63rd European High Pressure Research Group Meeting

23-28 August 2026, Palavas, France

63rd European High Pressure Research Group Meeting

EHPRG 2026

Conference Program and Abstract Book

23–28 August 2026

Palavas-les-Flots, France

A unique opportunity to explore the latest advances in high-pressure science while enjoying the exceptional Mediterranean setting of southern France.

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science under pressure

BETSA

All for very high pressure experiments


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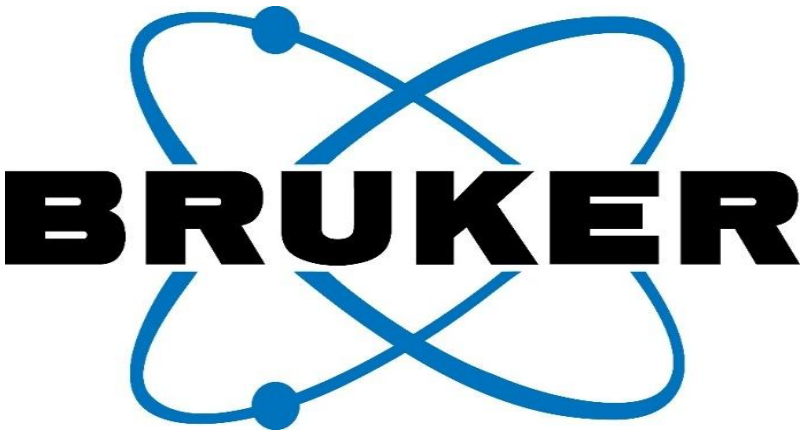
MECATRONICS


Sanchez
Technologies
Thermodynamics &
Core Analysis
Laboratory Instruments

Our SILVER sponsors



Our BRONZE sponsors

MG63
MÉCANIQUE GÉNÉRALE DE PRÉCISION

SITEC
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DAC Tools
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WELCOME

Welcome to EHPRG 2026

Dear Colleagues,

It is our great pleasure to welcome you to the **63rd European High Pressure Research Group Meeting (EHPRG 2026)**, taking place from **23 to 28 August 2026** in **Palavas-les-Flots**, on the Mediterranean coast of southern France.

For more than six decades, EHPRG has brought together scientists from across Europe and around the world to exchange ideas, present the latest discoveries, and foster collaborations in every field of high-pressure science. The meeting has become a unique forum where physicists, chemists, geoscientists, materials scientists, crystallographers and life scientists share advances in experimental techniques, theoretical developments and emerging applications.

EHPRG 2026 continues this tradition while offering an inspiring environment that encourages scientific discussion and networking. Hosted at the iconic **Phare de la Méditerranée**, overlooking the sea, the conference combines an outstanding scientific programme with the relaxed atmosphere of one of the Mediterranean's most attractive coastal destinations.

Throughout the week, participants will enjoy plenary lectures delivered by internationally recognised experts, invited talks, contributed oral presentations, poster sessions, and dedicated opportunities for young researchers to present their work. The conference will also feature the traditional EHPRG Award lecture, the commercial exhibition of high-pressure equipment, social events, and numerous occasions to strengthen existing collaborations and establish new ones.

Beyond the scientific programme, we hope you will take time to discover the unique character of Palavas-les-Flots and the surrounding region. From its sandy beaches and vibrant harbour to the historic city of Montpellier, the area offers an exceptional blend of culture, gastronomy and Mediterranean lifestyle.

We sincerely thank all members of the Organising Committee, the Scientific Committee, our sponsors, institutional partners and volunteers whose dedication has made this meeting possible.

We wish you an inspiring conference, stimulating discussions and an enjoyable stay in France.

We look forward to welcoming you to EHPRG 2026.

Julien Haines

Jérôme Rouquette

Conference Chairs

TOPICS

T1 Bio/Life Sciences, Food Science and Technology

T2 Chemistry, Synthesis, Novel materials

T3 Electronic, Magnetic, Caloric and Transport properties

T4 Geo- and Planetary Sciences

T5 Instrumentation, Metrology and Techniques

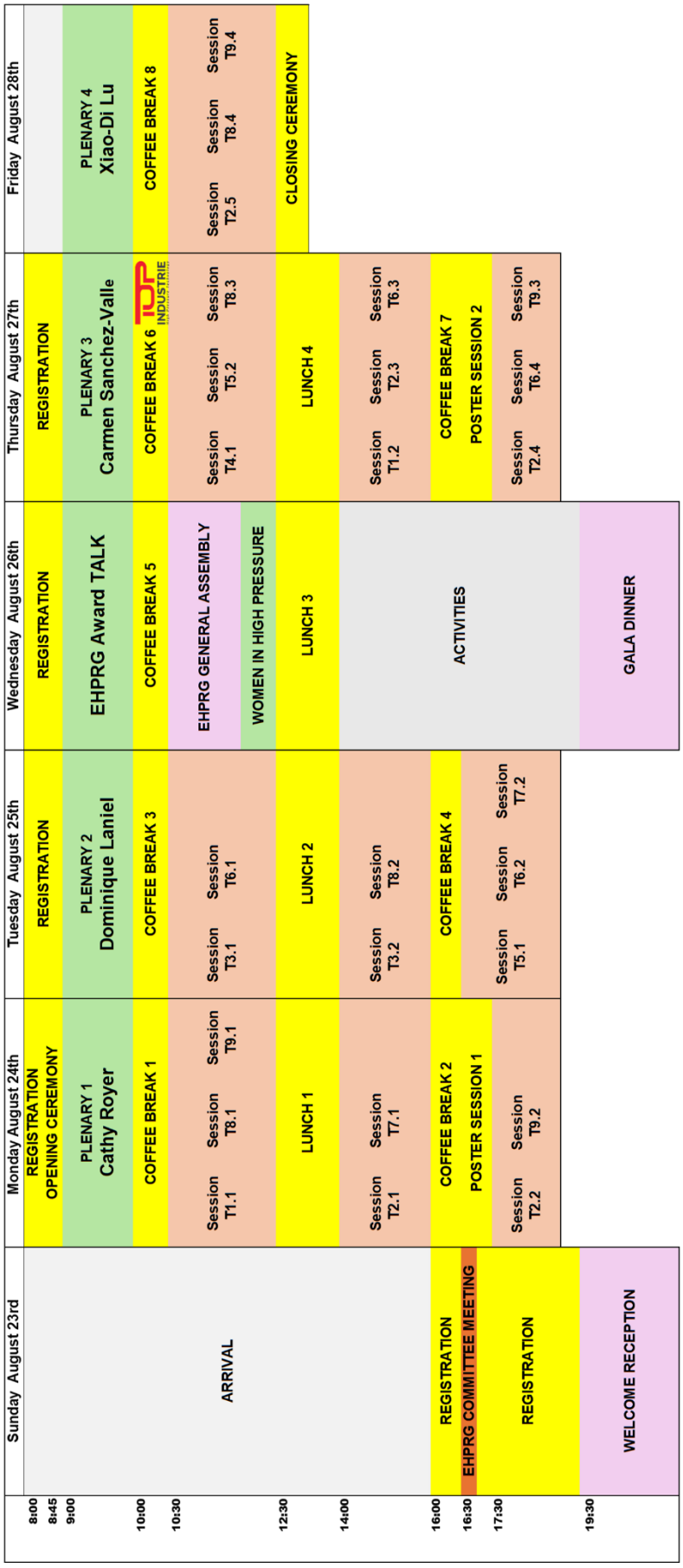
T6 Crystallography at High Pressure

T7 Simple Systems and Experiments at extreme conditions

T8 Spectroscopic and Structural studies

T9 Theoretical and Computational approaches

PROGRAM OVERVIEW



THE CONFERENCE CENTER

The amphitheater

CONGRESS - SEMINAR - CONFERENCE - GENERAL ASSEMBLY

The Odyssey Space - The Nausicaa Rooms

SEMINAR - MEETING - WORKSHOP - TRAINING

A 3-IN-1 SPACE

The Odyssée space offers you a modular space, divisible into three committee rooms called Nausicaa.
A 3-in-1 space, adaptable to your wishes, to offer you maximum comfort for your work sessions.

THE STRONG POINTS

- The layout of the rooms according to the configuration of your choice: U-shaped, theater-shaped, pole-shaped, etc.
- The possibility of joining rooms or closing them off depending on your daily schedule thanks to a system of removable partitions
- High-speed Wi-Fi
- Hot/cold air conditioning

BUSINESS DESTINATION 2023

NAUSICAA 1	NAUSICAA 2	NAUSICAA 3
60 M2	100 M2	60 M2

The Mezzanine

RECEPTION - CAFÉ - EXHIBITION - LOUNGE

A MULTIFUNCTIONAL PLACE AT YOUR DISPOSAL

This multifunctional space offers numerous design possibilities for all types of events. The Mezzanine features four entrances from the reception hall, direct access to the Amphitheater, and a spacious, light-filled and fully modular space for welcoming your participants, setting up stands, or organizing a breakfast reception for up to 200 people.

THE STRONG POINTS

- A modular and very bright space
- Hot/cold air conditioning
- High-speed Wi-Fi

BUSINESS DESTINATION 2023

SURFACE	CAPACITY	LIVING ROOM CONFIGURATION
260 M2	200 PAX.	16 STANDS MAX.

PLENARY SPEAKERS

Monday 9.00 -10.00

Pressure-based mapping of protein functional landscapes

Catherine Royer
Rensselaer Polytechnic Institute Troy, USA
royerc@rpi.edu

Tuesday 9.00 -10.00

A First Foray into High-Pressure Carbonitride Wonderland

Dominique Laniel

Centre for Science at Extreme Conditions
School of Physics and Astronomy
University of Edinburgh, UK
Dominique.Laniel@ed.ac.uk

Thursday 9.00 -10.00

Hot compressed ices in exoplanetary interiors

Maria del Carmen Sanchez Valle
Institut für Mineralogie
Universität Münster,
Münster, Germany
sanchezm@uni-muenster.de

Friday 9.00 -10.00

Novel Properties of Dense Hydrogen and Magnetic measurements with quantum sensors at high pressures

Xiao-Di Liu
Laboratory of Materials Physics
Institute of Solid State Physics
Chinese Academy of Sciences
Hefei, China. *xiaodi@issp.ac.cn*

EHPRG AWARD

Wednesday 9.00 -10.00

Single-crystal X-ray diffraction under high pressure

Akun Liang
College of Science
Eastern Institute of Technology, Ningbo, China
akliang@eitech.edu.cn

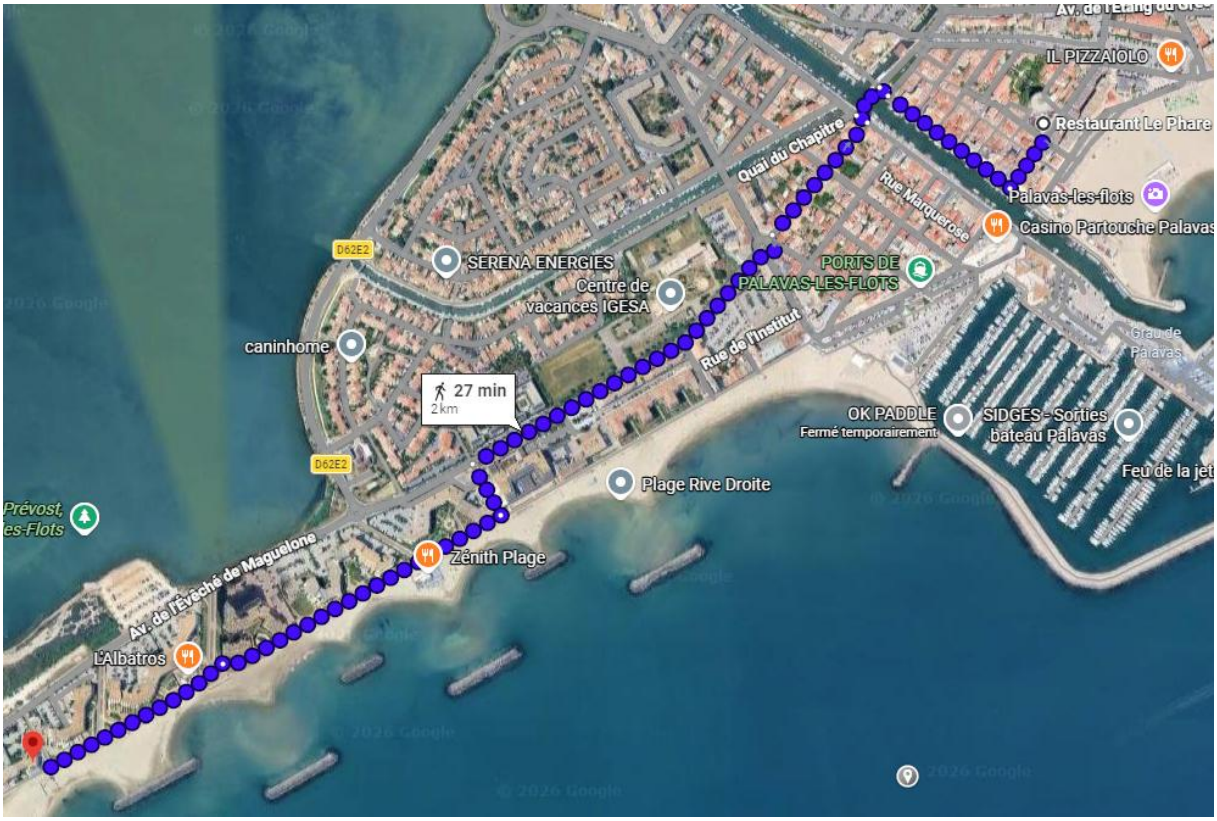
PROGRAM

Sunday 23 August 2026

4:00 Registration (also possible during the conference from Monday onwards)

4:30 EHPRG Committee Meeting (Nausica 3)

7:00 Welcome Reception (La Plage des Lézards)



Monday 24 August 2026

Auditorium Nausica 2 Nausica 3

8:00 Registration

8:45 **Opening Ceremony**

Plenary 1 (Chair: Hans Robert KALBITZER) (Auditorium)

9:00 **Catherine Royer**, Rensselaer Polytechnic Institute, ***Pressure-based mapping of protein functional landscapes***

10:00 **Coffee Break**

T1.1 Bio/Life Sciences, Food Science and Technology (Chair: Catherine Royer) (Nausica 3)

10:30 **Mohamed JEBBAR**, University of Brest, ***Thermococcales in the Deep Sea: Adaptation to High Hydrostatic Pressure, (invited)***

11:00 **Antonio Diego MOLINA-GARCIA**, ICTAN-CSIC, ***Different activities of a hydrolase under pressure***

11:20 Tone Mari **RODE**, NOFIMA, Stavanger, ***The use of HPP as a tool for microbial control and quality preservation in modern food systems, (invited)***

11:50 **Laurence POTTIER**, Oniris, Nantes, ***Effect of High Pressure on pea protein digestibility***

12:10 **Christian ROUMESTAND**, University of Montpellier, ***Do similar folding pathways mean similar folds ? A comparative High-Hydrostatic-Pressure NMR folding study of ß-sandwich proteins.***

T8.1 Spectroscopic and Structural studies (Chair: Katarzyna Jarzembska) (Nausica 2)

10:30 **Mael GUENNOU**, University of Luxembourg, ***Infrared Spectroscopy Studies of Perovskite Oxides at High Pressures***

10:50 **Mohamad Baker SHOKER**, University of Luxembourg, ***Re-emergence of a Polar Instability at High Pressure in $KNbO_3$***

11:10 **Suvashree MUKHERJEE**, Indian Institute of Science Education and Research, Kolkata, ***Probing Pressure-Induced Structural Evolution and Its Impact on the Optical Behavior of Rb_2TeBr_6***

11:30 **Fernando RODRÍGUEZ**, University of Cantabria, ***Pressure-Enhanced Ferromagnetism in Cs_2CrCl_4 Studied by Optical Spectroscopy***

Monday 24 August 2026

11:50 Yang SONG, University of Western Ontario**, *Pressure-Induced Structural and Optoelectronic Modulations in 2D Dion-Jacobson Hybrid Lead Iodide Perovskites with a Rigid Spacer***

12:10 Anna CELESTE, ENS Paris Saclay, ***X-Ray Pump-Probe Study of Diamond Formation with and without Color Centers***

T9.1 Theoretical and Computational approaches (chair: Sergei Simak) (Auditorium)

10:30 **Eva ZUREK**, University at Buffalo, ***High Pressure Electrides and Core-Electron Chemistry, (invited)***

11:00 **Stanislaw KRUKOWSKI**, Institute of High Pressure Physics, Polish Academy of Sciences, ***High Pressure Melting vs Decomposition of GaN: ab initio Molecular Dynamics Study and comparison to the experimental data***

11:20 **Valery LEVITAS**, Iowa State University of Science and Technology, ***Atomistic Mechanisms of Shear-Induced LDA↔HDA Transformations and Shear Banding in Amorphous Silicon under High Pressures***

11:40 **Francisco Javier MANJÓN,** Universitat Politècnica de València, València, ***Hydrogen bond disappearance and electron-deficient multicenter bond formation in compressed hydrogen halides***

12:00 **Timothy LEES**, Linköpings University, Linköping, ***Rapid Mechanical Property Prediction using Wyckoff Set Regression for Scalable Materials Exploration***

12:30 **Lunch**

T2.1 Chemistry, Synthesis, Novel materials (chair: Mathieu Marchivie) (Nausica 2)

2:00 **Frederico ALABARSE**, Sincrotrone ELETTRA Trieste, ***Tuning thermal expansion and mechanical properties by high pressure insertion of guest molecules***

2:30 **Igor ABRIKOSOV**, Linköping University, Sweden, ***Metastable states of matter: a path towards new 2D and 1D materials***

2:50 **Stanislow KRUKOWSKI**, Institute of High Pressure Physics, Polish Academy of Sciences, ***Nitrogen dissolution in Liquid Ga and Fe at high pressure by ab Initio analysis – application to crystallization of GaN and BN***

3:10 Elena BYKOVA, Goethe-Universität Frankfurt, ***Influence of volatiles on the chemistry of Fe-O system***

3:30 Dominik KURZYDLOWSKI, Cardinal Stefan Wyszyński University in Warsaw, ***High-pressure experiments on XePtF6 – the first noble gas compound***

Monday 24 August 2026

T7.1 Simple Systems and Experiments at extreme conditions (Chair: Eva Zurek) (Auditorium)

2:00 **Frédéric DATCHI**, IMPMC, ***Experimental x-ray studies of liquid polymorphism, (invited)***

2:30 **Guglielmo MARCHESE,** CSIC - ICMAB**, *Raman fingerprint of high-temperature superconductivity in compressed hydrides, (invited)***

3:00 **Mélissa TECHER,** LuMIn, ENS Paris-Saclay, **Probing superconductivity at very low temperature and high pressure using NV centers in diamond**

3:20 **Roman MARTONAK,** University in Bratislava**, From diamond to BC8 to simple cubic and back: Kinetic pathways to post-diamond carbon phases from metadynamics**

3:40 **Wan Xu,** Institute of Solid State Physics, Chinese Academy of Sciences**, *High pressure studies of dense oxygen and nitrogen binary mixtures***

4:00 **Coffee Break**

T2.2 Chemistry, Synthesis, Novel materials (Chair Frederico Alabarse) (Nausica 2)

5:30 **Foramben PRAJAPATI**, ICMCB-CNRS, ***Shaping Spin-Crossover Molecular Ceramics through Cool-SPS for Efficient Barocaloric Refrigeration***

5:50 **Cristian MARINO**, UniFi-LENS, European Laboratory for Non-linear Spectroscopy, ***Abiotic formation of organic complexity from multicomponent ice analogue via high-pressure photochemistry***

6:10 Yolanda SABATER ALGARRA, University of Kent, ***Towards Sustainable Spin-Crossover Materials through Mechanochemical One-Pot Synthesis***

T9.2 Theoretical and Computational approaches (chair: Alfonso Muñoz Gonzalez) (Auditorium)

5:30 **Julia CONTRERAS**, LCT, Université Sorbonne, ***Machine-learned electron localization in dense hydrogen***

5:50 **Leonid BURAKOVSKY**, Los Alamos National Laboratory, ***Model for equation of state and solidus and liquidus for a mixture for description of high-entropy alloys***

6:10 **Ethan TURNER**, Curtin university of Perth, ***Machine-learning simulations predict phase transformation of fullerite in a diamond-anvil cell***

Tuesday 25 August 2026

8:30 Registration

Plenary 2 (Chair: Francisco Javier Manjón) (Auditorium)

9:00 **Dominique Laniel**, University of Edinburgh, ***A First Foray into High-Pressure Carbonitride Wonderland***

10:00 **Coffee Break**

T3.1 Electronic, Magnetic, Caloric and Transport properties (Chair: Jiri Prchal) (Nausica 2)

10:30 **Dmitrii SEMENOK**, HPSTAR, Beijing, ***Ultrastable Metal Polyhydrides Below 60 GPa, (invited)***

11:00 **Chunhui YE**, University of Science and Technology of China, China, ***Pressure-Induced Flat Bands and Zero-Field Chern States in Large-Angle Twisted Bilayer Graphene***

11:20 **Yupeng WANG**, University of Science and Technology of China, ***High-Pressure Tuning of Dynamic Magic-Angle Correlated States in Twisted Bilayer Graphene***

11:40 **Matthias LAMP,** Experimentalphysik II, University of Augsburg, ***Charge dynamics in the Weyl semimetals $NbIrTe_4$ and $TaIrTe_4$ under pressure: Signatures of an electronic phase transition***

12:00 **Guy MAKOV**, Ben Gurion University, **Universal origin of anomalies in compressed liquid alkalis**

T6.1 High-Pressure Crystallography: Session in honor of Michael Hanfland (chair: Marco Merlini) (Auditorium)

10:30 **Anna PAKHOMOVA**, ESRF, ***Clathrate hydrates at high pressure: The cases of methanol enclathration, (invited)***

11:00 **Daniel ERRANDONEA,** Universidad de Valencia, ***Theory-guided discovery of pressure-induced transitions in the fast-ion conductor $BaSnF_4$***

11:20 **Benedetta CHRAPPAN SOLDAVINI,** Università degli Studi di Milano, ***High Pressure and High Temperature polymorphism of Na_2CO_3 up to 10 GPa***

TBA 11:40 **Davide COMBONI,** Università di Milano, ***ID15b and Hydrated borates at High-pressure,* TBA**

12:10 **Tomasz POREBA,** EPFL, Lausanne, ***Cryogenic stabilization of molecular hydrogen in dense cubic ice***

12:30 **Lunch**

T3.2 Electronic, Magnetic, Caloric and Transport properties (Chair: Daniel Errandonea) (Auditorium)

2:00 **Jonathan BUHOT**, H.H. Wills Physics Laboratory, Bristol, ***Thin-Film Hydride Superconductors: A New Platform to Study Near-Room-Temperature Superconductivity at Megabar Pressures, (invited)***

Tuesday 25 August 2026

2:30 **Alexander TSIRLIN**, Leipzig University, Leipzig, Germany, ***Herbertsmithite: pressure evolution of a spin liquid***

2:50 **Jaroslav VALENTA**, Institute of Physics of the Czech Academy of Sciences, ***Pressure dependence of tricriticality in $UIrSi_3$***

3:10 **Naveen DHAMI,** Synchrotron Soleil, ***Pressure dependence of Eu valence, crystal structure and electrical resistivity of $EuTGe_3$ (T = Co, Rh and Ir)***

3:30 **Manisha YADAV**, Bhabha Atomic Research Centre, Homi Bhabha National Institute, ***Superconducting Phase of BiTe at High pressure***

T8.2 Spectroscopic and Structural studies (Chair: Barbara Lavina) (Nausica 2)

2:00 **Neha BURA**, Universidad de Valencia, ***Hydrated Carbonates under Pressure, (invited)***

2:30 **Vittoria PISCHEDDA**, Université Lyon1, ***High-Pressure Multi-Probe Studies of Lithium-Ion Battery Materials*.**

2:50 **Ece UYKUR**, Helmholtz-Zentrum Dresden, ***Kagome Metals under Pressure: Dimensionality Crossover and Fermi Surface Reconstructions***

3:10 **Ganesh BERA**, Universidad de Valencia, ***Pressure-Triggered Molecular Organization in Tsaregorodtsevite, a Natural TMA-Sodalite Zeolite***

3:30 **Harsha KUMAWAT**, High Pressure & Synchrotron Radiation Physics Division, Bhabha Atomic Research Centre; Homi Bhabha National Institute, ***Pressure–Temperature Phase Diagram of Diglycine Perchlorate***

4:00 **Coffee Break**

T5.1 Instrumentation, Metrology and Techniques (Chair: Karen Appel) (Auditorium)

4:30 **Nicolas Guignot**, SOLEIL synchrotron, ***A multi-technical approach to the study of the physical properties of materials. Examples from the PSICHE beamline, Synchrotron SOLEIL, (invited)***

5:00 **Raffaella TORCHIO**, ESRF, **The High-Power Laser Facility at ESRF: local and electronic structure of matter up to Mbar range**

5:20 **Samuel Marre**, ICMCB, ***Multi-Scale Transparent High Pressure Laboratory Experimental Approaches: Applications In Deep Environments Studies***

5:40 **Ioannis TZIFAS**, GSI Helmholtz Center for Heavy Ion Research GmbH, Darmstadt, ***Structural transformations under coupled extremes of pressure and swift heavy ion irradiation***

6:00 **Robert FARLA**, Deutsches Elektronen-Synchrotron DESY, ***P61B LVP: The Large Volume Press station for in-situ X-ray diffraction and imaging on materials at HPHT***

Tuesday 25 August 2026

T6.2 High-Pressure Crystallography (Chair: Michael Hanfland) (Nausica 3)

4:30 **Anna Krawczuk,** University of Göttingen, ***From Intermolecular Interactions to Functional Properties: Pressure-Tuned Behavior of π-Conjugated Molecular Crystals***

5:00 **Milo AGATI**, ESRF, ***How subtle differences in organic molecular crystals influence their structural evolution in compression***

5:20 **Ewa PATYK-KAZMIERCZAK,** Adam Mickiewicz University, Poznań, ***Putting Pressure on Multicomponent Crystals: Tuning Single-Crystal-to-Single-Crystal Transformations via Compositional Engineering***

5:40 **Sarah BOLTON**, University of Edinburgh, ***Pushing the 10 GPa Pressure Boundary for Organic Solids: Crystal Structure Determination of α-Glycine Above a Megabar***

6:00 **Barbara LAVINA,** University of Chicago and Argonne National. Lab**, The crystal structure of ruby up to 170 GPa**

6:20 **Roman GAJDA**, University of Warsaw, ***New look at phase diagram of cuprite under pressure,*** **TBA**

T7.2 Simple Systems and Experiments at extreme conditions (Chair: Nenad Velisavljevic) (Nausica 2)

4:30 **Emanuele COLONNA**, ESRF, ***Microscopic Investigation of laser shocked glassy GeO_2***

4:50 **Amrita CHAKRABORTI,** Université de Lille, ***Nanosecond timescale plasticity in shock-compressed polycrystalline MgO up to pressures above 100 GPa***

5:10 **Valery LEVITAS,** Iowa State University of Science and Technology**, *Combined Strain- and Stress-Induced Phase Transformations and Microstructure* Evolution under High Pressure**

5:30 **Jun KONG,** Center for High Pressure Science and Technology Advanced Research**, *Compositions, structures, and properties of chlorides system under high pressure***

5:50 **Duanwei HE,** Sichuan University, **Phosphorus-Doped N-Type Diamond Semiconductors through High-Pressure Thermal Diffusion**

6:10 **Simon AYRINHAC**, IMPMC, Sorbonne Université**, *Thermoelastic properties of liquid Bi determined by picosecond acoustics***

Wednesday 26 August 2026

8:30 Registration

EHPRG Award Lecture (chair: Matteo Ceppatelli) (Auditorium)

9:00 **Akun LIANG**, Eastern Institute of Technology, ***Single-crystal X-ray diffraction under high pressure***

10:00 **Coffee Break (sponsored by Irian Mecatronics)**

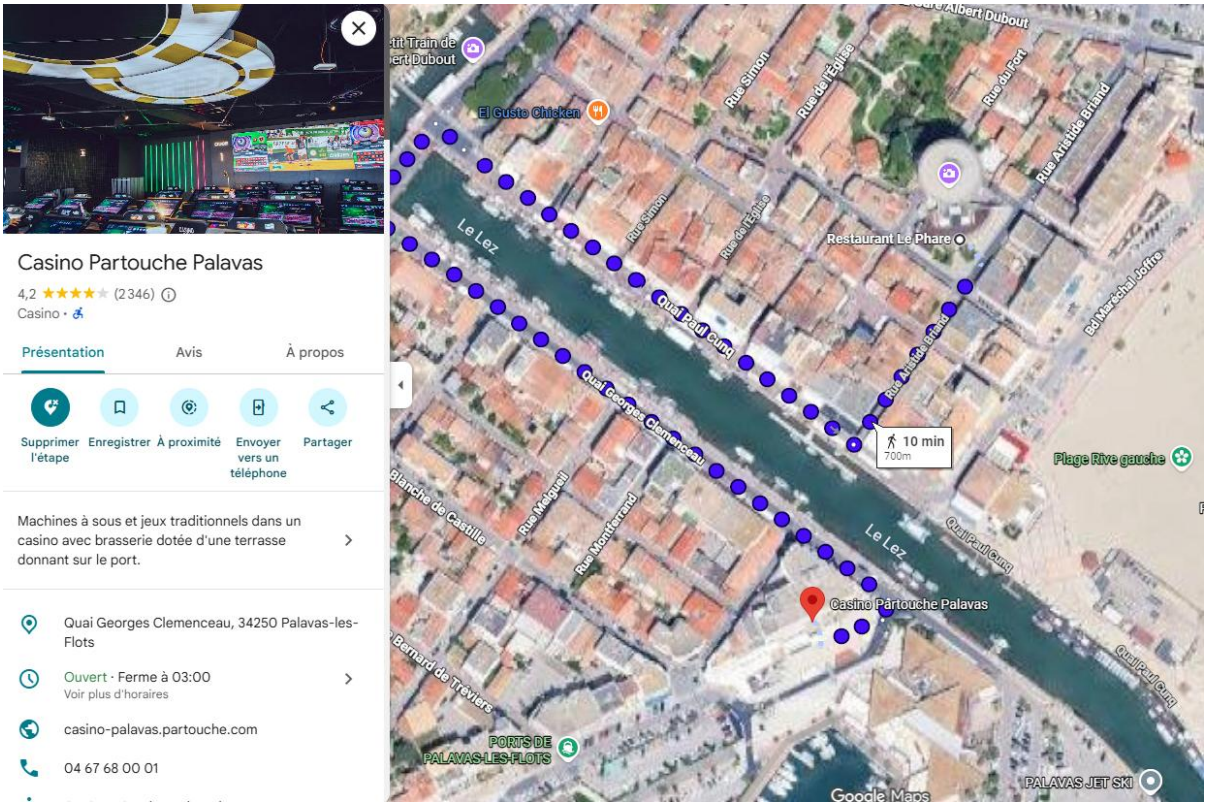
10:30 **EHPRG General Assembly** (chair: Matteo Ceppatelli) (Auditorium)

11:30 **Women in High Pressure** (chair: Julia Contreras) (Auditorium)

12:30 **Lunch**

2:00 **Activities**

7:00 **Gala dinner (Casino Partouche)**



Thursday 27 August 2026

8:30 Registration

Plenary 3 (chair: Vitali Prakapenka) (Auditorium)

9:00 **Maria del Carmen SANCHEZ VALLE**, University of Edinburgh, ***Hot compressed ices in exoplanetary interiors***

10:00 **Coffee Break sponsored by TOP Industrie**

T4.1 Geo- and Planetary Sciences (chair: Anna Pakhomova) (Nausica 2)

10:30 **Isabelle DANIEL**, U. Lyon, ***Forms of organic carbon at depth***

11:00 Vitali **PRAKAPENKA,** The University of Chicago**, *Polymorphism of Superionic Ice at Planetary Interior***

11:30 **Ben KALMAN,** The University of Western Ontario**, *Heat flow within terrestrial cores from electrical resistivity measurements of Fe-Si to 24 GPa***

11:50 **Konstantin SOLOVEV,** GFZ Helmholtz Centre for Geosciences, Potsdam, ***Influence of Iron on the Stiffness of Silicate Glasses: Insights from All-Optical Density Measurements of Enstatite–Ferrosilite Glasses at High Pressure***

12:10 **Anastasiia KALUGINA**, GFZ Helmholtz Centre for Geosciences, Potsdam, ***Insights into the Structure of Mn^{2+}-dopped K_2CO_3-$MgCO_3$ Glass at High Pressure from Time-resolved Laser Fluorescence***

T5.2 Instrumentation, Metrology and Techniques (Chair: Raffaella Torchio) (Auditorium)

10:30 **Jose Luis RODRIGO RAMON**, Universidad de Valencia, **Benchmark melting behavior of rhodium under megabar pressures**

10:50 **Jodie BRADBY**, Research School of Physics, Australian National University, **Simple measurement of the hardness of C60 samples recovered after compression to 75 GPa**

11:10 **Evrard PEYRAQUE**, ICGM, ***In situ*** **Raman thermometry for temperature determination in externally heated diamond anvil cells**

11:30 **Nenad VELISAVLJEVIC**, Lawrence Livermore National Laboratory and High Pressure Collaborative Access Team, **New X-ray Light Sources, Innovative Pressure Platforms, and Advances in AI: Opportunities for High-Pressure Research**

11:50 **Ingo Loa**, Centre for Science at Extreme Conditions University of Edinburgh, **X-Ray Thermal Diffuse Scattering under High Pressure**

12:10 **Nicolas JAISLE,** Centre for Science at Extreme Conditions University of Edinburgh, **Determining thermal conductivity at extremes using X-ray Free Electron Lasers**

T8.3 Spectroscopic and Structural studies (chair: Fernando Rodríguez) (Nausica 3)

10:30 **Katarzyna JARZEMBSKA**, University of Warsaw, ***Red-to-NIR Optical Tuning in Rhodium(I) Complexes, (invited)***

Thursday 27 August 2026

11:00 **Stepan TIAGLO**, Institut Lumière Matière, UMR5306 Université Lyon 1-CNRS, ***High-Pressure Study of Wurtzite InP Nanowires***

11:20 **Chiara COPPI**, ESRF, ***High-Pressure Study of Ferroelectric SbSI: From Long-Range Order to Local Probes***

11:40 **Agata KAMINSKA**, Institute of Physical Sciences, Cardinal Stefan Wyszynski University in Warsaw, ***Application of High-Pressure Spectroscopy to Identify the UV Color Center in 2D Boron Nitride***

12:30 **Lunch**

T1.2 Bio/Life Sciences, Food Science and Technology (Chair: Isabelle Daniel) (Nausica 3)

2:00 **Evina GONTIKAKI**, Foundation for Research and Technology-Hellas, ***Simulating the Deep Sea: High-Pressure Experiments on Indigenous Microbial Bioremediation of Hydrocarbons, (invited)***

2:30 **Anaïs CARIO**, ICMCB, ***Fluid chemistry and mineral interactions as dual interfaces of microbial life in deep-sea vents under high-pressure conditions***

2:50 **Judith PETERS**, Institut Laue Langevin, ***High pressure equipment for neutron scattering and applications, (invited)***

3:20 **Hans Robert KALBITZER**, University of Regensburg, Germany, ***Use of high pressure in drug design***

3:40 **Werner KREMER**, University of Regensburg, Germany, ***Insights into the structure of invisible conformations of large methyl group labeled molecular machines from high pressure NMR***

T2.3 Chemistry, Synthesis, Novel materials (Chair Anna Krawczuk) (Auditorium)

2.00 **Demitrio SCELTA**, LENS, Sesto Fiorentino, ***From CO_2 clathrate hydrate to solid carbonic acid: high-pressure chemistry in astrochemical ices, (invited)***

2:30 **Dominik SPAHR**, Goethe University Frankfurt, ***New carbonic acid compounds in the H-C-O system at elevated pressures***

2:50 **Matteo CEPPATELLI,** ICCOM-CNR, LENS, Sesto Fiorentino, ***Interlayer bond formation in arsenic at high pressure***

3:10 **Alexander SOLDATOV**, State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, ***Carbon materials design using high-pressure toolkit***

3:30 **Xuejing HE**, Eastern Institute for Advanced Study, Ningbo, ***High-pressure synthesis of a hafnium carbonitride hosting a hexazine ring***

Thursday 27 August 2026

T6.3 High-Pressure Crystallography (Chair: Elena Bykova) (Nausica 2)

2.00 **Robin FRÉVILLE,** ESRF, ***Phase transition mechanism of the pressure-induced β↔γ transformations in tin***

2.20 **Alexandre COURAC,** IMPMC**,** ***Na-Si phase diagram at HPHT***

2.40 **Camino MARTÍN-SÁNCHEZ,** University of Geneva, ***Is gold really stiffer at the nanoscale?***

3.00 **Benjamin BERTIN**, ICMCB, ***Surfing Between Structure and Spin State: High-Pressure Studies of Spin Crossover Compound***

3.20 **Apostolos PANTOUSAS**, ESRF, University of Bayreuth**,** ***From [CO_3] towards [CO_4]: a high-pressure study of two novel hydrous carbonates***

3.40 **Milo DIXON**, University of Edinburgh, ***Assessing Synthesis Pathways to Superconducting Mg_2IrH_6***

4:00 **Coffee Break**

T2.4 Chemistry, Synthesis, Novel materials (Chair: Vittoria Pischedda) (Nausica2)

5:30 **Loïc TORAILLE**, CEA/DAM, ***Looking for ambient pressure superhydrides: application to the Y-Fe-H system***

5:50 **Leon SCHÜTTE**, ICGM, ***In-situ characterization of the High-Pressure High-Temperature synthesis of tetragonal Na_2Si_3***

6:10 **Joao Pedro FALK DE CAMPOS**, ICGM, ***Amorphous Silica obtained from the Zeolite Chabazite due to Structural Collapse under Mild Pressure-Temperature Conditions***

T6.4 High-Pressure Crystallography (Chair: Maria del Carmen Sanchez Valle) (Auditorium)

5:30 CANCELLED -**Agnieszka HUĆ**, Univerisity of Warsaw, ***High-pressure studies of hydrogen bonding in gypsum via Quantum Crystallography methods***

5:30 **Dougal MCCULLOCH**, RMIT University (AU), ***Shear-driven formation of diamond during cold compression of graphite and glassy carbon***

5:50 **Maxime JUIN**, IMPMC, ***Understanding quartz polymorph's formation during impact events using dynamic compression***

T9.3 Theoretical and Computational approaches (Chair: Florian Trybel) (Nausica 3)

5:30 **Morgan REDINGTON**, ICM2P, Poitiers, ***Exploration of the Na-Si phase diagram and theoretical structure prediction of a layered sodium Zintl phase Na_2Si_3***

Thursday 27 August 2026

5:50 **Ilia SHOLIN**, Independent researcher, Bahrain, ***Introducing high-pressure physics into physics education through digital simulations***

6:10 **Shir BEN SHALOM,** Ben-Gurion University of the Negev**,** ***The Anomalous Melting of Antimony Hides a Liquid-State Transformation***

Friday 28 August 2026

8:30 Registration

Friday August 28th

Plenary 4 (Chair: Ingo Loa) (Auditorium)

9:00 **Xiao-Di LU**, Chinese Academy of Sciences, ***Novel Properties of Dense Hydrogen and Magnetic measurements with quantum sensors at high pressures***

10:00 **Coffee Break**

T2.5 Chemistry, Synthesis, Novel materials (Chair: Samuel Marre) (Nausica 2)

10:30 **Lukasz ROGAL**, Institute of Metallurgy and Materials Science PAS, ***Medium-range ordering in Mg–Cu–Gd glasses induced by annealing at the glass transition temperature and high pressure***

10:50 **Kseniia KONDRINA**, DESY, ***Formation of Mo-Ta Solid-Solution Nitrides under Extreme Conditions***

11:10 **Ken NIWA**, Nagoya University, ***High-Coordinate Transition Metal Phosphides via High-Pressure Synthesis***

11:30 **Qian ZHANG**, University of Edinburgh, ***High-pressure synthesis of alkali metal carbodiimides***

11:50 **Andrey ASLANDUKOV**, Goethe University Frankfurt, ***Inorganic tricarbonate: high-pressure synthesis of $K_2C_3O_7$***

T8.4 Spectroscopic and Structural studies (Chair: Elen Duverger) (Nausica 3)

10:30 **Almudena INCHAUSTI**, Université de Bordeaux, ***Unlocking hidden phases in Fe(II) spin crossover complexes under pressure***

10:50 **Beatrice D'ALÒ**, Synchrotron Soleil, ***Absence of charge density wave transition in $SnSe_2$ at extreme conditions***

11:10 **Murugeswari ANDICHAMY**, Anna University, ***High Pressure Raman Spectroscopy of $IrTe_2$ up to 25.9 GPa: Spectroscopic Mapping of Lattice Destabilization and Amorphization***

Friday 28 August 2026

T9.4 Theoretical and Computational approaches (Auditorium) (chair: Julia Contreras)

10:30 **Sergei SIMAK**, Linköpings University, Linköping, ***A Continuous-Path Approach to Crystal Structure Prediction, (invited)***

11:00 **Francisco Javier MANJÓN,** Universitat Politècnica de València, ***Unconventional multicenter bonds in gold halide perovskites at room and high pressure***

11:20 **A R Atique ULLA**, Homi Bhabha National Institute, Bhabha Atomic Research Centre, ***Exploring structural and non-trivial electronic properties of Ta_2NiSe_5 under pressure***

11:40 **Henricus TEN EIKELDER,** Linköpings University, Linköping, ***Efficient Approach to Nuclear Quantum and Anharmonic Thermal Effects in Pressure-Constrained Relaxations***

12:00 **Florian TRYBEL**, Linköpings university, Linköping, ***CrysViz: a lightweight browser-based platform for on-device crystal structure visualization and simulation***

12:20 Closing Ceremony

12:30 **Lunch**

POSTER SESSIONS

4:00 – 5:30 **POSTER SESSIONS (MEZANINE)**

The following topics (T1, T2, T3, T5, T9) will be presented during the Monday and (T6, T7, T8,) during the Thursday poster sessions. We request that the presenters from the first poster session remove their posters on Tuesday evening at the latest.

T1 Bio/Life Sciences, Food Science and Technology

P01 Anais CARIO, ICMCB - CNRS, ***High hydrostatic pressure as a modulator of microplastic–microbiome interactions: a deep-sea analogue approach***

P02 Christian ROUMESTAND, University of Montpellier, ***The HHP-NMR unfolding study of the yeast Frataxin Yfh1 at variable temperature gives essential clues on the heat- and cold-induced denaturation of the protein.***

P03 Laetitia PICART-PALMADE, University of Montpellier - UMR IATE, ***Influence of high hydrostatic pressure on Mexican jackfruit seed proteins***

T2 Chemistry, Synthesis, Novel materials

P04 Antoine BELLOUARD, Institut de Chimie de la Matière Condensée de Bordeaux ICMCB, Univ. Bordeaux, CNRS, Bordeaux- INP, ***Continuous Flow Synthesis of Spin Crossover Materials for Solid-State Green Refrigeration***

P05 Dario FLORIO, Institut Charles Gerhardt Montpellier, ***HP/HT synthesis and in situ investigation of K doped Pb_2FeMoO_6 perovskite: tuning properties via A-site substitution***

P06 Elen DUVERGER-NÉDELLEC, ICMCB-UMR 5026, CNRS, Univ. Bordeaux, Bordeaux INP, ***Keep Cool with Crystals: Crystals under Pressure for the Refrigeration of the Future.***

P07 Sean S. SEBASTIAN, Goethe Universtity Frankfurt, ***Caffeine enabling high-pressure research on new light element compounds***

P08 Sam CROSS, University of Bristol, ***Synthesis and characterisation of high-Tc metal hydride thin films at megabar pressure***

P09 Milo DIXON, University of Edinburgh, UK - ***High pressure synthesis of manganese superhydride MnH_7***

P30 Yuqing YIN, University of Beyreuth, Germany **-** ***Halogen Chains with One-Dimensional Semi-Metallic Electronic Structure and Peierls Physics in Polymorphs of Na4X5 (X = I, Br, Cl) Compounds***

T3 Electronic, Magnetic, Caloric and Transport properties

P10 Adnan KAREEM, Jožef Stefan International Postgraduate School (IPS), Ljubljana, Slovenia, ***Pressure and Field Tuned Magnetism in the Honeycomb Antiferromagnet $Na_3Ni_2BiO_6$***

P11 Alexandre COURAC, Sorbonne université, Quantitative and qualitative high pressure calorimetry for in situ studies

P12 Govindaraj LINGANNAN, University of Doha for Science and Technology, ***Pressure-Enhanced Charge Density Wave Order and Anisotropic Lattice Strain in $BaFe_2Al_9$***

T4 Geo- and Planetary Sciences

T5 Instrumentation, Metrology and Techniques

P13 Christophe GUILLAUME, Almax easyLab, Belgium, ***Almax easyLab Solutions for Extreme Pressure Science***

P14 Efim KOLESNIKOV, University of Lille, ***Periodic dynamic oscillations of iron in diamond anvil cells***

T6 Crystallography at High Pressure

P15 Juan Angel SANS, Technical University of Valencia, ***Pressure-Induced Helium Trapping in Sr_2FeIrO_6 Double Perovskite***

P16 Bishnupada GHOSH, Diamond Light Source, ***Low-temperature High-pressure Sample Environment for Single Crystal and Powder X-ray Diffraction -for I15 beamline of Diamond Light Source***

P17 Christoph OTZEN, Albert-Ludwigs-Universität Freiburg, ***Structural characterization of amorphized quartz resulting from diamond anvil cell and shock experiments***

P18 Estelle LEDOUX, Department of Earth Sciences, University of Oxford, UK, ***The stishovite to post-stishovite phase boundary studied by stress cycling experiments in a dDAC***

P19 Jirí PRCHAL, Charles University, Faculty of Mathematics and Physics, ***Crystal structure of $EuZn_2X_2$ Zintl phases in elevated pressure***

P20 Robin FRÉVILLE, European Synchrotron Radiation Facility, France, ***Extreme conditions X-ray diffraction and imaging beamline ID15B on the ESRF extremely brilliant source***

P31 Agnieszka HUĆ, Univerisity of Warsaw, Poland, **High-pressure studies of hydrogen bonding in gypsum via Quantum Crystallography methods**

T7 Simple Systems and Experiments at extreme conditions

P21 Shir BEN SHALOM, Ben-Gurion University of the Negev, Israel, ***Determining High-Pressure Binary Phase Diagram Evolution through Thermodynamics and Electrical Measurements***

P22 Simon AYRINHAC, IMPMC, Sorbonne Université, Paris, ***Periodic table of phase diagrams of the elements***

T8 Spectroscopic and Structural studies

P23 Dimitrios CHRISTOFILOS, Aristotle University of Thessaloniki, Greece, ***Raman study of $[Ru(bpy)(CN)_4Mg(H_2O)_5]\cdot H_2O$ crystal at high pressure***

P24 Gunnar WECK, CEA-DAM, DIF, LMCE, Bruyères-le-Châtel, France, ***Metallization of Solid Oxygen: Optical Gap Closure and Structural Evolution up to 100 GPa***

P25 Mayssoune MINA, Université de Lorraine, LCP-A2MC, ER 4632, F-57000 Metz, France**,** ***Zn1-xMnxTe & Zn1-xBexSe High-pressure lattice structure/dynamics***

P26 Rebecca NICHOLLS, University of Bristol, ***High Pressure as a Potential Route to Correlation Physics in Mott Insulator Nb_3Cl_8***

P27 Selene BERNI, CNR-IFAC, ***Pressure-induced hydrogen formation and phase transitions in H_2S-THF clathrate hydrate***

P28 Taras PALASYUK, Warsaw University of Technology, ***Anomalous pressure modulation of the lowest B_{1g} lattice vibration in semimetal zirconium diphosphide, ZrP_2***

T9 Theoretical and Computational approaches

P29 Alfonso MUNOZ GONZALEZ, Universidad de La Laguna, ***Pressure-dependent structural, elastic, electronic and vibrational studies of Sr_2InSbO_6 from first principles simulations.***

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
A1 EHPRG Award

Single-crystal X-ray diffraction under high pressure

Akun LIANG (Eastern Institute of Technology, Ningbo, China),

Abstract

Accurate determination of the crystallographic structure of materials under high pressure is of fundamental importance, both for understanding pressure-induced physical phenomena and for guiding the synthesis of novel compounds that are inaccessible at ambient conditions. Single-crystal X-ray diffraction (SCXRD) remains one of the few in-situ probes capable of delivering this level of structural accuracy inside the diamond anvil cell (DAC).

In this talk, I will present the single-crystal X-ray diffraction method under high pressure and illustrate its application in two complementary contexts. The first concerns single crystals that are already obtainable at ambient conditions, a few micrometres in size, and loaded directly into the DAC. Using examples from $MAPbBr_3$, $Ba(IO_3)_2{\cdot}H_2O$, $B_{13}C_2$, and $Cd(IO_3)_2$, I will show how high-pressure SCXRD, performed up to megabar pressures, resolves subtle structural changes that have been misassigned or overlooked by other in-situ probes.

The second concerns a newer approach: SCXRD performed directly on polycrystalline samples synthesized in a laser-heated diamond anvil cell, wthout the need to load a pre-formed single crystal. I will discuss how this method has enabled the discovery of an emerging family of metal carbonitrides, including the guanidinate anion $[CN_3]^{5-}$ [1], its corner-sharing polymerized form [2], the fully deprotonated melaminate anion $[C_3N_6]^{6-}$, and previously unknown CN_4-based anions in which an additional nitrogen atom is appended to a terminal N of the tetrahedron, extending the stoichiometry to $[CN_5]^{4-}$ and $[CN_6]^{5-}$ polycarbonitride species [3].

Together, these results demonstrate that high-pressure single-crystal X-ray diffraction, whether applied to pre-existing single crystals or directly to the products of in-situ high-pressure synthesis, is a uniquely powerful tool, it reveals structural details invisible to other techniques, and it opens a route to entirely new classes of compounds that do not exist at ambient conditions.

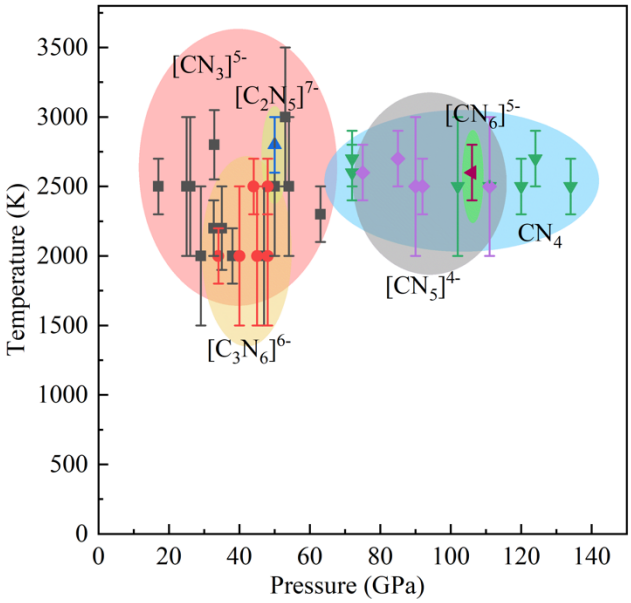


Figure 1. The synthesis conditions for various carbon-nitrogen species.

References :
[1] *A. Aslandukov et al., Angew. Chem. Int. Ed.* ***62****, 2023, e202311516*
[2] *L. Brüning et al., Angew. Chem. Int. Ed.* ***62****, 2023, e202311519*
[3] *F. I. Akbar et al., J. Am. Chem. Soc.* ***148,*** *2026, 11915-11924*

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
P1 High Pressure and Bio/Life Sciences, Food Science and Technology

Pressure-based mapping of protein functional landscape

Tejaswi Koduru, Philippe Barthe, Karyn De Guillen, Luke Fisher, Carleton Coffin, Noam Hantman, Pierce Leonardi, Jack Foland, Scott A. McCallum, Joel E. Morgan, Estella Yee, Christian Roumestand, Douglas H. Bartlett, Catherine A. Royer
(Rensselaer Polytechnic Institute, Troy, USA)

Abstract
Over 80% of the microbial biomass on Earth exists in high pressure environments. However, it is known that high pressure destabilizes the interactions and structure of proteins from mesophilic organisms. The question thus arises as to how microbes living at high pressure have adapted to their environments, which include very hot temperatures at hydrothermal vents or in the oceanic or continental crusts, as well as the low temperatures of the cold deep sea. Here we compare the enzymatic and structural properties of homologous exonucleases from the mesophilic Staphylococcus aureus and from Carnobacterium AT7 from the cold deep Aleutian trench under varying thermodynamic and chemical conditions. Results are discussed in light of recent work probing adaptive mutations in a strain of E. coli (AN62) which was evolved in the laboratory for growth under pressure.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
P2 Chemical Sciences

A First Foray into High-Pressure Carbon Nitride Wonderland

Dominique Laniel (University of Edinburgh, UK)

Abstract

The recently discovered C_3N_4 polymorphs, consisting exclusively of corner-sharing CN_4 tetrahedra, were synthesized after more than three decades of effort.[1,2] These materials exhibit exceptional physical properties, including superhardness, ultraincompressibility, piezoelectricity, and photoluminescence, while being recoverable to ambient conditions. However, aside from chemical doping, the three known polymeric C_3N_4 polymorphs offer limited opportunities for tuning their physical and chemical properties.

A natural route toward expanding the chemistry of such CN_4-based carbon nitrides is to draw inspiration from silicon nitrides, which originally motivated the prediction of these C_3N_4 structures.[3] In particular, nitridosilicates constitute a large family of silicon nitride materials built from corner-sharing SiN_4 tetrahedra that form extended, often porous, anionic frameworks hosting metal cations. The incorporation of these cations not only enables remarkable structural diversity but also strongly influences the physical properties of the resulting materials, underpinning applications ranging from solid-state lighting to other advanced technologies. Given carbon's propensity to behave like silicon at high pressures, carbon-based analogues of nitridosilicates, termed nitridocarbonates, are expected to exist.

In this talk, we explore whether nitridocarbonates can be realized in ternary C–N systems using high pressures and high temperatures. To achieve this, carbon, nitrogen and various transition metals were compressed in diamond anvil cells and subsequently laser heated. The resulting compounds were characterized by synchrotron single-crystal X-ray diffraction and density functional theory (DFT) calculations.

Remarkably, several synthesized ternary phases contain extended anionic frameworks of corner-sharing CN_4 tetrahedra and are direct structural analogues of known nitridosilicates. Other novel compounds display a far richer structural chemistry, incorporating not only CN_4 tetrahedra but also $C(CN_3)$ and $C(C_2N_2)$ tetrahedral units, as well as N–N bonds. Their physical properties, including stability ranges, compressibility, and electronic band gaps, will also be presented.

Together, these findings establish nitridocarbonates as a new class of pressure-stabilized materials. Compared with their nitridosilicate counterparts, they offer enhanced chemical flexibility while retaining attractive physical properties, opening new opportunities for the design of functional materials and future technological applications.

References:

1. Laniel *et al*. Advanced Materials **36**, 2308030 (2024)
2. Laniel *et al*. Advanced Functional Materials **35**, 2416892 (2025)
3. Liu *et al*. Science **245**, 841-842 (1989)

Hot compressed ices in exoplanetary interiors

Carmen SANCHEZ-VALLE (University of Münster, Germany)

Abstract

'Ices' of water, ammonia and methane (and mixture thereof) are major components of interstellar and planetary bodies, from comets to the icy moons of the Jovian planets or the thousands of newly discovered water/ice-rich exoplanets [1-3]. Current models of the internal structure of water-rich exoplanets assume the existence of thick ice mantle layers overlaying a rocky and/or metallic core [3]. Understanding the behaviour of hot compressed ice phases at relevant conditions (>50 GPa and 2000 K) is thus critical to model the internal structure and dynamics of large icy bodies from the growing number of remote geophysical observations [4,5]. Despite extensive investigation, experimental studies have largely focused on end-members, while the behaviour of more complex systems remains less well resolved.

Here I will discuss our recent results on the phase relations, chemical reactivity and thermal properties of HCNO ices achieved by static and dynamic compression approaches in diamond anvil cells coupled with X-ray diagnostics at PETRA III and the European XFEL. Specifically, I will present studies that show 1) chemical reactions in the H_2O-NH_3 system that stabilize ultra-water rich ammonia hydrates in the icy mantle layers of water/ice-rich exoplanets; 2) the effect of compression rates on the crystallization pathway and the stability of phases in the H_2O-NH_3 system; and 3) complexities in the phase relations of CH_4 at extreme conditions. Moreover, I will illustrate new opportunities for the study of the thermal conductivity of planetary ices that leverage the unique characteristics of the XFEL source to directly heat and probe samples with consecutive X-ray pulses. The picture that emerges from these studies is a large compositional and structural diversity in simple systems, and provides evidence for complex interactions between H_2O ice and volatiles at high pressure-high temperature conditions. The implications of these results to interior modelling of ice exoplanets will be discussed.

[1] Borucki et al. Science 327:977 (2010).

[2] Noack et al. *Space Sci. Rev.* 212, 877–898 (2017).

[3] Sotin et al. *Icarus* 191, 337–351 (2007)

[4] Nettelmann et al. *ApJ* 733, 2 (2011).

[5] Helled et al. *Exp. Astron.* 53, 323–356 (2022).

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
P4 Physcial Sciences

Dense Hydrogen and Quantum Sensing under Extreme Pressure

Xiao-Di Liu (Institute of Solid State Physics, Chinese Academy of Sciences, Hefei, China),

Abstract

Dense hydrogen has long been regarded as one of the most fascinating systems in condensed matter and high-pressure physics because of its predicted metallic, superconducting, superfluid, and other exotic quantum states. Owing to its light mass, strong nuclear quantum effects, and pronounced isotopic dependence, hydrogens exhibit an exceptionally rich phase diagram and novel properties that remains far from fully understood.

Using high-pressure and low-temperature Raman spectroscopy together with optical transmission measurements, we have systematically investigated the phase behavior of H_2, D_2, and HD mixtures up to 350 GPa over the temperature range of 10–300 K. We report the first observation of the **ΔJ = 0** rotational excitation in dense hydrogen, providing new insight into molecular rotational dynamics under extreme compression [1]. Our studies also reveal an unusual isotope-doping effect in H_2–HD–D_2 molecular alloys below 200 GPa, originating from the nuclear quantum effects and exchange symmetry[5-7]. At higher pressures, the HD mixture exhibits the same phase-transition sequence (III–IV–V) as pure hydrogen, while its pressure-dependent band gap remains comparable to those of H_2 and D_2, indicating that isotopic alloying has little influence on the metallization pressure[3]. These results provide new insights into the quantum behavior of dense hydrogen approaching the metallic regime.

The definitive confirmation of superconductivity at very high compressions in diamond anvil cell ultimately requires local magnetic measurements, which remains a major experimental challenge. To address this challenge, we have developed quantum sensing techniques based on nitrogen-vacancy centers in diamond and silicon-vacancy/divacancy defects in 4H-SiC for in situ magnetometry in diamond anvil cells. These quantum sensors enable highly sensitive local magnetic detection in microscopic samples under multi-gigapascal pressures and have been applied to pressure-induced magnetic phase transitions in $Nd_2Fe_{14}B$ [8], the pressure-dependent superconducting phase diagram of $YBa_2Cu_3O_{6.6}$[4], and the direct observation of the Meissner effect in $La_3Ni_2O_{7-\delta}$ by combining local magnetometry with four-probe electrical transport [2]. Spatial mapping of the Meissner response further visualizes superconducting inhomogeneity and provides complementary magnetic and electrical evidence for superconductivity.

Together, these advances establish quantum sensing as a powerful platform for exploring magnetism and superconductivity under extreme conditions and open new opportunities for future studies of dense hydrogen and hydride superconductors at ultrahigh pressures.

References:

1. Jie Feng , **Xiao-Di Liu*** , Haian Xu, Pu Wang, Graeme J. Ackland , and Eugene Gregoryanz, Observation of ΔJ = 0 Rotational Excitation in Dense Hydrogens, **Physical Review Letters** 136, 016101 (2026).
2. Lin Liu, Jianning Guo, Deyuan Hu, Guizhen Yan, Yuzhi Chen, Lunxuan Yu, Meng Wang* , **Xiao-Di Liu*** , and Xiaoli Huang*, Evidence for the Meissner Effect in the Nickelate Superconductor La3Ni2O7-δ Single Crystal Using Diamond Quantum Sensors, **Physical Review Letter**s 135, 096001 (2025).
3. Hai-An Xu, Wan Xu, Pu Wang, Lin Liu, **Xiao-Di Liu***, Eugene Gregoryanz. Phase transitions in H_2-HD-D_2 mixtures up to 350 GPa. ***Physical Review B*** 111, 024109(2025).
4. Jun-Feng Wang, Lin Liu, **Xiao-Di Liu*** et al.. Magnetic detection under high pressures using designed silicon vacancy centres in silicon carbide. **Nat. Mater.** 22, 489-494 (2023).
5. **Xiao-Di Liu*,** *et al*, Counterintuitive effects of isotopic doping on the phase diagram of H_2-HD-D_2 molecular alloy, ***PNAS***, 117, 24(2020).
6. **Xiao-Di Liu**, *et al*, Comment on “Observation of the Wigner-Huntington transition to metallic hydrogen”, ***Science*** 357, 2286(2017).
7. **Xiao-Di Liu*,** *et al*, High-Pressure Behavior of Hydrogen and Deuterium at Low Temperatures, ***Phys. Rev. Lett.*** *119, 065301(2017*).
8. Lin Liu, Jun-Feng Wang, **Xiao-Di Liu***, et al. Coherent Control and Magnetic Detection of Divacancy Spins in Silicon Carbide at High Pressures. **Nano. Lett.** 22, 9943-9950 (2022)

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T1.1-O1 Bio/Life Sciences, Food Science and technology

Thermococcales in the Deep Sea: Adaptation to High Hydrostatic Pressure

Mohamed JEBBAR (Brest University, FRANCE),
Yann MOALIC (ISEN Brest, FRANCE)
Trinetra MUKHERJE (Brest University, FRANCE)
Sebastien LAURENT (Ifremer, FRANCE)
Violette DA CUNHA (Evry University, FRANCE)

Abstract

Background: The deep-sea hydrothermal vents, characterized by extreme pressure, temperature, and redox gradients, are hypothesized as cradles of early life (Martin et al., 2008). Thermococcales archaea—strictly anaerobic, hyperthermophilic, and often piezophilic—are key models for studying adaptation to these environments (Bertoldo and Antranikian, 2006). Traditionally classified into three genera, their taxonomy and adaptive mechanisms remain underexplored.

Methods: We employed a multidisciplinary approach, combining omics, culture-based physiology, biophysics, and genetics, to dissect the adaptive strategies of Thermococcales under deep-sea vent conditions.

Results: Sequencing of 69 new Thermococcales genomes, alongside existing data, yielded over 100 high-quality, closed chromosomes—one of the most comprehensive datasets for an archaeal order. Pangenomic and bioinformatic analyses reclassified these genomes into five distinct genera, challenging current taxonomy. Integration of pangenomic data with metabolic predictions revealed the distribution, evolutionary history, and metabolic specializations across species and ancestors. Notably, the piezophilic *Thermococcus barophilus* thrives under high hydrostatic pressure (HHP), unlike the piezosensitive *Thermococcus kodakarensis*. Comparative studies uncovered proteome structural adaptations and unique hydration dynamics under HHP (Martinez et al., 2016). In *T. barophilus*, HHP induces repression of amino acid biosynthesis genes, resulting in auxotrophy for 17 amino acids, and upregulates energy and carbohydrate metabolism (Cario et al., 2015; Vannier et al., 2015). The mechanism for amino acid acquisition under HHP remains unresolved; ongoing genetic, physiological, and omics investigations aim to clarify this.

Conclusions: This work redefines Thermococcales taxonomy and elucidates HHP adaptation mechanisms, including metabolic shifts and amino acid auxotrophy. Their stable enzymes and pathways offer promising biotechnological applications for industrial catalysis and bioremediation under extreme conditions. Continued omics studies will further illuminate their adaptive and applied potential.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T1.1-O2 Bio/Life Sciences, Food Science and technology

Different activities of a hydrolase under pressure

Aline SCHNEIDER-TEIXEIRA (CIDCA-CONICET, Argentina; ICTAN-CSIC, Spain; ICP-CSIC, Spain),
Sara JUAREZ (ICTAN-CSIC, Spain; CIB-CSIC, Spain)
Francisco Javier PLOU (ICP-CSIC, Spain)
Beatriz GALAN (CIB-CSIC, Spain)
Jose Luis GARCIA (CIB-CSIC, Spain)
Pilar RUPEREZ (ICTAN-CSIC, Spain)
Antonio Diego MOLINA-GARCIA (ICTAN-CSIC, Spain)

Abstract

The general effect of High Hydrostatic Pressure on biopolymers and, especially, on proteins, is the well-known destabilization of their solution structures, leading, depending of pressure, temperature and treatment time, to dissociation of structural elements or partial or total denaturation (with the implicit reduction or loss of enzymatic activity). These effects can be reversible after return to atmospheric pressure or longer lasting, depending on factors kinetically controlling the process. However, in a number of enzymatic systems, the effect can be an enhancement of the activity or, at least, an overall performance improvement. This behavior deserves our attention, both as a technological improvement and as a chance for advancing in our understanding of pressure effects on biopolymers and of their structure-function-stability relationships, themselves.

Cellulases, hydrolases able to cut (1→4)-β-D-glucosidic bonds present in many polysaccharides, such as cellulose, are known to be sensitive to pressure, in given conditions improving its catalytic performance. It has been reported in the fungal origin (Trichoderma reesei) endoglucanase II, reacting with several plant substrates. Here, its effect on artichoke cellulose-rich is reported.

T. reesei hydrolytic activity is actually carried out by an enzymatic complex, containing different activities, cleaving polysaccharides in different positions. It is commercially produced under the name Celluclast™. Additionally, different domains carry out different functions, some of them catalytic, but others related to interactions with substrates. To obtain information on the mechanism in which activity is modified by pressure, the catalytic domain of T. reesei endoglucanase II was heterologously expressed in E. coli and purified. Its cellulose-cleaving activity was extensively characterized at atmospheric conditions, showing a behavior and stability similar to that within the complex, in spite of not being associated to the rest of proteins. Its activity was found to be enhanced by pressure.

These pressure-promotion effects on cellulose-cleaving activity were observed when the reaction took place under pressure, by measuring reactants and products before and after given periods of pressure treatment.

Celluclast™ commercial cocktail also shows a somehow unexpected hydrolytic activity towards chitosan. This linear, chitin-derived polymer by partial deacetylation, is also bound by (1→4)-β-D-glucosidic bonds, after all, not so different from cellulose bonds, but steric differences, as well as the net charge of chitosan in solution are differential factors to be noted.

In a different type of experiment, Celluclast™ previously treated in solution under pressure showed a significant increase of activity towards chitosan. The possible action mechanisms under these similar but not equal responses to pressure are discussed, proposing lines of research to ascertain the ways to increase this enzyme performance, as well as to understand pressure-related proteins structure-function relations.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T1.1-O3 Bio/Life Sciences, Food Science and technology

The use of high pressure processing (HPP) as a tool for microbial control and quality preservation in modern food systems

Tone Mari RODE (Nofima, Norway),

Abstract

High pressure Processing (HPP) has become one of the most important non-thermal preservation technologies in the food industry, enabling microbial control while maintaining many of the sensory and nutritional attributes associated with fresh foods. Today, HPP is applied commercially across a broad range of refrigerated products, including juices, ready-to-eat meals, meat products, seafood, and fruit- and vegetable-based foods. However, its suitability and effectiveness is product-specific, depending on the characteristics of the target microorganisms, food matrix, processing conditions, and subsequent storage environment.

This presentation will explore the role of HPP as a tool for microbial safety, shelf-life extension, and quality preservation in modern food systems. The influence of key processing variables – including pressure level, holding time, temperature, and product composition – will be discussed in relation to microbial responses such as inactivation, sublethal injury, and recovery during chilled storage. Particular attention will be given to vegetative pathogens, spoilage microorganisms, and *Listeria monocytogenes*, a major concern in refrigerated ready-to-eat foods.

The limitations of conventional HPP for controlling bacterial spores will also be addressed, together with emerging approaches such as pressure-assisted thermal processing and germination–inactivation strategies. In parallel, the presentation will examine how HPP can help preserve desirable quality attributes, including flavour, aroma, colour, texture, and nutritional value, while also highlighting product-specific challenges related to enzyme activity and pressure-induced quality changes.

Finally, HPP will be considered within a broader framework of integrated food preservation. The future of HPP lies not only in achieving microbial inactivation, but in enabling the design of food systems that simultaneously deliver safety, quality, sustainability, and consumer value.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T1.1-O4 Bio/Life Sciences, Food Science and technology

Effect of High Pressure on pea protein digestibility

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GEPEA, Oniris, Nantes, France

Abstract

In the context of increasing global interest in plant-based diets, pea protein represents a promising alternative to animal protein due to its relatively high protein content and balanced amino acid profile (Amat, 2023). While plant proteins are often limited in essential amino acids, peas can provide a complete amino acid profile especially when combined with cereals. However, their digestibility remains a key limitation. This study examines the nutritional potential and digestibility of pea protein, with a particular focus on the effects of High Pressure (HP) processing.

To carry out the experiment, pea protein powder (85% protein) and fresh green pea (5% protein) were used. Samples of pea protein powder suspensions were introduced in PA/PE bags and underwent a vacuumization. Then, they were treated by High Pressure (15°C, 5 min, 200 MPa, 400 MPa or 600 MPa). Protein digestibility was assessed as described by Gatellier & Santé-Lhoutellier (2009). Analysis of proteins and peptides was conducted using SDS-PAGE electrophoresis in denaturing conditions according to Laemmli (1970). Determination of total amino-acids in samples was performed according to Guyon (2018).

Above all, the *in vitro* digestibility of pea protein powder and green peas using pepsin digestion are compared. Results show that green peas are digested more rapidly in the early stages, whereas pea protein powder is initially less accessible to enzymatic action. However, over time, pea protein powder reaches a higher overall digestibility, suggesting structural differences that influence enzyme accessibility. Despite this, both forms exhibit relatively low digestibility compared to theoretical expectations, highlighting the need for improvement strategies.

High Pressure processing is investigated as a method to enhance digestibility. This non-thermal technology, commonly used in the food industry, can modify protein structure without significantly affecting other nutrients. The results demonstrate that HP treatment significantly improves pea protein digestibility. At pressure between 200 and 400 MPa, digestibility increases moderately, while at 600 MPa, a substantial improvement is observed, with more than half of the protein being digested. This effect is attributed to partial protein denaturation, which exposes new enzymatic cleavage sites and facilitates peptide release.

Electrophoresis analysis reveals that HP treatment does not destroy protein fractions but likely alters their conformation. After digestion, new low-molecular-weight peptides appear, especially at higher pressure, confirming enhanced enzymatic activity and protein breakdown. These findings support the hypothesis that HP improves enzyme accessibility rather than changing protein composition.

Amino acid analysis shows that pea protein is rich in key amino acids such as glutamic acid, lysine, leucine, and aspartic acid. Importantly, HP treatment does not alter the overall amino acid profile of undigested samples. However, after digestion, higher pressure increase the release of certain essential amino acids, particularly lysine and valine. This suggests that HP processing enhances not only digestibility but also the nutritional availability of important amino acids.

In conclusion, pea protein is a valuable plant-based protein source with a favorable amino acid composition but limited digestibility. High Pressure processing significantly improves its digestibility and promotes the release of nutritionally beneficial peptides and amino acids. These findings highlight the potential of HP technology to enhance the nutritional quality of plant proteins and support their use as sustainable alternatives to animal protein.

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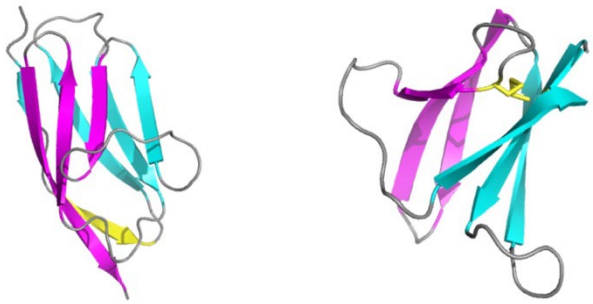
23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T1.1-O5 Bio/Life Sciences, Food Science and technology

Do similar folding pathways mean similar folds ? A comparative High-Hydrostatic-Pressure NMR folding study of ß-sandwich proteins.

Christian ROUMESTAND (Montpellier University, France),

Abstract

If we know from Anfinsen laws that the 3D structure of a protein is encoded in its sequence, the paths taken by the polypeptide to fold into a well-defined native structure are far to be well understood. This issue is particularly important in the case of proteins having a similar 3D fold, but very divergent sequences. For instance, all the proteins from the Immunoglobulin Super Family (IgSF) are built on a common fold: a 7-stranded ß-sandwich called Ig-fold, but they differ in their distribution, biological role, and also in their amino acid composition. Similarly, MAX effectors are a family of proteins widely distributed in the phytopathogen fungus *Magnaporthe oryzae* that share a conserved common 6-stranded ß-sandwich fold, despite low sequence identity. These effectors constitute the molecular arsenal for the fungus infection and contribute to the pathogenicity of the plant pathogen.



The ß-sandwich 3D Structure of Titin I27 (left) and AVR-Pib (right)

In the present study, we compared the folding pathways of two Ig-like folds (I27 module from Titin, a multi-modular protein found in vertebrate striated muscle, and ED3, a domain from the Dengue virus envelope E-protein), and 3 MAX effectors (AVR-Pia, AVR-Pib and MAX60). We used High-Hydrostatic-Pressure NMR (HHP-NMR), a technique particularly well suited to decipher protein folding landscapes [1,3], allowing the identification of folding intermediates that could be otherwise rubbed out by harsher method as chemical denaturation, for instance.

Steady-state HP-NMR experiments show that the unfolding of both Ig-like modules start with the disruption of connections between the N- and C-termini, yielding a similar folding intermediate, even though real-time HP-NMR kinetics studies suggest a markedly more hydrated transition state ensemble (TSE) for ED3 than for I27 [4,5]. In the case of MAX effectors, we found that AVR-Pia and AVR-Pib display a similar folding intermediate formed by the ß-sheet ß3ß4 [6]. On the other hand, MAX60 exhibits a different folding intermediate, consisting in its additional C-terminal helical extension and the ß-sheet ß1ß6 [7]. Thus, proteins with similar topology can present similar folding pathways, but in the frame of a similar structural context. In the case of MAX60, the C-terminal extension that makes close contacts with the protein core is able to change the folding pathway of the ß-sandwich.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T1.2-O1 Bio/Life Sciences, Food Science and Technology

Simulating the Deep Sea: High-Pressure Experiments on Indigenous Microbial Bioremediation of Hydrocarbons

Evina Gontikaki, Institute of Geoenergy, Foundation for Research and Technology - Hellas,

Abstract

Deep-sea oil spills present persistent ecological challenges in environments defined by high pressure, low temperature, and limited nutrient availability. Despite these constraints, such extreme ecosystems harbor diverse microbial communities naturally capable of degrading hydrocarbons. In this invited talk, I will present experimental work conducted by my group focusing on high-pressure simulations designed to replicate in situ conditions in the deep Eastern Mediterranean Sea. Our results shed light on how indigenous microbial communities respond to hydrocarbon inputs, revealing patterns of community succession, key functional traits, and the environmental constraints that influence bioremediation efficiency under realistic deep-sea conditions. Framed within a broader sustainability perspective, this work highlights how leveraging native microbial diversity and experimentally grounded insights can inform environmentally responsible strategies for mitigating hydrocarbon pollution in remote and sensitive marine ecosystems.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T1.2-O2 Bio/Life Sciences, Food Science and Technology

Fluid chemistry and mineral interactions as dual interfaces of microbial life in deep-sea vents under high-pressure conditions

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Abstract

Deep-sea vents (DSVs) are among the few environments on Earth where life thrives independently of sunlight, sustained entirely by the chemistry of the hydrothermal fluid and the minerals that precipitate along chimney walls. In these systems, microorganisms do not merely tolerate extreme condition, they rather exploit them, drawing energy and carbon directly from the fluid while actively reshaping the surrounding mineral matrix. Deciphering these two intimately coupled interactions, under the high hydrostatic pressures that prevail in the deep ocean, is central to understanding both the limits of life and the biosignatures it leaves behind.

In this PhD project, carried out within the ANR HOTDOG, we reproduce DSV conditions at lab scale using milli- and micro-fluidic devices built from sapphire (a material that withstands pressures up to 300 bar while remaining optically transparent). A porous microreactor geometry mimics the architecture of hydrothermal chimneys, enabling *in situ* monitoring by Raman spectroscopy and optical microscopy, alongside *ex situ* analyses (gas chromatography, TEM).

To probe fluid-driven metabolism, we cultivated the methanogen *Methanothermococcus okinawensis* under increasing H_2/CO_2 partial pressures (2–50 bar). Methane production rose sharply with pressure (from 14.04 ± 1.12% at 2 bar to 48.06 ± 1.75% at 10 bar, the maximum yield) with no inhibitory effect on growth, demonstrating that pressure amplifies the metabolic exploitation of hydrothermal gases.

To probe mineral interactions, the hyperthermophilic archaeon *Thermococcus barophilus* was incubated with abiotically stable FeS_2 within a microreactor. *In situ* microscopy revealed progressive FeS_2 dissolution over 135 h in the presence of cells (an effect absent in abiotic controls [1]) pointing to an active cell–mineral interaction, possibly related to the biomineralization processes previously described in Thermococcales [2].

Together, these results frame DSV microorganisms as active agents at two interfaces: i) the fluid they metabolize and ii) the mineral they transform. High pressure emerges not as a mere environmental constraint, but as a key parameter shaping both interactions. These findings shed new light on microbial habitability in extreme environments, from the Hadean Earth to potential extraterrestrial settings.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T1.2-O3 Bio/Life Sciences, Food Science and Technology

Studies of biological systems under high hydrostatic pressure and the instrumentation required for that

Judith PETERS (Univ. Grenoble Alpes, ILL, IUF, France)

Abstract

High hydrostatic pressure (HHP) is one of the stressors, which can perturbate or denaturate proteins. To investigate the impact of HHP, incoherent neutron scattering is a well-adapted method giving access to information on molecular dynamics. In this overview, I will first present some instrumental setups taking particularly into account the requirements by neutron scattering experiments. In a second time, I will show applications in several domains:

The question of protein adaptation to HHP environments is extremely important to shed light on evolutionary questions and for the understanding of functioning under such harsh conditions. Some recent results will be presented here [1, 2]

Moreover, proteins undergo a series of transitions as a function of temperature, including the dynamical transition cold and heat denaturation. As cold denaturation occurs for most proteins at negative temperatures, HHP is a tool to shift the transition to more accessible temperatures, i.e. higher temperatures for the cold denaturation and lower temperatures for the heat denaturation. We investigated the impact of HHP on the transition and energy landscape [3] for some model proteins, what will also be discussed here (see figure 1).

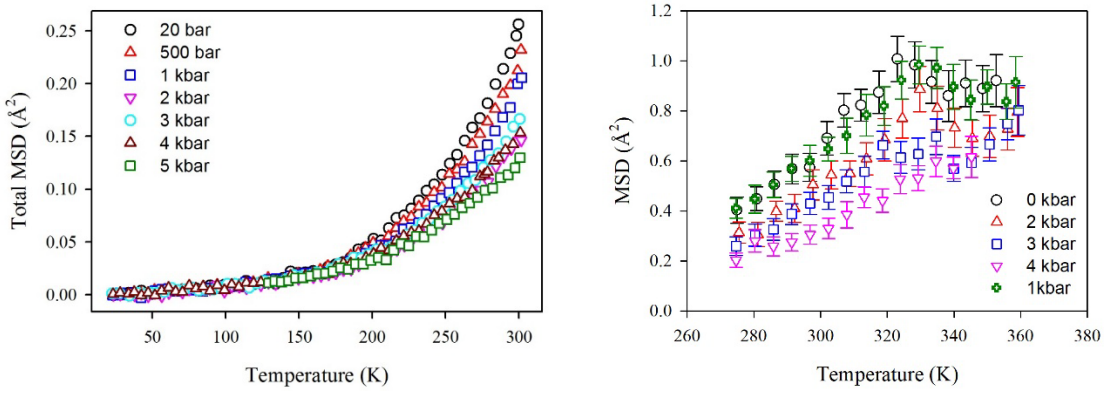

Figure 1: Mean square displacements (MSD) extracted from elastic incoherent neutron scattering under HHP on myoglobin in a large temperature range.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T1.2-O4 Bio/Life Sciences, Food Science and Technology

Use of High Pressure in Drug Design

Hans Robert Kalbitzer (University of Regensburg, Germany)

Abstract

High-pressure NMR spectroscopy (HPNMR) is a powerful technique for characterizing conformational equilibria of biological macromolecules in solution [1]. High-pressure X-ray crystallography (HPMX) provides a complementary and orthogonal approach, enabling the direct visualization of pressure-induced conformational changes with atomic resolution under well-defined thermodynamic conditions [2]. From a physical perspective, hydrostatic pressure selectively stabilizes low-volume conformational states and thus shifts equilibria toward sparsely populated substates that are often inaccessible under ambient conditions. The application of high pressure has therefore emerged as a unique and non-invasive tool for detecting rare, low-population “excited” conformational states of proteins that are particularly relevant for functional regulation and drug discovery.

These excited states constitute attractive targets for intrinsic allosteric inhibition, in which small molecules selectively bind to a non-dominant conformational state and thereby redistribute the conformational equilibrium away from the catalytically competent form toward a less active state of the catalytic cycle [3]. Here, we demonstrate how the combined application of HPNMR and HPMX allows not only the identification and thermodynamic characterization of such rare states, but also their direct structural characterization in complex with small-molecule ligands.

As a proof of principle, we study Ras, a key regulator of cellular signal transduction involved in proliferation and differentiation. Oncogenic Ras mutants are constitutively active due to impaired regulatory control. Ras activation is mediated by guanine nucleotide exchange factors (GEFs), which promote the exchange of GDP for GTP, whereas inactivation is driven by GTPase-activating proteins (GAPs), which stimulate GTP hydrolysis.

Using high-pressure NMR spectroscopy in the pressure range from 0.1 to 300 MPa, four conformational states of Ras were detected and characterized: state 1(0), the nucleotide-releasing state; state 1(T), the GEF-binding state; state 2(T), the effector-binding state; and state 3(T), the GAP-interacting state. One of the earliest Ras inhibitors identified was Zn^{2+}–cyclen. The three-dimensional structure of its complex with Ras was previously inferred from chemical shift perturbation and paramagnetic relaxation enhancement experiments on wild-type Ras and engineered state 1(T) mutants, followed by docking calculations [4]. However, crystallographic characterization of this cmplex had remained elusive because the ligand-binding site is closed in conventional crystal structures.

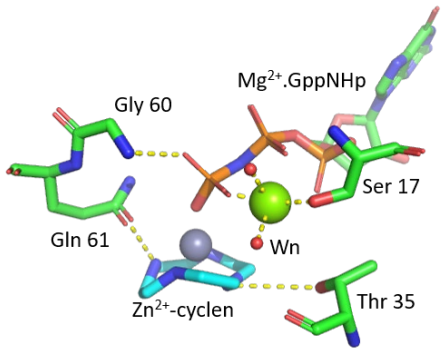

Fig. 1. Coordination of Zn^{2+}-cyclen in a single crystal of Ras.Mg^{2+}.GppNHp in state 1(T) induced by high pressure (500 MPa) [5].

We show that the application of high pressure to Ras crystals induces a conformational opening of the binding site, enabling high-resolution visualization of the Ras–Zn^{2+}–cyclen complex (Fig. 1) by HPMX [5]. These results highlight the methodological complementarity of solution- and crystal-based high-pressure techniques and illustrate the broader potential of high pressure as a controllable thermodynamic variable in structure-based drug discovery. Based on these findings, we propose a general strategy for integrating high-pressure methods into drug development workflows targeting rare, functionally relevant conformational states.

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Insights into the Structure of Invisible Conformations of Large Methyl Group Labeled Molecular Machines from High Pressure NMR

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Most proteins are highly flexible and can adopt conformations that deviate from the energetically most favorable ground state. Structural information on these lowly populated, alternative conformations is often lacking, despite the functional importance of these states. Here, we study the pathway by which the Dcp1:Dcp2 mRNA decapping complex exchanges between an autoinhibited closed and an open conformation. We make use of methyl Carr-Purcell-Meiboom-Gill (NMR) relaxation dispersion (RD) experiments that report on the population of the sparsely populated open conformation as well as on the exchange rate between the two conformations. To obtain volumetric information on the open conformation as well as on the transition state structure we made use of RD measurements at elevated pressures. We found that the open Dcp1:Dcp2 conformation has a lower molecular volume than the closed conformation and that the transition state is close in volume to the closed state. In the presence of ATP the volume change upon opening of the complex increases and the volume of the transition state lies in-between the volumes of the closed and open state. These findings show that ATP has an effect on the volume changes that are associated with the opening-closing pathway of the complex. Our results highlight the strength of pressure dependent NMR methods to obtain insights into structural features of protein conformations that are not directly observable. As our work makes use of methyl groups as NMR probes we conclude that the applied methodology is also applicable to high molecular weight complexes.

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T2.1-O1 Chemistry, Synthesis, Novel materials

Tuning thermal expansion and mechanical properties by high pressure insertion of guest molecules

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Benoît BAPTISTE (IMPMC, UMR7590-CNRS, Sorbonne Université, IRD, MNHN, FR)
Julien HAINES (ICG, Université de Montpellier, CNRS, ENSCM, FR)

Abstract

Zeolites are aluminosilicates built up of corner-sharing TO_4 (T = Si, Al, ...) tetrahedra, which form a network of pores with typical diameters between 3 and 8 Å. These microporous materials are used at a large scale for applications in, for example, catalysis, adsorption, separation, and ion exchange. If zeolites are compressed in the presence of fluids containing atoms or molecules small enough to enter the pores, pressure-induced guest insertion can be observed. This can provide important information on the maximum possible filling of these porous materials and can be of interest in the fields of CO_2 capture[1-3] and hydrogen storage[4,5]. Guest insertion also strongly modifies the phase stability and the mechanical properties, such as compressibility and thermal expansion, of filled as compared to empty-pore zeolite. The rhombohedral, zeolite chabazite (CHA) with small 3.7 Å pores based on 8-membered rings of tetrahedra, is a promising candidate for CO_2 capture[3] due to the small difference between the pore size and the kinetic diameter of CO_2 (3.3 Å) and the loading of CO_2 has been studied, stabilizing its structure up to 12 GPa with a high degree of filling[3]. The aluminophosphate $AlPO_4$-17, with the hexagonal, erionite structure (ERI), space group $P6_3/m$ and cell parameters a and c of 13.1113 Å and 15.3600 Å, respectively,[6] is another example of a zeolite-type material with even smaller 3.4 Å, 8-membered ring pores, which are even closer to the kinetic diameter of CO_2, differing from chabazite in the stacking sequence of 6-membered rings in the c-direction (AABBCC for CHA and AABAAC for ERI). This material could be expected to have a very promising CO_2 and H_2 capture performance. Anhydrous $AlPO_4$-17 has been found to exhibit a very strong Negative Thermal Expansion (NTE) coefficient, *the highest known for an oxide*, of -35.1×10^{-6} K^{-1} over the temperature range of 18-300 K [7], and complete pressure-inducing amorphisation (PIA) near 2.5 GPa in non-penetrating pressure transmitting media [6]. Structural studies on insertion in $AlPO_4$-17 at high pressure (HP) shed light on deactivation of PIA on this system: recently we have performed the insertion of Ar, N_2 and O_2 on $AlPO_4$-17 (see ref. 8) and on the study of its structural behavior to HP and low T (see ref. 9). Accurate isobaric scans at low T were performed and analysis from the data were able to precisely locate the inserted molecules and determine the structure of O_2-filled $AlPO_4$-17 at HP. Thermal expansion was measured precisely at 0.38 GPa by synchrotron powder XRD. Spectacular results were obtained: whereas the overall volume thermal expansion only exhibits a small change with respect to empty $AlPO_4$-17 at ambient pressure, the expansion along the a direction decreases almost to zero and the expansion along c increases by a factor of 7 [9]. Very recently we were able to perform HP CO_2 insertion on $AlPO_4$-17, measured by synchrotron XRD single crystal under HP and high-T, being able to localize the guest molecules. Now, on-going experiments are investigating the structural response of $AlPO_4$-17 to pressure, temperature and guest insertion by using H_2 and He as penetrating PTM. In this Invited Talk we will present the latest obtained results and perspectives.

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Metastable states of matter: a path towards new 2D and 1D materials

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Abstract

Materials are at the heart of modern scientific and technological development. To participate in and to contribute to the solution of existing and future global challenges, we must explore novel design concepts. In this respect, exploration of metastable states of matter greatly enhances opportunities to design new advanced materials. Combining theoretical simulations with experiment and broadly varying external parameters, pressure, temperature and composition allows one to discover phases which could not be synthesized otherwise. In this talk, we pay special attention to one of the major challenges of the high-pressure synthesis in terms of applications: the need to recover the synthesized materials at ambient conditions. We demonstrate feasibility of using high pressure in a search for materials with reduced dimensionality. Starting with 2D materials, we discuss a discovery of a new Dirac material, layered van der Waals bonded BeN_4 polymorph [1], followed by a realization of an ideal Cairo tessellation in NiN_2, which is a pentagonal 2D material [2].

Next, we turn out attention to 1D materials, which attract great attention since the pioneering works of Peierls. Still, the synthesis of truly monoatomic chains remains elusive. We have explored a novel path of experimental synthesis of monoatomic one-dimensional chains by their chemical stabilization in ionic compounds. We have demonstrated that in synthesized at high pressure sodium halides Na_4X_5 (X = I, Br, Cl) with *hP*18 Ga_4Ti_5-type structures, transfer of valence electrons from cations to anions has led to the formation of halogen chains connected with other atoms only by ionic interaction and having one-dimensional electronic structure. The Peierls physics in the systems is confirmed by theoretical calculations, newly synthesized incommensurately modulated *i-hP*18-Na_4X_5 (X = I, Br, Cl) compounds, as well as by the discovered *hP*36 phases of Na_4Cl_5 and Na_4Br_5 [3].

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T2.1-O3 Chemistry, Synthesis, Novel materials

Nitrogen dissolution in Liquid Ga and Fe at high pressure by *ab Initio* analysis – application to crystallization of GaN and BN

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Abstract ()

Presently available experimental data indicate that very high solubility of nitrogen in Fe can be achieved in contrast to III group metals (Ga, In, Al) where the solubility is orders of magnitude lower. In this study, dissolution of molecular nitrogen in Ga and Fe metals was investigated by *ab initio* calculations. It was found that both metals strongly attract nitrogen that leads to N_2 molecule decomposition before dissolution. However the N bonding inside these solvents is different. For Ga it is between *Ga4s* and *Ga4p* and *N2p* states whereas for Fe this is by *N2p* states to *Fe4s, Fe4p* and also *Fe3d* states. Accordingly, the calculated energy of dissolution of molecular nitrogen for arbitrary chosen starting atomic configurations, was 0.535 eV/mol. and -0.299 eV/mol. for Ga and Fe, respectively. Expressions for configurations optimized with molecular dynamics contained additional terms, but the difference between the corresponding energy values, 1.107 eV/mol. and 0.003 eV/mol was similar. Full thermodynamic analysis of chemical potential was made employing entropy derived terms in Debye picture. As it has been confirmed, the Debye temperatures are similar: for Ga, $\theta_D = 552\ K$ and for Fe, $\theta_D = 512\ K$. These values indicate that temperature dependent terms are large but not much different, their contribution is: $G_{S-therm} = -0.488\ eV$ and $\Delta G_{S-therm} = -0.475\ eV$ at *T = 1000 K* for Ga and Fe respectively. The entropy dependent terms were obtained ~~by~~ via normal conditions path to avoid singularity of ideal gas entropy at zero K. From these data, nitrogen solubility was obtained, being indeed much higher for Fe than for Ga at similar temperature. In ideal solution approximation, the N concentration in Ga was about $3 \times 10^{-3}\ at\ fr$ at $T = 1800\ K$ and $p = 10^4$ bar whereas for Fe, it was about $9 \times 10^{-2}\ at\ fr$. at the same conditions, which is in very good agreement with experimental evaluations. The high solubility in iron indicates that liquid Fe could be perspective solvent to crystallize GaN from metallic solution at high pressures of nitrogen.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T2.1-O4 Chemistry, Synthesis, Novel materials

Influence of volatiles on the chemistry of Fe-O system

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Abstract

Being the only geochemically abundant element in Earth's interior with multiple stable oxidation states, iron plays a key role in controlling oxygen fugacity and, consequently, in regulating redox equilibria, phase relations, and volatile cycles in the deep Earth. Numerous mixed-valence iron oxides with unexpected compositions have recently been identified under high-pressure and high-temperature conditions, revealing rich crystal chemistry and intriguing physical properties, including pressure-induced spin transitions, charge ordering, and the emergence or collapse of magnetic order [1–4]. The chemical behaviour of iron-bearing compounds is particularly sensitive to the presence of volatiles such as H_2O and CO_2, which are continuously recycled into Earth's interior through subduction processes. In recent years, novel iron carbonates [5–7] and hydroxide/oxyhydroxide phases [8,9] have been synthesized at high pressures and high temperatures. Hydrous phases such as pyrite-type FeO_2H_x ($x \leq 1$) are considered possible carriers of water and hydrogen to the lowermost mantle [8,9] and have been proposed as a potential origin of ultralow-velocity zones and seismic anomalies near the core–mantle boundary [10]. Despite intensive research, the role of volatiles in controlling the chemistry of Fe-bearing compounds at extreme conditions remains insufficiently understood.

In this study, we applied single-crystal X-ray diffraction in laser-heated diamond anvil cells (DACs) to investigate the high-pressure behaviour, chemical reactivity, and thermal stability of Fe-bearing compounds, including oxides and carbonates, in the presence of H_2O and CO_2 at pressures up to 75 GPa and temperatures up to 3000 K. Recent advances in multi-grain single-crystal XRD enable the detection of minor phases and reliable determination of their crystal structures, thereby significantly improving the accuracy of phase identification in complex high-pressure assemblages. We compare the chemical reactions between iron compounds and volatiles with those occurring in inert pressure media under conditions relevant to Earth's deep interior. Our results show that volatiles can substantially alter reaction pathways at extreme conditions, even when they are not incorporated into the final crystalline products.

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T2.1-O5 Chemistry, Synthesis, Novel materials

High-pressure experiments on $XePtF_6$ – the first noble gas compound

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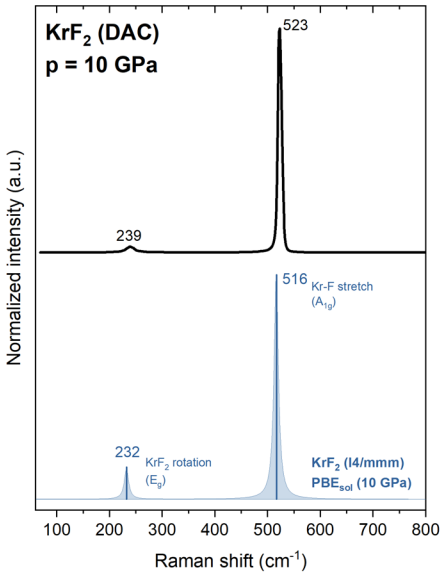
Abstract

Although the demonstration of noble-gas reactivity represents one of the most significant breakthroughs of 20th-century inorganic chemistry, the first noble-gas compound, $XePtF_6$ ($XeF_2 \cdot PtF_4$) [1], lacks comprehensive structural characterization, and its geometry and atom connectivity remain to be elucidated [2]. Ternary Xe-Pt-F compounds, however, could serve as important systems for benchmarking theoretical methods and deepening our understanding of Lewis acid-base interactions and chemical bonding in noble-gas compounds [3].

In a recent study, we proposed several structural models of $XePtF_6$ through density functional theory calculations, which were derived from experimentally determined crystal structures of XeF_2–MF_4 (M = Cr, Mn) analogues [4]. Here, we present diamond anvil cell experiments in which laser-heated recrystallization, single-crystal diffraction, and confocal Raman microscopy were combined with solid-state modelling, resulting in the first successful structural determination of $XePtF_6$. Furthermore, we experimentaly explored the high-pressure reactivity within the Xe–Pt–F system, as well as the thermodynamic stability of compressed krypton difluoride.



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T2.2-O1 Chemistry, Synthesis, Novel materials

Shaping Spin-Crossover Molecular Ceramics through Cool-SPS for Efficient Barocaloric Refrigeration

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Abstract

As the global demand for energy-efficient cooling solutions grows in response to climate change, tranditional vapor-compression system, responsible for significant energy consumption and greenhouse gas emission, are under increasing scrunity. Everyday refrigeration devices (air conditioners, refrigerators, heat pumps) accounted for up to 20% of the world's electricity production in 2025 and 7.5% of its greenhouse gas emission[1]. One of the most promising new energy-saving technologies for cooling systems used the mechanocaloric effect, which describes adiabatic temperature variations brought on vy pressure (barocaloric) or stress (elastocaloric). Using non-critical, inexpensive, pleintiful, and non-toxic elements, mechanocaloric research has created advanced materials in the past ten years that can readily overcome electrocaloric and magnetocaloric materials[2]. In molecular Spin Crossover (SCO) complexes, a stimulus-induced (*T*, *p*, light,etc.) variation in electronic configuration triggers a transition in properties (mechanical, magnetic, optical, electronic) along with structural and entropy changes[3]. Most interestingly, this transition can be triggers by low pressure stimuli of less than few kilobars, due to volume changes of up to 11%[4]. These characteristics position SCO materials as highly promising canditates for barocaloric application as anticipated in breakthrough reserach published on 2016[5].

Such materials, which are typically only availble as polycrystalline powders, must be shaped into macroscopic (poly)centrimetric forms in order to be used technologically. We have demostrated on variety of respresentative samples that Cool-SPS processing (SPS : Spark Plasma Sintering, $50 \leq T \leq 600$°C ; $40 \leq p \leq 900$ MPa) can sinter powders into "molecular ceramics"[6], with relative densities that satisfactorily range from 85 to 95% of the corresponding crystal structures. Singnificant differences have been observed regarding the morphology, phase identity (when dealing with polymorphs) with the initial materials, whether during the sintering process or in the properties of the resulting ceramics. For molecular materials, the results will be compared with the (*p,T*) phase diagrams derived from X-ray diffraction data. In fact, a key tool for monitoring and managing sintering processes is the maping of those complexes phase diagram, which is primarily accomplished through spectroscopic and diffraction studies on single crystals or polycrystalline powder to examine and comprehend the nature of the species seen when combining pressure and temperature changes.

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T2.2-O2 Chemistry, Synthesis, Novel materials

Abiotic formation of organic complexity from multicomponent ice analogue via high-pressure photochemistry

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Abstract

Complex, multicomponent ice mixtures featuring simple molecules such as, water (H_2O), ammonia (NH_3), methane (CH_4), carbon monoxide (CO), carbon dioxide (CO_2), methanol (CH_3OH), are widespread across the Universe. Their presence has been revealed in several astrochemical environments such as molecular cloud ices [1], comets [2] or asteroids [3]; furthermore, this icy material constitutes the crustal layers and interiors of icy moons [4–6] and planets [7].

Besides their diffusion, these mixtures are appealing because they represent an ideal starting system for prebiotic synthesis of interesting biological precursors, such as alcohols (R-OH) and amines ($R\text{-}NH_2$), or chemicals featuring carbonylic (R_2-C=O), carboxylic (R-COOH) and amide ($R\text{-}CONH_2$) functionalities, up to amino acids and sugars. Prebiotic studies are typically performed under low pressure/low temperature conditions [8], and density is rarely considered in triggering or orienting this reactivity. There are a certain number of reports about thermodynamic stability of simple ice mixtures, mainly clathrate hydrates [9], but the combined effect of high pressure, generated by diamond anvil cells (DACs) and UV irradiation must be considered to have a full picture of the possible reaction scenarios. In fact, the photodissociation of many of these simple chemicals by UV radiation [10–12], may trigger chemical reactivity under high pressure on complex mixtures relevant to the astrochemical domain, thus extending the reactive conditions beyond those typical of the surfaces and first crustal layers of icy worlds, simulating those experienced during dynamics events such as superficial impact of high or medium intensity.

Here we present our results about the high-pressure, photoinduced reactivity of a planetary model ternary mixtures of water, ammonia and methanol in different compositions. The molar ratios of the three components have been chosen to accurately mimic the chemical composition of volatiles suggested for icy planets and giant planets of solar-like systems[6]. The reactivity has been triggered by the two-photon absorption of near UV wavelength at pressures below 1.5 GPa, and the samples have been characterized by optical spectroscopy (Raman, FTIR) along the various irradiation cycles, revealing the formation of a variety of products such as methoxyamine, amonimethanol, formamide, N-methylformamide and glycine, the simplest amino acid, along with the production of molecular hydrogen sequestered in the form of its hydrates. These results highlight the role of pressure in modulating photochemical pathways initiated by radicals formed through methanol, ammonia, and water photodissociation, ultimately promoting the formation of small organic molecules from simple ice mixtures. These findings support the idea that transient high-pressure events, such as impacts, may enhance chemical complexity in icy environments [13].

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Towards Sustainable Spin-Crossover Materials through Mechanochemical One-Pot Synthesis

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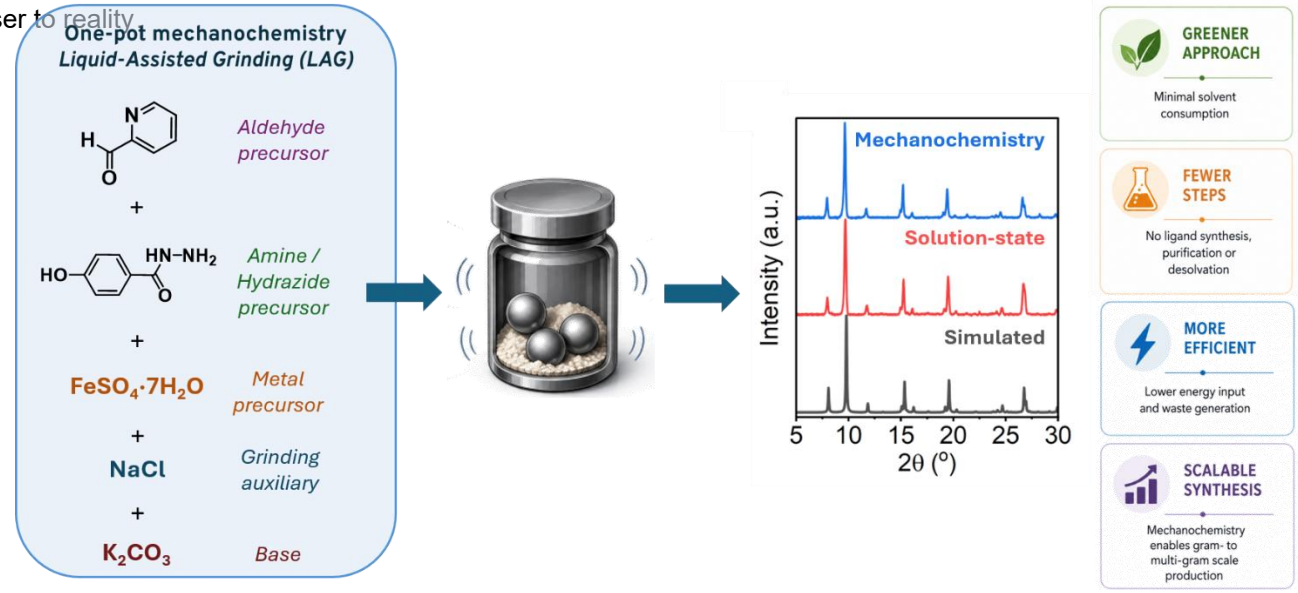
Abstract

Spin-crossover (SCO) compounds are molecular materials capable of reversibly switching between high-spin and low-spin electronic configurations in response to external stimuli such as temperature, pressure, light, and guest molecules. Among them, Fe(II)-based SCO complexes are particularly attractive due to their potential applications in molecular electronics, spintronic devices, and, more recently, barocaloric refrigeration technologies. The latter application is especially promising because pressure-induced spin-state switching is accompanied by significant entropy and volume changes, making SCO materials attractive candidates for solid-state cooling.

Schiff-base ligands offer a versatile platform for the design of SCO materials, as subtle modifications of the ligand framework can finely tune the transition temperature and cooperativity. However, the development of practical barocaloric materials requires not only suitable functional properties but also sustainable and economically viable synthetic routes. Mechanochemistry has emerged as a greener and more sustainable alternative to conventional solution-based synthesis, significantly reducing solvent consumption, energy requirements, and waste generation.

Here we report the first one-pot mechanochemical synthesis of Fe(II) SCO complexes in which both Schiff-base ligand formation and metal coordination occur simultaneously during liquid-assisted grinding (LAG). Three tridentate Fe(II) Schiff-base complexes, $Fe(L1)_2$, $Fe(L2)_2$ and $Fe(L3)_2$ [L1 = 4-hydroxy-N′-(pyridin-2-ylmethylene)benzohydrazide (HMPB), L2 = 1-((quinolin-8-ylimino)methyl)naphthalen-2-ol (HQNAL), and L3 = (4-chloro-2-((quinolin-8-ylimino)methyl)phenol) (4Cl-QSAL)], were obtained quantitatively through this direct synthetic approach.

Powder X-ray diffraction and magnetic measurements demonstrate that the mechanochemically prepared materials retain the same structural phases and spin-crossover behaviour as their conventionally synthesised counterparts, while directly yielding the desired desolvated phase. By eliminating multiple synthetic, purification and desolvation steps, this one-pot approach provides a robust, efficient and sustainable route to Fe(II) SCO materials. In addition, the inherent scalability of mechanochemical synthesis makes this methodology particularly attractive for the production of SCO materials beyond the laboratory scale, bringing their practical application in barocaloric refrigeration technologies a step closer to reality.



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T2.3-O1 Chemistry, Synthesis, Novel materials

From CO_2 clathrate hydrate to solid carbonic acid: high-pressure chemistry in astrochemical ices

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Abstract

Water-rich ices containing simple volatile molecules are widespread throughout the Solar System and the interstellar medium, making their chemistry highly relevant to astrochemical processes [1]. Among these systems, carbon dioxide (CO_2)–water (H_2O) mixtures are of particular interest due to the abundance of CO_2 on icy planetary bodies, comets, and interstellar ices [2]. Moreover, the chemical reactivity between CO_2 and H_2O may result in the formation of their 1:1 adduct, carbonic acid (H_2CO_3), a key intermediate in carbon chemistry. The synthesis of H_2CO_3 from its constituents has long remained challenging and has often been carried out under very drastic conditions starting from fluids: only a few recent works have encompassed high-pressure in this complex framework [3-5].

We recently identified a particularly effective route for the formation of solid hydrated carbonic acid through the cold compression of pristine CO_2 clathrate hydrate [6-7]. Under moderate pressure and temperature conditions (130–270 K, <5 GPa), this process leads to the formation of diverse hydrated phases, including crystalline ε-H_2CO_3, amorphous ε-H_2CO_3, and crystalline ε_m-H_2CO_3. These phases were characterized using Raman spectroscopy together with synchrotron and laboratory X-ray diffraction. A detailed investigation of the ε_m-H_2CO_3 formation pathway [7] reveals a complex multistep mechanism involving dense amorphous intermediates with remarkable thermal and pressure stability, as well as the transient appearance of metastable ice phases [8]. The observed transformations highlight the rich structural landscape accessible in compressed CO_2–H_2O systems and provide new insight into the behavior of carbon-bearing ices under planetary interior conditions.

The relatively mild pressure–temperature regime required for these reactions is compatible with processes occurring within icy worlds, such as the subduction of surface materials into deeper layers. These findings therefore suggest previously unrecognized pathways for carbonic acid formation and storage in extraterrestrial environments, with important implications for the chemical evolution of icy bodies and the diversity of astrochemical processes beyond Earth.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T2.3-O2 Chemistry, Synthesis, Novel materials

New carbonic acid compounds in the H-C-O system at elevated pressures

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Abstract

Due to its great relevance for astrophysical research carbonic acid (H_2CO_3) and its monohydrate ($H_2CO_3 \cdot H_2O$) have recently been studied intensively [1-5]. However, no single-crystal structure determination of water-free H_2CO_3 had been reported, while for $H_2CO_3 \cdot H_2O$ a structural model based on single crystal diffraction data had been determined at 6.5 GPa [5]. Hence, no lattice dynamical calculations for H_2CO_3, needed for unambiguous vibrational spectrum assignment and, consequently, for remote sensing of its presence in meteorites or on icy bodies, could be carried out [1,2]. The high-pressure behaviour of H_2CO_3 has long been disputed [6-9]. At pressures between 1-44 GPa the crystal structure of H_2CO_3-*Pnma* has been predicted by density functional theory (DFT) calculations [6]. However, this structural model substantially differs from the structure of H_2CO_3-$P2_1/c$ derived from a combined neutron powder diffraction and DFT-based study at ~2 GPa [7].

In our studies we used a combination of single crystal X-ray diffraction, Raman spectroscopy and DFT-based calculations, in order to study the formation and crystal structure of H_2CO_3 at elevated pressures in laser-heated diamond anvil cells (LH-DAC). We determined for the first time the crystal structure of a H_2CO_3 phase ($P2_1/n$) using single crystal X-ray diffraction (Fig. 1R) and derived the positions of the hydrogen atoms experimentally [8]. Fig. 1L shows our 2D-Raman mapping before and after laser-heating a H_2O + CO_2 mixture at 8(1) GPa. Using the same approach, we confirmed that H_2CO_3-$Cmc2_1$ with polymerized [CO_4]-chains can be obtained at 40(2) GPa [9]. Its crystal structure was successfully refined from single crystal X-ray diffraction data, including the hydrogen position and is in agreement with a structural model predicted earlier [6]. Further experiments, carried out in the H-C-O system between 5-50 GPa, show that other novel carbonic acid phases can be obtained by laser-heating a H_2O + CO_2 mixture in this pressure range and that the phase diagram of carbonic acid is more complex than previously assumed.

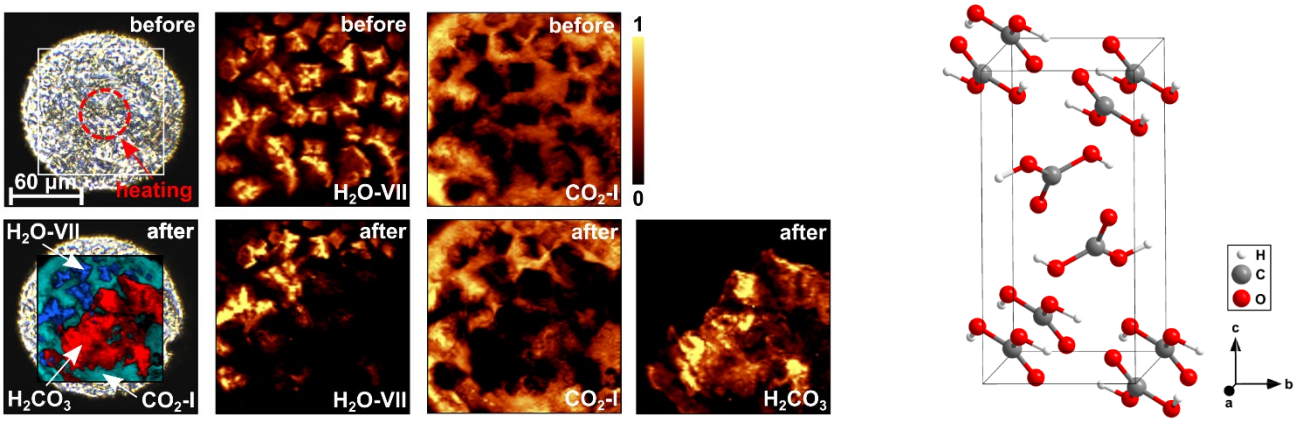

Fig. 1 (L): Synthesis of H_2CO_3 at 8(1) GPa from a H2O + CO2 mixture in a LH-DAC. **(R)** Structure of H_2CO_3-$P2_1/n$ [3].

We acknowledge funding by the DFG (BA4020, WI1232, BY101/2-1, BY112/2-1), the Johanna-Quandt-Stiftung, the LOEWE program and the Fulbright Program. BW is grateful for the Dassault Systemes Science Ambassador program. We acknowledge DESY, ESRF and APS for provision of experimental facilities and beam time.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T2.3-O3 Chemistry, Synthesis, Novel materials

Interlayer bond formation in arsenic at high pressure

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Abstract

The high-pressure behavior of arsenic has been explored in literature up to 250 GPa. Upon room temperature compression, ambient pressure hexagonal As-I (A7), commonly known as gray arsenic, transforms into simple cubic (sc) As-II, then into host-guest incommensurately modulated As-III and ultimately into bcc As-IV [1]. The first transformation from A7 As-I to sc As-II represents a prototypical phase transition in structural chemistry, which is particularly relevant for group 15 elements, inherently featuring the characteristic ns^2np^3 outer shell orbital electronic configuration. This transformation represents indeed the transition from a layered structure (A7 As-I), in which As atoms exhibit three first-neighbor distances in the same layer and three second-neighbor distances in the adjacent layer, highlighting trigonal-pyramidal coordination, to a non-layered structure (sc As-II), featuring six equivalent nearest-neighbor distances and octahedral atomic coordination. Nevertheless, after several decades of investigations, the A7 to sc transformation in As still remains elusive and debated, essentially due to the lack of conclusive experimental studies [2-4]. Here we report the results of single-crystal structure determination of As by synchrotron X-ray diffraction during room T compression up to 38 GPa, using a membrane diamond anvil cell for the generation of pressure and He as pressure transmitting medium. Our experiments enabled to finely and unambiguously track the pressure dependence of the lattice parameters, atomic positions and interatomic distances across the full pressure range of the transformation. Our data highlight a two-step pressure-induced inter-layer bonding mechanism, underlying the increase of the As coordination number, and reveal the existence of a pseudo-simple cubic (p-sc) structure between A7 As-I and sc As-II, which demonstrates structural consistency with lighter P in group 15 [5]. The results are interpreted according to literature theoretical studies and supported by additional data analysis, which adds focus on the key-role of *s-p* orbital mixing. While finally solving the long-standing debate on the elusive A7 to sc transformation in As, implications concern fundamental bond theory in pnictogens and the synthesis of As-based materials.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T2.3-O4 Chemistry, Synthesis, Novel materials

Carbon materials design using high-pressure toolkit

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Abstract

A rich variety of carbon-derived structural states originates not only from various hybridization motifs carbon atoms manifest, but also structural diversity of the precursors used in materials synthesis, including nanostructured molecular systems (fullerenes, nanotubes and graphene). These systems have been the focus of attention of the scientific community due to the rich assortment of outstanding chemical, optical, electrical and mechanical properties they exhibit [1]. High pressure provides a unique pathway to synthesize novel carbon-based materials that are unattainable under ambient conditions, transforming nanostructured van der Waals-bonded precursors into robust, covalently bonded networks.

In this talk, we review our recent results on the synthesis of a new class of carbon-based materials under high pressure from various precursors, including graphite nano-platelets, glassy carbon and fullerite C_{60}. These materials exhibit a remarkable combination of mechanical and electronic properties (ultra-hardness, superior wear resistance, and semiconducting behavior) [2-4]. They were characterized by multi-excitation Raman spectroscopy, SEM, XRD, high-resolution scanning TEM/EELS revealing the relationship between synthesis parameters and the resulting sp^2/sp^3 hybridized carbon frameworks. Application of torsion under high pressure to nano-graphite induces a phase transformation to hexagonal diamond allotrope (lonsdaleite) at ambient temperature, providing a unique alternative to the conventional high-pressure/high-temperature synthesis route [4-6]. Finally, we will discuss the potential of these materials for applications and present a viable route to the design of carbon materials with target mechanical and electronic properties.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T2.3-O5 Chemistry, Synthesis, Novel materials

High-pressure synthesis of a hafnium carbonitride hosting a hexazine ring

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Abstract

The formation of polymeric nitrogen and carbon-nitrogen configurations remains a long-standing challenge in chemistry. High pressure synthesis has emerged as an effective strategy, enabling the preparation of a range of polymeric nitrogen species and carbonitride anionic species in metal-C-N ternary systems (e.g., [1-10]). The *cyclo*-N_6 ring, one of the most sought-after yet elusive polymeric nitrogen species, has hitherto been identified only in metal-N binary systems and exhibits poor stability upon decompression, with no reports of recovery to ambient conditions.[8-10]

In this study, we report a novel hafnium carbonitride, synthesized using a laser-heated diamond anvil cell under near-megabar pressures and temperatures reaching several thousand kelvin. Solved by multigrain X-ray crystallography (**Figure 1**), its crystal structure features a 3D C-N anionic framework consisting of [CN_4] tetrahedral units interconnected by polymeric nitrogen chains. Remarkably, within this framework, a fully single-bonded armchair-shaped *cyclo*-N_6 anion is trapped. The hafnium carbonitride structure remained intact upon decompression down to below 10 GPa and is predicted to be dynamically stable at 0 GPa by DFT calculations.

Our results demonstrate that embedding a *cyclo*-N_6 ring within a carbonitride framework provides an effective route to enhance the stability of this otherwise highly labile species. This strategy open a new pathway for the synthesis of *cyclo*-N_6 rings and other novel nitrogen-based species that are typically accessible only under extreme conditions, potentially enabling their stabilization at ambient conditions.

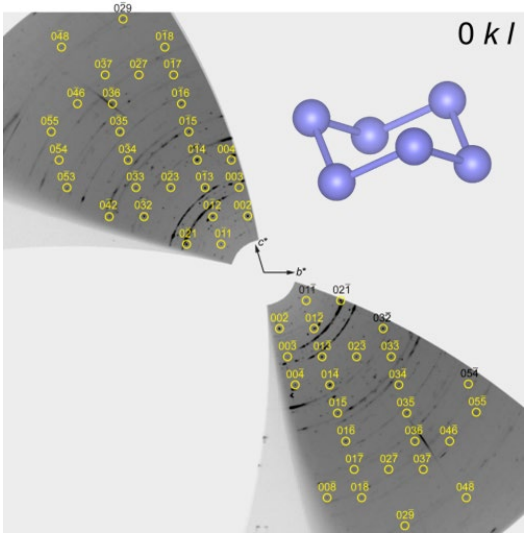

Figure 1. Reconstructed reciprocal lattice section 0*kl* based on the single-crystal X-ray diffraction data of a hafnium carbonitride crystallite collected at the synthesis pressure.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T2.4-O1 Chemistry, Synthesis, Novel materials

Looking for ambient pressure superhydrides: application to the Y-Fe-H system

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Abstract

Computational studies have successfully predicted the dramatic uptake of hydrogen by metals under pressure, leading to the experimental synthesis of superhydrides. These materials demonstrate exceptional properties, such as high-temperature superconductivity, hydrogen storage and superionicity, like in LaH_{10} [1,2,3]. Up to now, most of the studies have been performed on binary hydrides in the 100 GPa range and none of the discovered superhydrides could be recovered at ambient pressure. Ternary hydrides offer possibilities to stabilize such superhydrides at ambient pressure, and potentially recover their properties [4]. While many ternary superhydrides have now been predicted by calculations, a frustratingly low number of them have actually been synthesized, and none of them were recovered at ambient pressure.

We have undertaken the search of ternary superhydrides in the system Y-Fe-H. Our experimental strategy relies on the use of pre-hydrogenated precursors $YFe_2H_{4.2}$ [5]. Our first experiments showed a spontaneous hydrogen uptake under pressure up to 50 GPa, which plateaued at YFe_2H_7 [6]. Subsequent laser heating at 80 GPa on these samples lead to the discovery of the superhydride $Y_3Fe_4H_{20}$ [7], whose full structure was obtained by coupling calculations and experiments. Remarkably, this compound remains metastable upon decompression down to ambient pressure for more than a day.

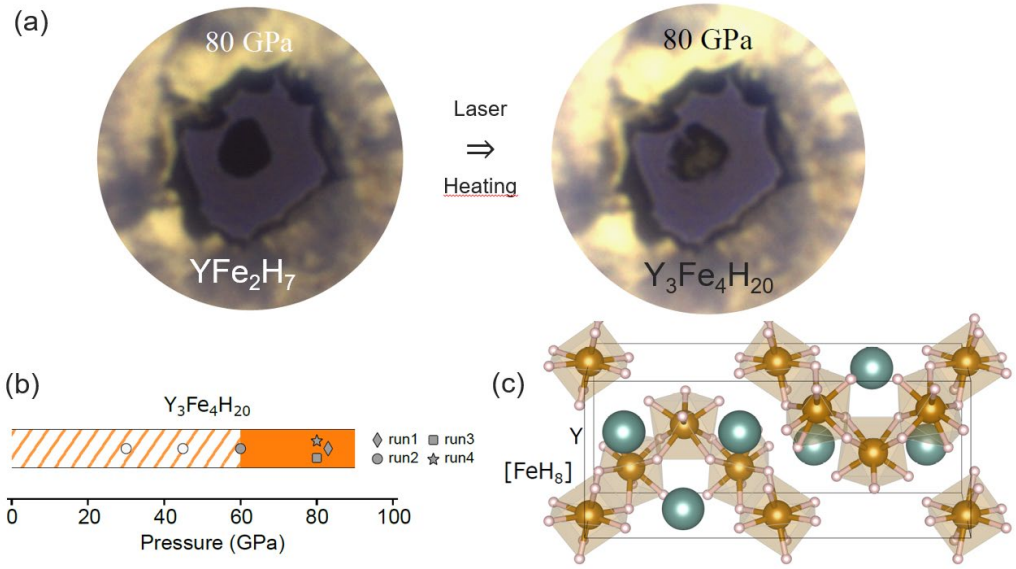

Figure 1: (a) Optical images taken before and after laser heating on a Y-Fe-H compound. (b) Stability (orange area) and metastability (dashed lines) phase diagram of $Y_3Fe_4H_{20}$, obtained after multiple heatings performed at different pressures. (c) Full structure of $Y_3Fe_4H_{20}$, which includes Y atoms and FeH_8 units.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T2.4-O2 Chemistry, Synthesis, Novel materials

In-situ characterization of the High-Pressure High-Temperature synthesis of tetragonal Na_2Si_3

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Dmitrii DRUZHBIN (ESRF, France),
Michael M. KOZA (ILL, France),
Jérôme ROUQUETTE (ICGM, France),
Mickaël BEAUDHUIN (ICGM, France),
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Abstract

In a world of climate change and limited natural resources, the urgent need for sustainable energy technologies drives the search for novel functional materials made of abundant, non-toxic, and low-cost elements. In this context, sodium silicides are emerging as promising candidates for photovoltaics, energy storage, and thermoelectric applications. While the Na-Si phase diagram has been relatively unexplored, *in-situ* synchrotron techniques and high-pressure high-temperature (HP-HT) synthesis have enabled the search for additional phases. [1, 2]

At ambient pressure, NaSi is the only thermodynamically stable phase, but three metastable phases have also been reported: Type I clathrate Na_8Si_{46} and type II clathrate $Na_{x<24}Si_{136}$ consists of a framework of Si cages that are filled with sodium ions. The third known structure, $NaSi_6$, was first discovered by Kurakevych *et al.* through *in-situ* monitoring of high-pressure high-temperature (HP-HT) synthesis. [1, 2, 3]

We report the discovery of a new Na_2Si_3 phase, formed under HP-HT conditions in the large volume press (LVP) located at the ID06-LVP beamline (ESRF) and identified using *in-situ* synchrotron X-ray diffraction. Na_2Si_3 was formed using a 10/5 multianvil assembly near 5 GPa at around 510 °C and is recoverable to ambient pressure and temperature. Additionally, we have explored different HP-HT synthesis paths for Na_2Si_3.

Na_2Si_3 adopts a tetragonal structure composed of two-dimensional layers of silicon, separated by sodium ions. The bonding can be rationalized within the Zintl-Klemm framework with a formal charge distribution $(Na^+)_2(Si^0)(Si^-)_2$. *Ab initio* calculations confirmed this structure and predicted an indirect band gap of ~1.14 eV at ambient pressure, making Na_2Si_3 interesting for applications in photovoltaics and thermoelectricity. [4]

These findings highlight the importance of combining *in-situ* HP-HT experimentation with theoretical modelling to discover novel metastable materials.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T2.4-O3 Chemistry, Synthesis, Novel materials

Amorphous Silica obtained from the Zeolite Chabazite due to Structural Collapse under Mild Pressure-Temperature Conditions

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Abstract

The siliceous zeolite chabazite, which has a very large void volume for a crystalline silica polymorph, was found by *in situ* synchrotron, x-ray diffraction in diamond anvils cells to collapse and become amorphous under mild, pressure-temperature conditions in the range of 0.5-1 GPa and 320-454 K. This procedure was scaled up under technologically-relevant conditions of around 0.7 GPa and 473 K in a standard pellet pressing die equipped with a band heater. The materials obtained are distinct from silica glass with first sharp diffraction peaks at close to 1.60-1.63 $Å^{-1}$, shorter intertetrahedral distances, and different infrared spectra. The mechanism for this collapse is dominated by the closure of the 8-membered rings of SiO_4 tetrahedra in the large chabazite cages in the structure resulting in a close to 40 % decrease in volume almost entirely due to the reduction of the c lattice parameter of rhombohedral chabazite. These results open the way to obtain novel amorphous forms of silica with characteristic medium-range order under mild *P-T* conditions, which could be expected to have distinct optical and mechanical properties with respect to silica glass.

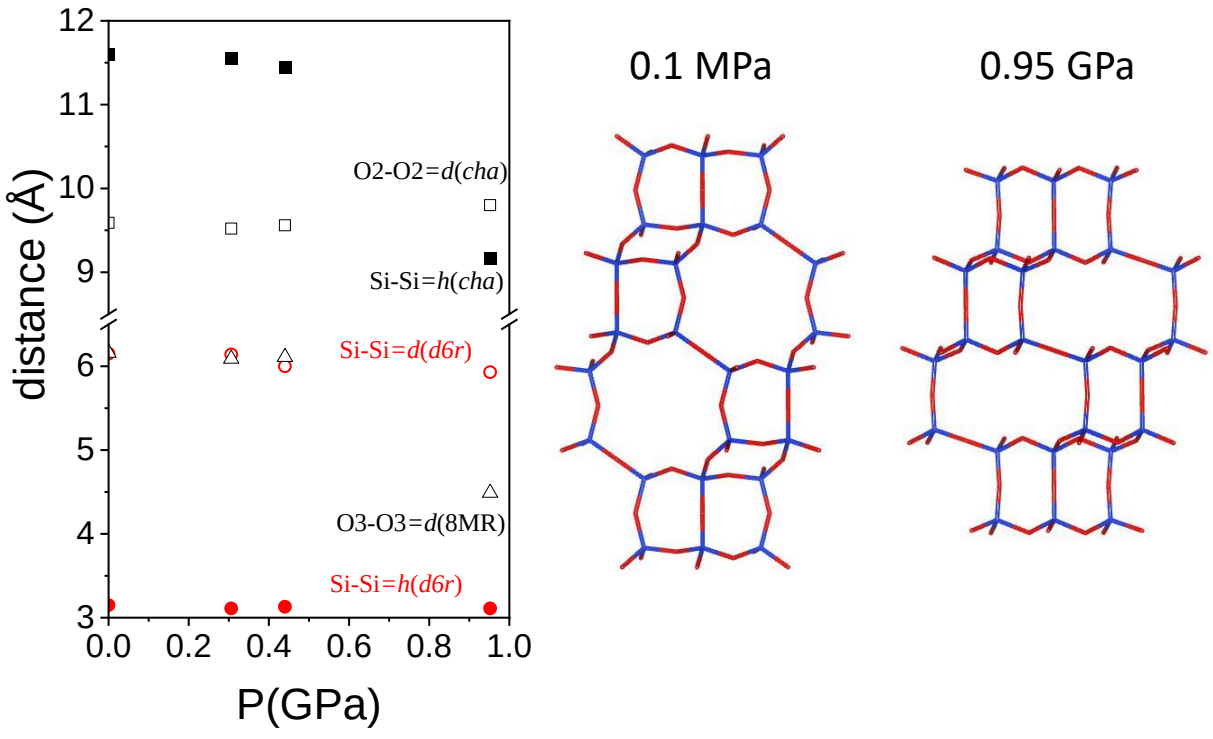

Figure 1 *Selected interatomic distances in CHA as a function of pressure (left). Details of the crystal structure (right) of CHA at 0.1 MPa and 0.95 GPa. Bonds are represented in blue (Si-extremity) and red (O-extremity).*

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T2.5-O1 Chemistry, Synthesis, Novel materials

Medium-range ordering in Mg–Cu–Gd glasses induced by annealing at the glass transition temperature and high pressure

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Abstract
The $Mg_{61}Cu_{28}Gd_{11}$ (at.%) metallic glass, characterized by a glass transition temperature of approximately 196 °C, was subjected to high-pressure/high-temperature treatment in order to investigate the early stages of structural reorganization preceding crystallization. The amorphous alloy was annealed in the range of, and above, the glass transition temperature, e.g., at 200 and 300 °C under a pressure of 7.8 GPa. Structural characterization of the recovered samples was performed by high-angle annular dark-field scanning transmission electron microscopy and high-resolution transmission electron microscopy at atomic resolution. HAADF-STEM imaging revealed nanoscale motifs enriched in Mg–Gd, indicating local chemical heterogeneity within the amorphous matrix. HRTEM analyses, supported by fast Fourier transform and inverse fast Fourier transform processing of selected micrographs, demonstrated the coexistence of distinct glassy states after pressure–temperature treatment. Additional analysis of selected-area electron diffraction patterns was performed to evaluate changes in medium-range order. Intensity profiles extracted from SAEDPs, together with the corresponding pair distribution function analysis, revealed variations in the width and shape of the diffuse halo rings. These changes indicate modifications in the degree of medium-range ordering within the amorphous structure, allowing the pressure–temperature-induced structural rearrangement to be distinguished even in the absence of detectable crystallization. The results show that high pressure and temperature promote structural reorganization in Mg–Cu–Gd metallic glass through local densification, chemical partitioning, and the formation of ordered amorphous motifs. A decrease in the effective glass transition temperature after high-temperature treatment further suggests a correlation between pressure-assisted densification mechanisms, enhanced medium-range ordering, and the thermal stability of the amorphous phase.

This work was financed by the National Science Center, Poland, project No. UMO-2022/47/B/ST8/03153 entitled: Tailoring properties and structure of Mg- and Zr-based metallic glasses by ultra-high pressure.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T2.5-O2 Chemistry, Synthesis, Novel materials

Formation of Mo-Ta Solid-Solution Nitrides under Extreme Conditions

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Abstract

Many transition metal (TM) nitrides are refractory ceramics. They are typically characterized by high melting temperature, oxidation resistance, chemical inertness, high electrical conductivity and remarkable catalytic properties. The binary nitrides based on either Ta or Mo have some remarkable properties, beyond applications just exploiting their high melting temperatures and oxidation resistance. For example, TaN exhibits exceptionally high thermal conductivity and therefore is widely used in the semiconductor industry (as a critical diffusion barrier and adhesion layer in copper interconnects), while Mo_2N is increasingly recognized for its catalytic properties.

It is interesting to study Mo-Ta-N ternary nitride compounds, as broader structure-property tunability is expected. Within this concept, either solid solutions of known nitrides or novel ternary phases can be of interest for fundamental and applied sciences. However synthesis of nitride compounds remains a challenging task, as typically high pressure conditions are required.

In this project, we explore reactions of Mo-Ta alloy with nitrogen and the resulting phases within the ternary Mo-Ta-N system, in the range of pressures and temperatures up to 50 GPa and 2000-3000 K. We employed laser heated diamond anvil cell (LH-DAC) was to achieve high pressure high temperature conditions, and synchrotron radiation of PETRA III, DESY allowed to study the crystalline products of the reaction.

An example of a diamond anvil cell (DAC) is shown in Figure 1. It is a Sym70 cell equipped with Boehler-Almax diamonds (300 μm diameter). The DAC was loaded with MoTa alloy (1:1 composition), ruby chips and gold powder that served as pressure markers, and filled with N_2 gas. We performed laser heating at the pressure 47 GPa by slowly raising temperatures up to 2600(200) K. The simultaneous collection of diffraction patterns showed the formation of new crystalline phases during heating. After temperature quenching, the reaction products were studied by X-ray diffraction imaging, which allowed to identify positions of the sample suitable for multigrain XRD data collection using ω-scans with $\Delta\omega = 0.5°$. Within our study we solved and refined crystal structures of several previously unknown nitride phases, including a phase crystallizing in the orthorhombic space group Pnma with a unit cell volume V~174 Å^3 as well as other phases (their crystal structures are shown in the Figure 1).

The most important observation is the presence of occupational disorder on the crystallographic metal sites, including both Mo and Ta. The new phases feature high incompressibility, and remain stable at the ambient conditions after pressure release.

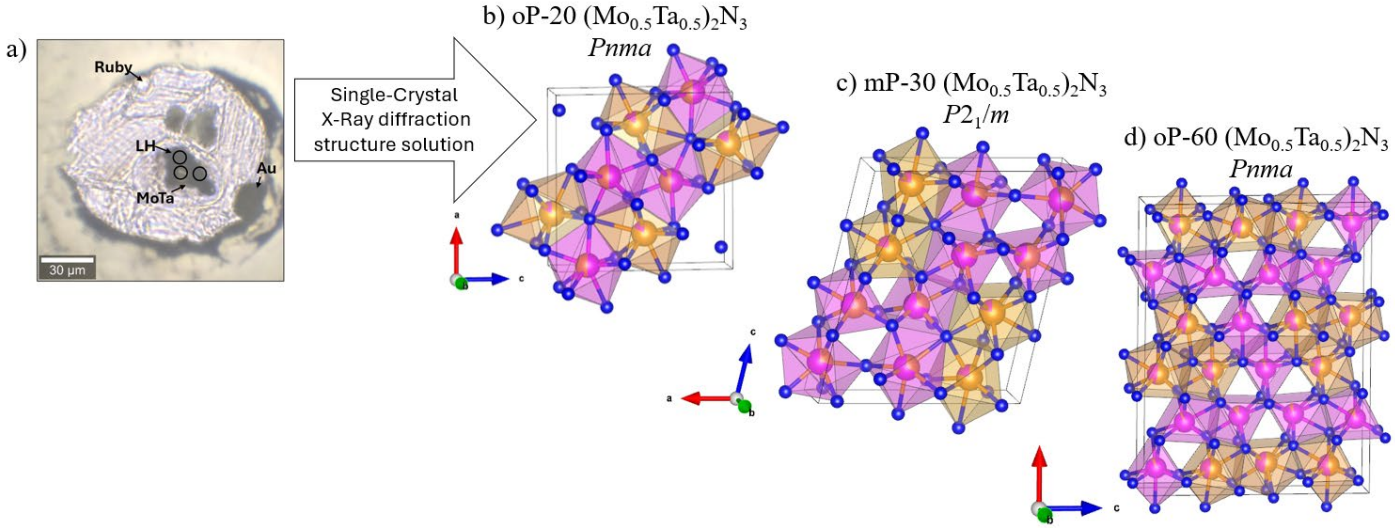

Fig 1. a) Photo of DAC chamber with laser-heated MoTa alloy. b) oP20-MoTaN3 Pnma phase. c) mP30-MoTaN3 phase. d) oP-MoTaN3 phase. Colors: orange – Ta, pink – Mo, blue – N; orange and pink polyhedra are bicapped and capped prisms with different volumes around 13 Å^3 and 16 Å^3 respectively.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T2.5-O3 Chemistry, Synthesis, Novel materials

High-Coordinate Transition Metal Phosphides via High-Pressure Synthesis

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Abstract ()

Similar to oxides and nitrides, the transition metal–phosphorus system offers a wide variety of functional materials. For instance, Ni–P–based compounds have been extensively studied as electrocatalysts for the hydrogen evolution reaction [1]. Meanwhile, the Mo–P system hosts various binary phosphides with distinct chemical compositions, several of which exhibit superconductivity [2]. To overcome the experimental challenges associated with phosphorus, ultrahigh-pressure synthesis is highly advantageous, as it allows the reaction of highly volatile phosphorus within a closed system. This approach is exceptionally effective for synthesizing high-crystallinity phosphides, while also enabling the development of novel ultrahigh-pressure phases that are inaccessible under ambient pressure.

In this study, we explored new high-coordinate phases within binary systems of phosphorus and early transition metals (e.g., Nb, Mo, Ta, and W), with a particular focus on TMP_2 (*TM*: transition metal) at pressures up to approximately 50 GPa. A recent room-temperature compression experiment on MoP_2 demonstrated that the ambient-pressure phase remains stable up to 55 GPa, although an anomalous change in the axial ratio was observed at around 36 GPa [3]. In contrast, theoretical calculations predicted the emergence of a novel, highly coordinated phase under high-pressure conditions. This discrepancy suggests that additional thermodynamic factors, such as temperature, may be crucial for overcoming kinetic barriers to synthesize the new high-pressure phase. Consequently, we investigated the high-pressure phase relations across a wide pressure and temperature regime using a laser-heated diamond anvil cell.

The starting materials were synthesized via a solid-state reaction of stoichiometric mixtures of the constituent metal and phosphorus. The mixed powder was pelletized, sealed in an evacuated silica glass tube, and subsequently heated in a furnace at 600–800 °C for several tens of hours. The phase purity of the synthesized products was verified using powder X-ray diffraction (XRD) measurements. For the high-pressure experiments, the starting sample was pelletized again and loaded into the sample chamber, sandwiched between alkali halide layers (e.g., NaCl or KCl) that served as both a pressure-transmitting medium and thermal insulator. After compression to the target pressure at room temperature, the sample was heated using an infrared laser for a few minutes. The laser-heated sample was characterized via high-pressure in-situ optical microscopy, Raman scattering spectroscopy, and synchrotron powder XRD measurements.

Raman scattering measurements during room-temperature compression revealed that MoP_2 remains stable up to approximately 40 GPa, consistent with a recent study reporting its stability up to around 60 GPa. In contrast, laser heating at approximately 40 GPa led to the disappearance of the starting phase, yielding numerous new diffraction peaks that could not be indexed to any known phases. The intensity of these novel peaks increased when the starting composition was shifted toward the metal-rich side. By screening reproducible peaks from multiple experiments, the new phase was successfully indexed to a tetragonal symmetry. A similar tetragonal profile was obtained for the W–P system at comparable pressures. The lattice parameters of the tetragonal phases in both the Mo–P and W–P systems were highly similar, consistent with the comparable atomic sizes of Mo and W. Upon decompression from 40 GPa, the diffraction peaks gradually broadened, accompanied by an anomalous compression behavior; however, the high-pressure phase was successfully recovered to ambient pressure. The lattice parameters and axial ratios of this tetragonal phase strongly resemble those predicted by theoretical calculations. On the day of the presentation, the crystal chemistry of the novel early transition metal phosphides synthesized under high pressure will be discussed.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T2.5-O4 Chemistry, Synthesis, Novel materials

High-pressure synthesis of alkali metal carbodiimides

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Abstract

Metal carbodiimides, comprised of the $[N=C=N]^{2-}$ anion, constitute a structurally versatile class of inorganic compounds. In many of these compounds,[1–6] metal cations and $[N=C=N]^{2-}$ anions are typically arranged in alternating layers, with the $[N=C=N]^{2-}$ units being perpendicular to the cation layers, producing structure types derived from metal oxides/chalcogenides (Figure 1a–d).[2,6] A particularly interesting subgroup of this class of materials are alkali metal carbodiimides (A_2CN_2, A = Li/Na/K). While Li_2CN_2[7] remains structurally related to oxide-derived archetypes (Figure 1e and 1f), Na_2CN_2[8] and K_2CN_2[9] display markedly tilted $[N=C=N]^{2-}$ units with respect to the layers of cations (Figure 1g and 1h), resulting in these structures having thus far no clear counterparts. Understanding the unique nature of these alkali carbodiimide compounds can presumably be understood through crystal chemical principles and high-pressure investigations; with alkali carbodiimide being fully *terra incognita* at extreme densities.

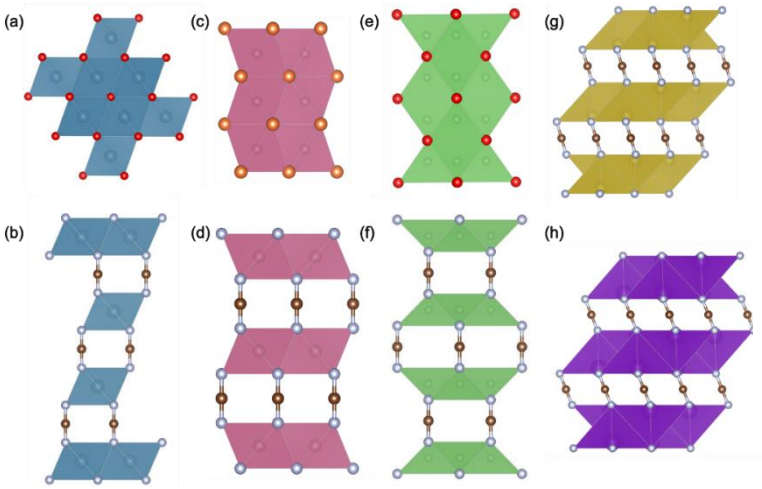

Figure 1. Analogies between the crystal structures of metal oxides/chalcogenides (O, S) and carbodiimides. Red, orange, grey, brown, blue, pink, green, yellow and purple spheres represent oxygen, sulfur, nitrogen, carbon, calcium, iron, lithium, sodium and potassium atoms, respectively, drawn using the atomic radii for O/S/N/C and the ionic radii for Ca/Fe/Li/Na/K. (a) CaO and (b) $CaCN_2$[2]. Ca-centered octahedra are shown in blue; (c) FeS[6] and (d) $FeCN_2$[6]. Fe-centered octahedra are shown in pink; (e) Li_2O[8] and (f) *I*4/*mmm* Li_2CN_2[7]. Li-centered tetrahedra are shown in green. The *C*2/*m* (g) Na_2CN_2[8] and (h) K_2CN_2[8]. Na/K-centered square pyramids are shown in yellow/purple. The latter two have no such direct counterparts.

In this talk, the unique nature of the Na_2CN_2[8] and K_2CN_2[9] compounds will first be rationalized based on i) the cation to anion ratio and ii) chemical precompression of the metal cation. Then, the investigation of the Li-, Na- and K-C-N systems up to 50 GPa using laser-heated diamond anvil cells (LHDACs) will be presented, demonstrating the synthesis of four novel carbodiimide polymorphs through synchrotron single-crystal X-ray diffraction (SCXRD). These novel compounds not only shed light on the interplay between cation size, pressure, and the orientation of the $[N=C=N]^{2-}$ units, but also demonstrate important trends across alkali metal carbodiimide compounds. These results will serve as a template for future investigations of metal carbodiimide studies, as well as provide knowledge on the thermodynamically stable A-C-N compounds up to 50 GPa.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T2.5-O5 Chemistry, Synthesis, Novel materials

Inorganic tricarbonate: high-pressure synthesis of $K_2C_3O_7$

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Yuqing YIN (University of Bayreuth, Germany),
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Gaston GARBARINO (ESRF, France),
Dominik SPAHR (Goethe University Frankfurt, Germany),
Bjoern WINKLER (Goethe University Frankfurt, Germany),
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Abstract

The synthesis of carbonates with novel anionic species is important for chemistry, geoscience, and materials science. Beyond common carbonates containing $[CO_3]^{2-}$ anions known at ambient conditions, high pressures can stabilize various sp^3-carbonates built of tetrahedral CO_4 units. At mild pressures, sp^2-pyrocarbonates with $[C_2O_5]^{2-}$ groups have also been reported. This suggests that the planar CO_3 unit, along with the tetrahedral CO_4 unit, can potentially also be a building block of exotic C-O anions at high pressure. This parallels borate chemistry, where diverse anions comprised of BO_3 and BO_4 building blocks exist. However, aside from the $[C_2O_5]^{2-}$ anion, no other species containing CO_3 units are known.

Here, we present the first inorganic tricarbonate salt, $K_2C_3O_7$, discovered in laser-heated diamond anvil cells at 55(3) and 45(2) GPa.[1] The crystal structure of $K_2C_3O_7$ was determined in situ using synchrotron single-crystal X-ray diffraction from a polycrystalline sample. It features non-planar $[C_3O_7]^{2-}$ anions, which consist of three corner-sharing planar CO_3 groups rotated relative to one another. This anion extends the homologous series of sp^2-carbonates: $[CO_3]^{2-}$ - $[C_2O_5]^{2-}$ - $[C_3O_7]^{2-}$. Raman spectroscopy establishes the characteristic vibrational fingerprint of the $[C_3O_7]^{2-}$ anion. Density functional theory (DFT) calculations corroborate the experimental results and suggest the thermodynamic stability of $K_2C_3O_7$ between 10 and 55 GPa. DFT calculations predict a phase transition between 80 and 90 GPa associated with a polymerization of the $[C_3O_7]^{2-}$ groups, accompanied by a change in the coordination polyhedra of two carbon atoms from triangles to tetrahedra. These findings highlight the rich structural chemistry accessible to carbonates under compression and suggest that additional sp^2- and mixed sp^2/sp^3-carbonates may be stabilized at high pressure.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T3.1-O1 Electronic, Magnetic, Caloric and Transport properties

Ultrastable Metal Polyhydrides Below 60 GPa

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Abstract

Application of external pressure to a system serves as an additional degree of freedom, expanding our knowledge about stable chemical compounds and chemical reaction pathways under extreme conditions. High-pressure techniques, using diamond anvil cells to reach millions of atmospheres, have revolutionized hydrogen chemistry. For decades, conventional hydrides like LiH, NaH, CaH_2, H_2S or CH_4 were thought to represent the limits of hydrogen content. But this does not exhaust the chemistry of hydrides.

In my talk, I will review a decade of experimental research showing that under pressure near 1 Mbar, elements form extraordinary polyhydrides—such as CsH_7 [1], RbH_9 [1], YH_6 [2], CeH_{10} [3], BaH_{12} [4], and even $La(Sc)H_{12}$ [5,6]—with far more hydrogen atoms per metal atom than previously imagined. I will show the latest results of attempts to reproduce room temperature superconductivity in the La-Sc-H system, and the recent achievement of T_c around 174 K below 100 GPa in the Th-H system. Moreover, by introducing Th into the La-H system, an even higher T_c of up to 230 K can be achieved at the same pressure of about 100 GPa.

I will pay special attention to Th-containing Ce-Th-H ternary polyhydrides (XH_{10}, XH_7, cF80-XH_{6+x}, A15 X_4H_{23}), which exhibit extraordinary stability down to 12 GPa and can be synthesized and characterized without damaging diamond anvils below 65 GPa. The recent trend of decreasing stabilization pressures for hydrogen-rich materials and superconductors [7] opens a realistic pathway toward their application, promising a transformative leap in hydrogen storage technology.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T3.1-O2 Electronic, Magnetic, Caloric and Transport properties

Pressure-Induced Flat Bands and Zero-Field Chern States in Large-Angle Twisted Bilayer Graphene

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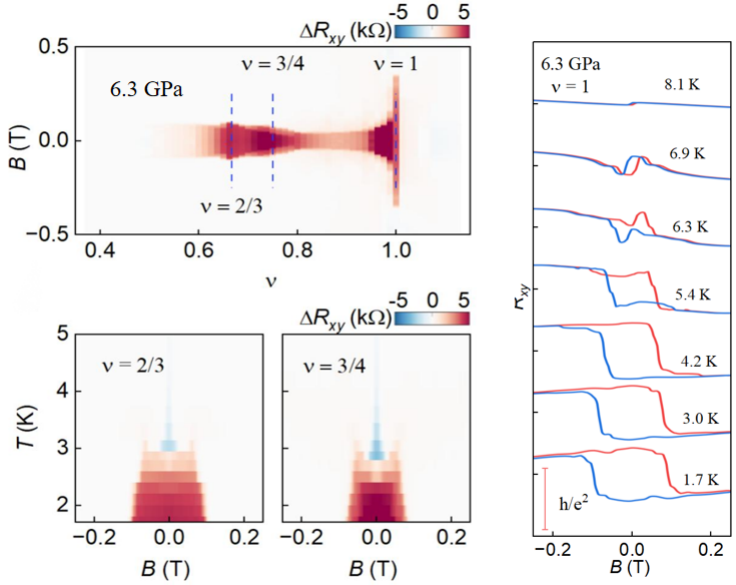
Abstract

Twisted bilayer graphene (TBG) is a moiré quantum material in which electron interactions can be dramatically enhanced by band flattening, giving rise to correlated states reminiscent of those discussed in the context of high-temperature superconductivity, as well as topological phases with quantized Hall response without an external magnetic field. Hydrostatic pressure offers a clean, non-invasive way to tune these electronic states by continuously modifying the interlayer coupling, yet its effects on large-angle TBG at multi-gigapascal pressures remain largely unexplored[1]. Here we develop a diamond-anvil-cell transport platform that enables continuous measurements on the same hBN-encapsulated TBG device up to ~10 GPa and apply it to samples with twist angles of $\theta \approx 1.37°–1.73°$. Pressure strengthens interlayer hybridization, shifts the effective magic-angle condition to larger twist angles, and drives these devices into an optimal flat-band regime near up to ~ 6 GPa, where correlated insulating states are strongly enhanced and the effective Fermi velocity is reduced to ~300 m/s. In this regime, zero-field anomalous Hall states emerge at integer fillings $\nu = 1$ and 2, corresponding to Chern insulators with $C = -1$ and -2 and Curie temperatures up to ~8 K. Near the optimal flattening condition, additional hysteretic anomalous Hall features appear at fractional fillings $\nu = 2/3$ and 3/4, with field dependence consistent with $|C| = 1$, pointing to interaction-driven symmetry breaking and topological charge-ordered states. These results show that hydrostatic pressure does more than recover flat bands in large-angle TBG: it opens access to a stronger-correlation regime in which new integer and fractional topological states can be stabilized.



Zero-Field Chern Insulators at integer and fractional fillings in twisted bilayer graphene under high pressure.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T3.1-O3 Electronic, Magnetic, Caloric and Transport properties

High-Pressure Tuning of Dynamic Magic-Angle Correlated States in Twisted Bilayer Graphene

Yupeng WANG (University of Science and Technology of China, PRC),
Chunhui YE (University of Science and Technology of China, PRC),
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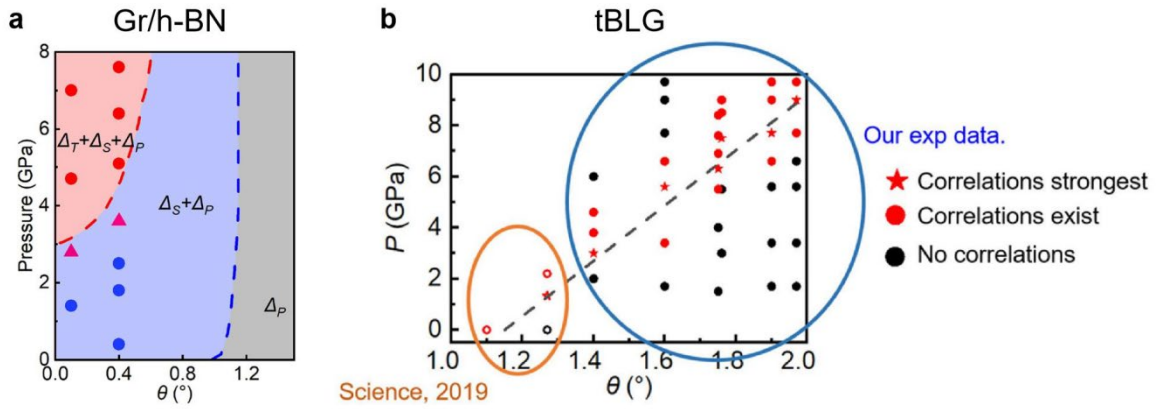
Abstract

Hydrostatic pressure offers a clean and reversible route to dynamically tune the magic-angle condition in twisted bilayer graphene (TBG) by modifying interlayer coupling and the bandwidth of moiré flat bands. Here we develop a diamond-anvil-cell-based multi-terminal quantum-transport platform, enabled by post-fabrication transfer and a custom transferable-electrode scheme, and use it to investigate pressure-controlled correlated and topological states in graphene moiré systems. As a benchmark, measurements on graphene/hBN superlattices reveal pressure-enhanced moiré potentials and the opening of higher-order Dirac gaps, in good agreement with first-principles structural relaxation and large-scale tight-binding calculations[1]. Applying this approach to TBG across different twist angles allows us to map a pressure–angle phase diagram of correlated insulators and establish a pressure-dependent magic-angle relation. In a 1.9° device, correlated insulating states emerge at integer fillings and are strongest near 7.7 GPa, consistent with maximal band flattening. In the same pressure window, transport near ν = -2 shows an enhanced superconducting dome with $T_{50\%}$ up to ~6 K and a Berezinskii–Kosterlitz–Thouless transition temperature of ~3 K. We further observe pressure-induced signatures of zero-field Chern insulating states at ν = 1 and 2, with large hysteretic anomalous Hall signals, Curie temperatures around 6 K, and anomalous Hall resistances reaching ~20 kΩ and ~10 kΩ, respectively, suggesting pressure-driven spontaneous breaking of $C_{2z}T$ symmetry. These results demonstrate that high pressure is a powerful control knob for engineering flat bands, strong correlations, and non-trivial topology in moiré graphene.



Our work on pressure-tuned moiré superlattices. This figure is partially adapted from Ref. [2].

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T3.1-O4 Electronic, Magnetic, Caloric and Transport properties

Charge dynamics in the Weyl semimetals $NbIrTe_4$ and $TaIrTe_4$ under pressure: Signatures of an electronic phase transition

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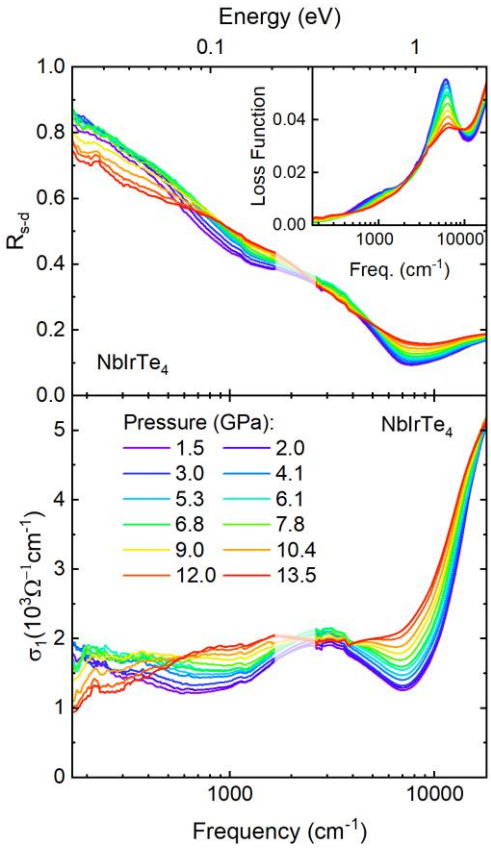
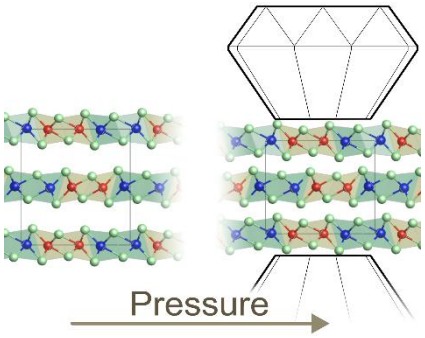
C. A. KUNTSCHER (University of Augsburg, Germany)

Abstract

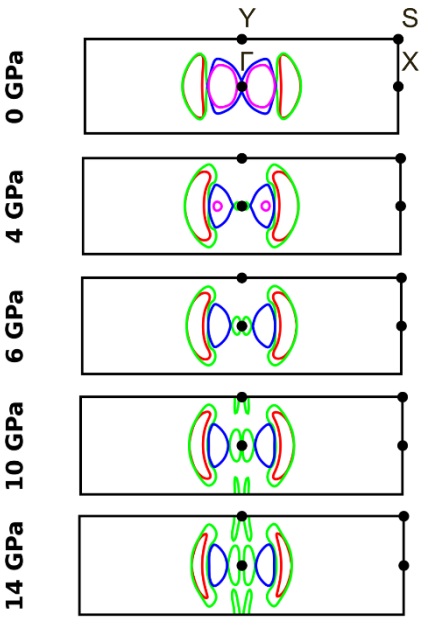
The ternary transition-metal iridium tellurides $NbIrTe_4$ and $TaIrTe_4$ are proposed as type-II Weyl semimetals. Applying external hydrostatic pressure is an effective method for tuning their electronic and structural properties. In this study, we present a high-pressure investigation of the charge dynamics in $NbIrTe_4$ and $TaIrTe_4$ using infrared spectroscopy supplemented by density functional theory calculations. Our experimental optical conductivity spectra reveal a clear phase transition occurring at a critical pressure of 7-8 GPa in both compounds. Above this critical pressure, we observe a significant redistribution of spectral weight in the optical conductivity spectrum. A Drude-Lorentz analysis indicates a sharp reduction in the free carrier concentration. Consequently, a previously obscured low-energy phonon mode emerges as a distinct feature, because the screening effect from the Drude contribution is weakened. Raman scattering measurements show no evidence of a significant structural phase transition, suggesting that the observed anomalies are predominantly electronic in nature. Our ab initio calculations support this conclusion; they indicate that the total density of states at the Fermi level remains remarkably constant. Instead, the reduction in Drude weight is driven by significant topological modifications of the Fermi surface, specifically the shrinking and fragmentation of electron and hole pockets. These purely electronic transitions involving topological changes to the Fermi surface are characteristic of a Lifshitz transition. Ultimately, these results provide collective evidence for a pressure-induced, Lifshitz-type electronic phase transition driven by tuned van der Waals interlayer coupling.



Evolution of the reflectivity and optical conductivity in $NbIrTe_4$ under pressure. The transition at P_c = 7-8 GPa is evidenced by a sharp decrease in Drude weight alongside an increase in interband transitions.



Schematic illustration of the high-pressure evolution. The application of hydrostatic pressure via a diamond anvil cell primarily compresses the soft van der Waals gap, leading to a significant decrease in the interlayer distance along the c-axis.



Evolution of the Fermi surface cross-sections of $NbIrTe_4$ under hydrostatic pressure.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T3.1-O5 Electronic, Magnetic, Caloric and Transport properties

Universal origin of anomalies in compressed liquid alkalis

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Abstract

Alkali metals are archetypal nearly-free-electron systems, yet compression drives them away from simple-metal behavior. In the liquid phase pressure induced structural transitions and thermodynamic compressibility anomalies have been reported experimentally in some systems. Independently, computational studies have indicated localization of charge and formation of electride-like states in the liquid. Considering all these phenomena as anomalies in compressed liquid alkalis, we apply first-principles molecular dynamics to liquid Na, K, Rb and Cs under pressure, to form a unified picture of all these phenomena across the alkali series. Specifically, we show that these phenomena are initiated by pressure induced electronic reconfiguration and interstitial electron localization and not just by densification. Compression transfers valence charge from delocalized *s*-like states into *p*-character states in Na and *d*-character states in K, Rb, and Cs, accompanied by the emergence of electride-like interstitial localization before the main structural rearrangement. The liquid structure subsequently opens, with the coordination number decreasing from 13-14 to 8-10, while the sound velocity exhibits a softening anomaly that appears prior to the coordination-number reduction. Furthermore, in K, Rb, and Cs, a quantitative electronic coordinate for the transitions is formulated. These results identify orbital reconfiguration and interstitial electron localization as the microscopic mechanism by which pressure drives both structural and compressibility anomalies in alkali-metal liquids and suggest a general pressure-driven route from simple metallic liquids to complex electride-like states.

Thin-Film Hydride Superconductors: A New Platform to Study Near-Room-Temperature Superconductivity at Megabar Pressures

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Abstract

The discovery of hydride superconductors has opened a new route towards room-temperature superconductivity [1-5]. Among those materials, LaH_{10} has attracted considerable interest due to its superconducting transition temperature around 250 K. However, hydride superconductors can only be synthesised at megabar pressures, making their study challenging and limiting the range of experimental techniques that can be applied. In particular, electrical transport measurements require electrodes integrated into a diamond anvil cell (DAC) that can survive both extreme pressures and laser-heating synthesis conditions whilst maintaining sufficiently low contact resistance with the sample for sensitive measurements.

To overcome some of these challenges, we have developed a method for synthesising hydride superconductors from elemental thin films deposited directly onto diamond anvils and using ammonia borane (NH_3BH_3) as a hydrogen source [6]. This approach led to the discovery of superconductivity in La_4H_{23} [7] and, more recently, enabled the synthesis of the first LaH_{10} thin films [8].

In this talk, I will present the methods used in our laboratory to synthesise and characterise high-T_c hydride superconductors. I will focus on thin-film LaH_{10} and its structural and superconducting properties, characterised using synchrotron X-ray powder diffraction and electrical transport measurements in magnetic fields. We find that thin-film LaH_{10} exhibits properties consistent with bulk samples. By combining high-resolution diffraction mapping with transport measurements, we can assign superconducting transitions to specific structural phases and distinguish between contributions from different phases. Finally, I will discuss the stability of both the structural and electronic properties of LaH_{10} thin film, based on measurements we carried out over almost a year.

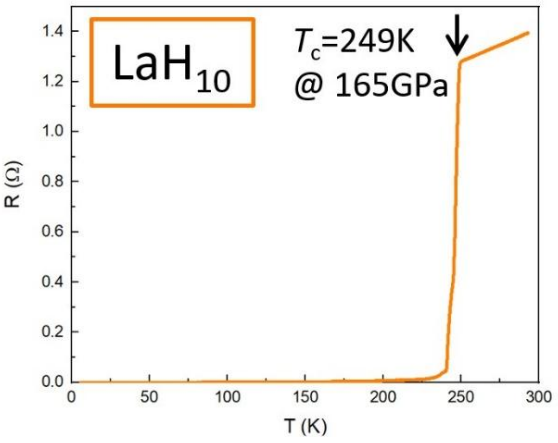

Figure 1: Electrical resistance in LaH_{10} film.

The thin-film approach provides a practical route to facilitate electrical measurements at extreme pressures and significantly improves the success rate of our transport experiments. Furthermore, the development of hydride superconductor thin films opens new possibilities for fabricating devices directly within DACs, enabling more advanced electrical and spectroscopic studies of superconductivity at ultrahigh pressures.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T3.2-O2 Electronic, Magnetic, Caloric and Transport properties

Herbertsmithite: pressure evolution of a spin liquid

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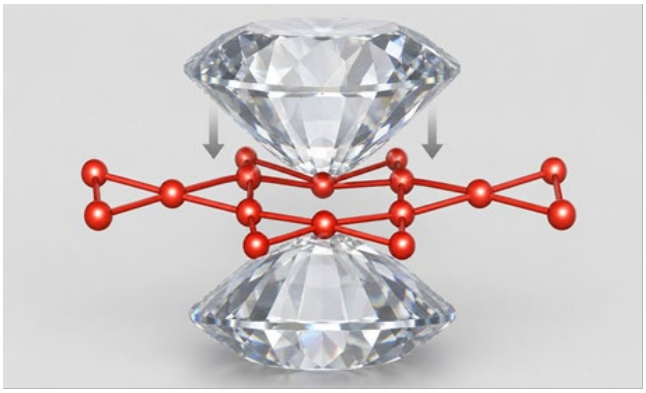
Abstract

Frustrated interaction geometry of magnetic moments can lead to unusual types of magnetic order and even to novel phases, such as quantum spin liquid where spins are dynamically correlated without forming a symmetry-broken long-range-ordered state. This theoretical prediction was extensively studied in various transition-metal compounds, including the Cu^{2+} mineral herbertsmithite, $Cu_3Zn(OH)_6Cl_2$, with a kagome network of interacting Cu^{2+} ions [1].

Whereas herbertsmithite lacks long-range magnetic order down to lowest temperatures, this observation received a conflicting assessment in the previous literature. On the one hand, a structural disorder of the magnetic Cu^{2+} and nonmagnetic Zn^{2+} ions was invoked as a plausible reason for the suppression of magnetic order. On the other hand, the occurrence of a pressure-induced transition toward a magnetically ordered state above 2.5 GPa [2] speaks in favor of a genuine spin-liquid scenario where competing interactions are detuned by the applied pressure, and magnetic order is stabilized. Abrupt structural changes around the critical pressure of 2.5 GPa [2] and at higher pressures [3,4] have been reported, but their origin could not be revealed.

Here, we revise pressure-dependent crystal structure and magnetism of herbertsmithite using single-crystal x-ray diffraction in a diamond anvil cell combined with high-pressure magnetometry. Contrary to the previous studies, we find that herbertsmithite evolves monotonically up to at least 10 GPa with no visible changes in its low-temperature magnetic behavior. It means that a disordered magnetic ground state persists above 2.5 GPa, at odds with the earlier findings. The reduction in the Cu-O-Cu bond angles at elevated pressures weakens nearest-neighbor magnetic couplings and increases the role of weaker interaction terms that should eventually stabilize magnetic order. The absence of this pressure-induced magnetic order in the experiment favors structural disorder as the driving force of the apparent spin-liquid behavior in herbertsmithite.

Intriguingly, at pressures above 10 GPa where monoclinic distortion was reported in the earlier studies [3,4], a robust trigonal symmetry is observed in our data. However, the *c*-parameter shows an anomalous increase upon compression. The possible origin of this negative anisotropic compressibility will be discussed.



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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T3.2-O3 Electronic, Magnetic, Caloric and Transport properties

Pressure dependence of tricriticality in $UIrSi_3$

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Abstract

Applying a magnetic field to an antiferromagnet can cause abrupt changes to its magnetic state. A metamagnetic transition to a paramagnetic state is accomplished in sufficiently high magnetic fields. This transition is usually of the second order. However, a first-order transition is observed at low temperatures well below the Néel temperature in some cases. The antiferromagnet - paramagnet transition line in the field-temperature magnetic phase diagram, having the first-order and second-order type segments, this is expected in Ising antiferromagnets with competing antiferromagnetic and ferromagnetic interactions. D. P. Landau has interpreted the point at which the two segments meet as a tricritical point (TCP) [1]. The TCP is observed only rarely in uranium compounds, for example, in $UIrSi_3$, [2], UIrGe [3], UAu_2Si_2 [4], USb_2 [5], UNiAl [6].

We will present a pressure study on $UIrSi_3$ single crystal. At ambient pressure, the Neél temperature (T_N) is 42 K. When the magnetic field is applied along the c-axis (easy magnetization axis), the AFM order is suppressed by the metamagnetic transition (MMT) at H_C = 7.3 T at 2 K, while a polarized paramagnetic phase emerges. At low temperatures, the metamagnetic transition is first-order type. In temperatures above 28 K, the hysteresis disappears; first-order type of the transition changes to the second-order type. The point at which the transition changes is TCP [2,7]. Applying pressure shifts H_C to a lower magnetic field, whereas the temperature of TCP (T_{TCP}) gradually increases as T_N (Fig. 1). The critical pressure for H_C = 0 T is estimated to be 8.6 GPa; the dependences of $T_N(p)$ and $T_{TCP}(p)$ merge near 9.5 GPa.

The pressure evolution of characteristic properties of $UIrSi_3$ and other uranium compounds is driven by magnetoelastic interactions. The presentation will discuss the origin of these phenomena and the underlying physics beyond critical pressures.

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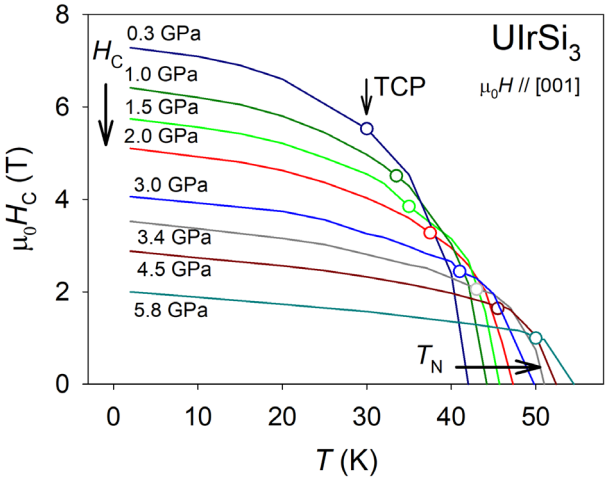

Fig. 1: Field-temperature phase diagram with enriched by result under high pressure.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T3.2-O4 Electronic, Magnetic, Caloric and Transport properties

Pressure dependence of Eu valence, crystal structure and electric resistivity of Eu*T*Ge$_3$ (*T*=Co, Rh and Ir)

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Strongly correlated 4*f*-electron systems exhibit a rich variety of emergent phenomena, including the Kondo effect, valence fluctuations, quantum criticality, and unconventional superconductivity. In such systems, pressure often serves as an effective tuning parameter to drive electronic instabilities and induce novel ground states. The non-centrosymmetric Eu*T*Ge$_3$ family (*T* = Co, Rh, Ir; space group I4mm) provides an attractive platform for investigating the interplay between magnetism, lattice degrees of freedom, and Eu valence evolution under compression. These compounds contain divalent Eu^{2+} ions ($4f^7$, J = 7/2) and order antiferromagnetically below ~15 K, with magnetic structures that depend sensitively on the transition-metal element [1].

We combined high-energy-resolution fluorescence-detected X-ray absorption spectroscopy (HERFD-XAS), synchrotron X-ray diffraction (XRD), and electrical transport measurements under hydrostatic pressure to probe the evolution of the electronic and crystal structures across the Eu*T*Ge$_3$ series. HERFD-XAS demonstrates a systematic pressure-induced transfer of spectral weight from Eu^{2+} to Eu^{3+} states, indicating a continuous increase of the mean Eu valence. The effect is least for the 3d compound, where the average Eu valence increases from ~2.2 at ambient pressure to ~2.25 at 40 GPa in EuCoGe$_3$ [2]. In contrast, the 4d and 5d analogues EuRhGe$_3$ and EuIrGe$_3$ exhibits a significantly stronger response, with the Eu valence reaching ~2.45 at 40 GPa [3]. These contrasting behaviors highlight the distinct influence of 3d, 4d, and 5d transition-metal electronic states on Eu valence instability. XRD measurements reveal that the non-centrosymmetric crystal structure remains remarkably robust up to 40 GPa, although signatures of a possible structural transition are observed in EuIrGe$_3$ [4]. Furthermore, equation-of-state (EOS) analysis of the pressure-dependent unit-cell volume was performed to determine the elastic properties and compressibility of the compounds.

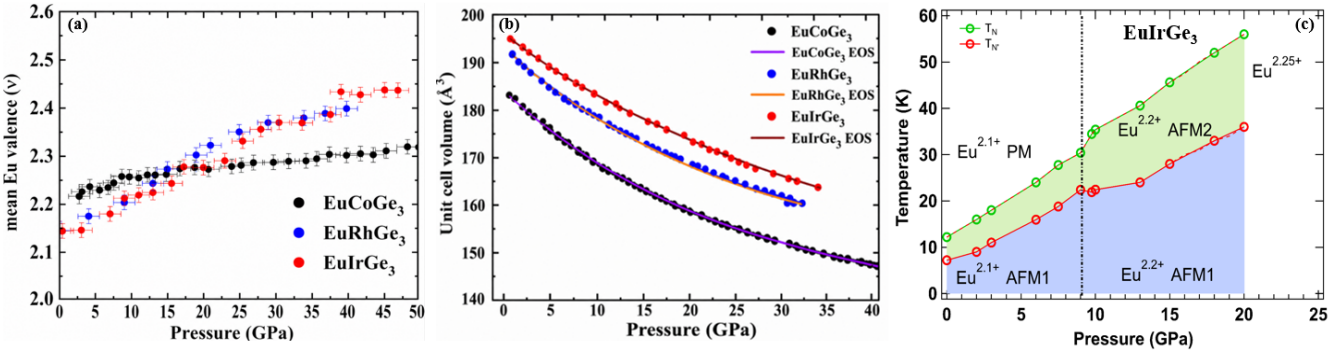

Figure 1. (a) Pressure dependence of the mean Eu valence obtained from HERFD-XAS, and (b) unit-cell volume with equation-of-state (EOS) fits for EuTGe$_3$. (c) temperature–pressure phase diagram of EuIrGe$_3$ derived from electrical resistivity measurements under pressure.

Electrical resistivity measurements performed up to 20 GPa on EuIrGe$_3$ reveal a substantial enhancement of resistivity with pressure, consistent with increased scattering from valence fluctuations and strengthened RKKY interactions. Simultaneously, the antiferromagnetic ordering temperature increases nearly fourfold, from 12 K at ambient pressure to approximately 48 K at 20 GPa. These results demonstrate that pressure drives Eu-valence evolution and strongly enhances magnetic ordering in non-centrosymmetric Eu*T*Ge$_3$ compounds, revealing a close coupling between electronic correlations, lattice compression, and magnetism.

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Superconducting Phase of BiTe at High pressure

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Abstract

Quasi-two-dimensional (2D) layered BiTe is a weak topological insulator having time-reversal symmetry protected conductive surface states on the side surfaces, while the layer surface is topologically protected due to the crystal mirror symmetry making it also a topological crystalline insulator [1]. Searching for superconductivity (SC) in diverse Topological insulators is of tremendous current interest for realization of topological superconducting surface states [2]. Efforts to induce SC at high pressure to obtain clean 3D topological SC without doping often lead to structural transitions into topologically trivial metallic phases prior to the emergence of SC [3,4].

Our high pressure investigations show that ambient quasi-2D trigonal ($P\bar{3}m1$) BiTe phase undergoes sequential structural transitions into various three dimensional (3D) network structures (SnTe-type) above 6 GPa and the atom-disordered bcc phase ($Im\bar{3}m$) emerges at 13 GPa through consecutive transitions to intermediate orthorhombic 3D phases ($Cmcm$) and($\gamma - Pnma$). Superconductivity emerges at 3 GPa, within the phase stability of the 2D layered BiTe phase. This also shows concurrent appearance of 2D weak anti-localization (WAL) feature in the normal state magneto-resistance, indicating the key role of the strong spin-orbit coupling in the emergence of SC in the layered phase [5]. SC T_c rapidly increases from 2.5K to 6K across the first structural transition to the 3D orthorhombic phase and further increases to 9K near 13 GPa across the structural transition to the bcc alloy phase. We identify the 2D and 3D BiTe phases with their distinct superconducting and normal state transport properties. Magneto-transport and Hall resistance measurements also indicate distinct transport behavior in the 2D and 3D phases.

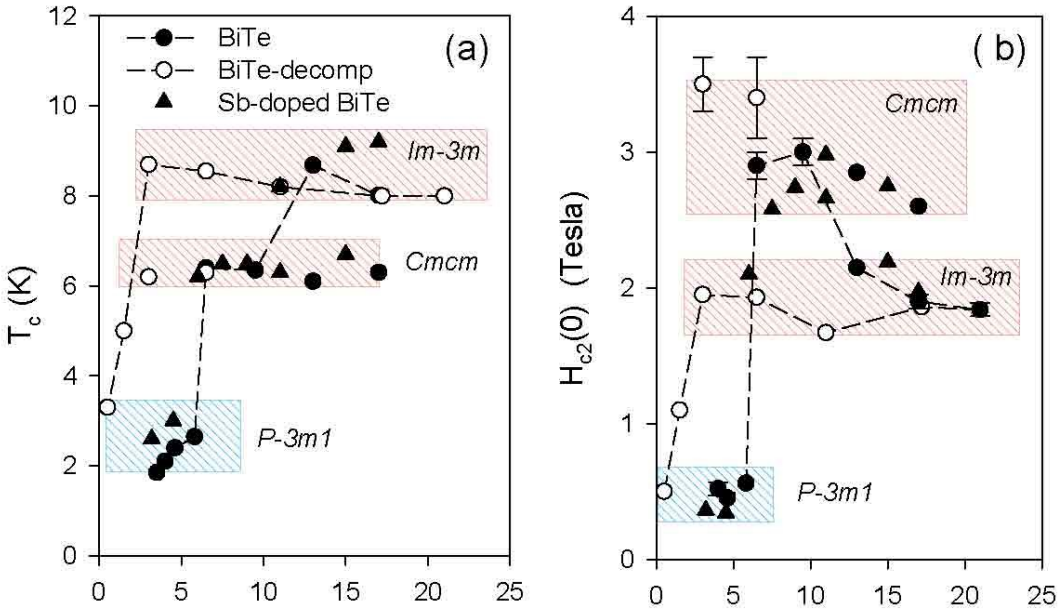

Fig. 1 *P*-variation of (a) SC T_c and (b) orbital upper critical field $H_{c2}(0)$ for BiTe and Sb-doped BiTe. The dashed lines indicate the *P*-variation of H_{c2} and T_c of the major phase at any *P*. The distinct T_c and $H_{c2}(0)$ values corresponding to the 2D and 3D phases fall in different shaded regions.

Acknowledgements: We acknowledge Prof. A. K. Sood for his support and S. Mondal and P. S. Anil kumar for providing single crystals. We thank S. Lupi, M. Zacchigna, and Veronica Stopponi for their assistance at the SISSI-Mat Science beamline and B. Joseph for his assistance at the XPRESS beamline. We gratefully acknowledge funding from ICTP (Italy) for high pressure XRD and IR measurements in Elettra Synchrotron (Italy).

Keywords: Topological Insulator, Superconductivity, X-ray diffraction, Magneto-transport measurements.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T4.1-O1 Geo- and Planetary Sciences

Forms of organic carbon at depth

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Abstract

In the subsurface, carbon has been largely assumed to exist as CO_2 for decades, though a few studies have shown that deep fluid-rock metamorphic reactions could generate other forms of carbon such as methane [1,2]. Over recent years, field and petrographic studies have revealed more diverse forms of organic carbon in sub-seafloor or subduction zones including organic acids [3] and condensed carbonaceous matter (CCM) [4,5].

In this study, we investigated the effect of pressure and water-rock ratio on the transformation of organic acids during the widespread serpentinization reaction of forsterite between 300 and 400°C. Experiments were performed in an externally heated diamond anvil cell and monitored in situ by Raman spectroscopy to characterize the kinetics of reactions between 1 and 40 kbar. Quenched products were analyzed by a suite of high-resolution analytical methods including but not limited to Raman and infrared mapping, XPS, SEM-EDX and TEM to characterize the variable composition of CCM, and structural relation with minerals.

Synthetic forsterite was chosen as the starting mineral in order to avoid focusing on redox reactions due to the ferrous iron content of olivine. Our study shows the rapid formation of CCM of variable composition and the lack of methane among products. The reaction kinetics is strongly influenced by pressure. The dehydration of the system by the serpentinization reaction contributes to carbon transformation by condensation as previously observed under lower pressure conditions in sub-seafloor [4]. Our results differ from those obtained for reaction between fayalite and aqueous acetate [6] that led to an organic composition very close to that obtained in the absence of the mineral phase, namely immiscible hydrocarbons [7,8]. Altogether, these studies highlight the wide range of organic compounds potentially occurring in sub-seafloor or subduction zones.

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T4.1-O2 Geo- and Planetary Sciences

Polymorphism of Superionic Ice at Planetary Interior

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Abstract

The behavior of water under extreme pressure and temperature is crucial for modeling the internal structure, stratification, and magnetic field generation of ice giant planets. At high pressures and temperatures, ice transforms into a superionic state characterized by a solid oxygen lattice with highly mobile protons. Defining the exact pressure-temperature boundaries of the superionic phases and their ultimate melting curve is critical for accurate modeling of gas planets. Recent static and dynamic experiments [1-5] utilizing laser-heated diamond anvil cells technique have confirmed the existence of *bcc* and *fcc* superionic phases (SI), although the precise pressure-temperature boundaries and the ultimate melting curve remain subjects of intense debate.

In our work [1-3], we have reported a significant increase in the melting curve in conjunction with the superionic phase transition and an extended temperature stability field for superionic ice, suggesting that the *fcc*-SI phase remains solid at high temperatures (approaching ~3000 K near 150 GPa). However, other studies [4-5] report a significantly lower melting curve for superionic phases. Most recently, a structural signature with an anomalously large thermal expansion crossover for the superionic transition in metastable *fcc*-SI ice was observed. Their results point to much lower transition temperatures for the *fcc*-SI phase, confirming its stability at approximately 2000 K beyond 150 GPa.

In our work [1-3], we have reported a significant increase in the melting curve in conjunction with the superionic phase transition and an extended temperature stability field for superionic ice, suggesting that the *fcc*-SI phase remains solid at high temperatures (approaching ~3000 K near 150 GPa). However, other studies [4-5] report a significantly lower melting curve for superionic phases. Most recently, a structural signature with an anomalously large thermal expansion crossover for the superionic transition in metastable *fcc*-SI ice was observed. Their results point to much lower transition temperatures for the *fcc*-SI phase, confirming its stability at approximately 2000 K beyond 150 GPa.

This discrepancy of up to ~1000 K at extreme pressures highlights critical challenges in high-pressure metrology, particularly concerning temperature gradients during laser heating and potential chemical effects. Resolving these controversies is very important for determining whether planetary mantles sustain solid superionic ice or transition to a fully fluid state fundamentally alters our understanding of ice giant evolution and interior dynamics.

Here, we will present results of recent measurements on superionic phase boundaries determined at different experimental conditions with extensive comparison to available static and dynamic data, including theoretical simulations. Unique properties of superionic phases will be discussed in the light of understanding the interior structure and dynamo processes in icy exoplanets.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T4.1-O3 Geo- and Planetary Sciences

Heat flow within terrestrial cores from electrical resistivity measurements of Fe-Si to 24 GPa

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Wenjun YONG (University of Western Ontario, Canada)
Richard A. SECCO (University of Western Ontario, Canada)

Abstract

Within the Earth and other terrestrial planetary bodies, the convection of a liquid metallic outer core is the driver of the dynamo-produced magnetic field which surrounds these bodies. It is widely accepted that these cores are composed primarily of Fe, with ~10% Ni, and one or more potential light elements including Si, S, and C. The dynamo within the liquid outer core can be driven by either chemical convection—which occurs as pure Fe freezes onto a solid inner core and the residual light elements rise—or thermal convection—which occurs as heat rises from the solid inner core, through the liquid outer core, and into the mantle. By quantifying the thermal conductivity of core-relevant alloys, the adiabatic heat flow in the liquid core can be calculated. By comparing this value with the heat flow through the core-mantle boundary (from other studies), the likely mechanism of outer core convection may be inferred, along with the likely duration of this convection.

The physical properties, including electrical resistivity, of Fe-Si alloys have been investigated previously, as Si has been stated to be the most likely light element within the inner solar system. From compositional constraints provided in previous studies, Fe-13 wt% Si is within the range of Si suggested for the cores of Mercury and the Moon. Additionally, this composition is likely also applicable to Mercury-like exoplanets, based on formation models. However, the electrical resistivity of this particular composition has not yet been investigated at high pressures.

Experiments are underway to be conducted in a 3000-ton multi-anvil press at pressures up to 24 GPa and temperatures into the liquid state. Octahedral pressure cells will be used which will contain continuous, porosity-free Fe-13 wt% Si wires, confirmed by computed tomography (CT) scans. These wires were produced from sample powder of the same composition. Using two sets of thermocouples, the four-wire method will be used to measure electrical resistivity and temperature within the sample at constant pressure. Using the Wiedemann-Franz law, these measurements will be used to calculate the electronic component of thermal conductivity, which can then used to calculate core adiabatic heat flow and then be compared to estimates of heat flow through the core-mantle boundaries within these bodies.

By the time of the meeting in August, CT scans of sample wires, high pressure-temperature resistivity experiments, and electron microprobe chemical composition analysis of recovered samples are expected to be completed and the following results obtained. Adiabatic heat flow within the cores of Mercury, the Moon, and two Mercury-like exoplanets will be estimated, and the likely convection mechanisms and durations within them inferred. In addition to the electrical resistivity data, the pressure-dependent melting boundaries will be determined for Fe-13 wt% Si at varying pressures, and combined with those of previous studies on other Fe-Si alloys.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T4.1-O4 Geo- and Planetary Sciences

Influence of Iron on the Stiffness of Silicate Glasses: Insights from All-Optical Density Measurements of Enstatite–Ferrosilite Glasses at High Pressure

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Abstract

The density of silicate melts is crucial for comprehensive modeling of the early Earth's evolution and for explaining mantle anomalies. It governs gravitational differentiation in the solidifying magma ocean, the migration of melts through the lithosphere, and their stabilization in the transition zone and near the core–mantle boundary. However, no systematic experimental data exists on the influence of iron on the compressibility of silicate melts — iron is one of the most abundant elements in the Earth's mantle — across the full mantle pressure range. This lack of systematic, self-consistent information about volume of silicate melts reflects significant experimental challenges in measuring the compressibility of silicate melts at mantle pressures and temperatures, including extremely small sample sizes, chemical reactivity of the melts, and the absence of long-range crystalline structure. Some of these experimental challenges may be overcome by using quenched glasses as structural proxies of their melts.

Here we report the compressibility of Fe-rich pyroxene glasses along the enstatite–ferrosilite compositional binary, with up to 7 at. % Fe ($En_{65}Fs_{35}$) and $Fe^{3+}/\Sigma Fe$ ratios of 0.45–0.55, measured at room temperature over a pressure range up to 60 GPa for all compositions and up to 120 GPa for the $En_{80}Fs_{20}$ composition. Compressibility was determined using the recently developed all-optical method in a diamond-anvil cell, where refractive-index and absorption-coefficient measurements are combined with image analysis of the sample inside the diamond anvil cell [1, 2].

Comparison of the compressibility of the studied Fe-rich pyroxene glasses with that of $MgSiO_3$ glass shows they are nearly indistinguishable within experimental uncertainty between 10 and 60 GPa (and up to 120 GPa for $En_{80}Fs_{20}$). Notably, the compressibility of MORB glass matches that of the studied glasses up to ~30 GPa. More generally, these results suggest that adding iron to silicate glasses— even in greater amounts than found in pyrolite or MORB — does not substantially alter their stiffness. Nevertheless, the individual roles of Fe^{2+} and Fe^{3+} require further careful examination: their ionic radii differ markedly, and they are expected to play different structural roles in silicate glasses, potentially affecting the stiffness.

Future all-optical measurements of the compressibility and optical properties of $MgO–SiO_2–Fe_2O_3–FeO$ glasses will provide experimental constraints for models of the physical properties of complex glasses and melts. Such data will substantially improve our understanding of primordial magma-ocean solidification, the evolution of physical and chemical heterogeneity in the mantle, and the migration or stabilization of melts at varying depths within Earth's interior.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T4.1-O5 Geo- and Planetary Sciences

Insights into the Structure of Mn^{2+}-dopped K_2CO_3-$MgCO_3$ Glass at High Pressure from Time-resolved Laser Fluorescence

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Abstract

The presence of carbonates in the mantle is supported by evidence from seismology, simulations, and natural samples. Deep carbonate melts exhibit extremely low viscosity and density, distinguishing them from silicate melts. High pressure experiments using K_2CO_3–$MgCO_3$ glass as an analogue for carbonate melts have suggested that pressure induces the formation of four fold coordinated carbon (CO_3 (sp^2-carbon) → CO^{3+1} (sp^3-carbon)) above ~30–40 GPa, implying potentially large changes in the physical properties of the glass (and possibly the melt) [1-3]. The formation of the CO_{3+1} configuration in the glass follows the strengthening of Coulombic attraction between K^+ and the oxygen atoms in distorted CO_3^{2-} anions [2]. Because Mg is a cation with a stronger cation field strength than K (at 1 atm: ~3.86 $Å^{-2}$ for Mg^{2+} vs ~0.53 $Å^{-2}$ for K^+), the pressure at which the CO_{3+1} configuration forms may also depend on changes in the local electronic environment of Mg. For example, one may expect that an increase in the Mg coordination number (CN) by oxygen could slow structural changes within the CO_3 anion and thus shift the onset of the carbon sp^2→sp^3 transition to higher pressures. However, resolving variations in Mg–O and Mg site in the glass using conventional structural probes remains challenging.

Here we report on the structural characteristics of Mn^{2+}-doped K_2CO_3-$MgCO_3$ glass probed by time-resolved laser fluorescence spectroscopy in a diamond anvil cell up to 37 GPa. The identical formal charge and intermediate ionic radius of Mn^{2+} allow it to serve as a proxy for common divalent cations (e.g., Mg, Fe^{2+}, Ca) in carbonates. The wavelength, intensity, and lifetime of the emission are sensitive to the Mn^{2+} CN and site symmetry, and show a strong pressure dependence. To interpret pressure induced changes in Mn^{2+} site, we performed reference measurements on Mn^{2+}-doped crystalline $CaCO_3$ and $MgCO_3$, whose high pressure behavior is well established. Our results show that upon compression the average Mn coordination increases from CN~6 at 1 atm to CN~7–8 at 13–14 GPa—well below the pressures reported for the carbon sp^2→sp^3 transition in the glass.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T5.1-O1 Instrumentation, Metrology and Techniques

A multi-technical approach to the study of the physical properties of materials. Examples from the PSICHE beamline, Synchrotron SOLEIL

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Abstract

The PSICHE beamline of the Synchrotron SOLEIL proposes a range of techniques for science at extreme conditions for a wide range of communities. The beamline specializes in combining diffraction, imaging and complementary techniques and can work in both polychromatic and monochromatic modes [1]. This presentation will showcase several recent developments, illustrated with examples from user experiments.

We will first present our large volume presses programs. The most innovative setup is the UToPEC system, a Paris-Edinburgh Cell designed for ultrafast tomography (> 1 tomo/s) at extreme conditions. The press can be continuously rotated by a high precision tomograph while heating, cooling the anvils and now controlling the pressure using an onboard compressor. A wide set of techniques are available, including CAESAR XRD, high-speed imaging, Beer-Lambert absorption measurements [2] and ultrasonic measurements. All are available almost simultaneously, creating new opportunities. For example, it is possible to perform Beer-Lambert absorption and ultrasonic measurements and control the sample geometry with tomography, giving access to the elastic properties of materials. While having access to XRD for structure analysis and pressure measurement.

Next, we will present our laser heated diamond anvil cell (LHDAC) setup, based on a technique that is widely used to generate temperatures of more than several thousands of K for pressures reaching tens and even hundreds of GPa. This technique is however known to generate high radial temperature gradients, that are detrimental for several reasons: 1/ they generate chemical diffusion (Soret effect) that are very problematic in the case of chemically complex samples; 2/ a very small X-ray beam is usually needed, which can be an issue when a good grain statistics is required; 3/ kinetic properties are very difficult to study; 4/ the sample microstructure may be difficult to interpret correctly.

For all these reasons, we have developed and implemented a new combination of techniques:

- Real-time sample surface temperature and emissivity mapping using an adapted 4 color pyrometry setup [3].
- Laser beamshaping to modify the power distribution of the laser focused spot. 4 color pyrometry can then be used to measure how this influences the temperature distribution at the sample surface, depending on the sample and environing materials thermal properties.

We will present a few examples of the opportunities that this innovative setup can bring to our users.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T5.1-O2 Instrumentation, Metrology and Techniques

The High-Power Laser Facility at ESRF: local and electronic structure of matter up to Mbar range

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Nicolas SEVELIN-RADIGUET (ESRF - European Synchrotron, Grenoble, France,FRANCE)
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Abstract

The High Power Laser Facility (HPLF) is a new platform at the ESRF that performs laser-driven dynamic compression probed by ultra-fast (<100 ps) X-ray Absorption Spectroscopy (XAS) at the energy dispersive beamline ID24-ED.

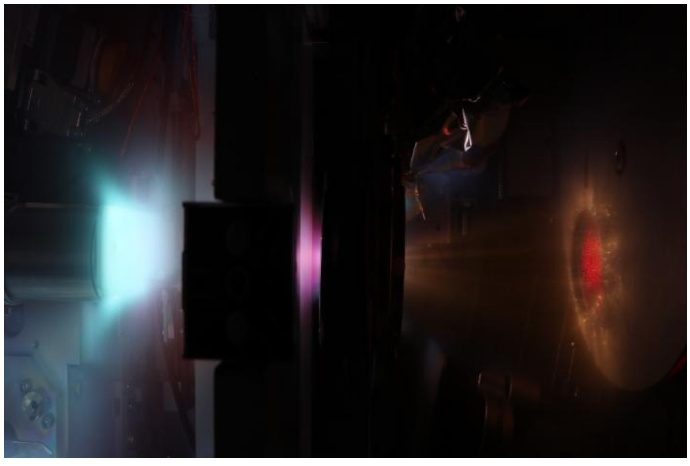
Dynamic compression provides a unique way to explore matter under extreme conditions of pressure and temperature up to several hundreds of GPa and tens of kK (for 100 J-class lasers), it also allows to explore the response of materials under high strain rates, and to generate over-liquidus states with non-eutectic composition, as the fast time scale (ns) allows to prevent chemical reaction and diffusion.

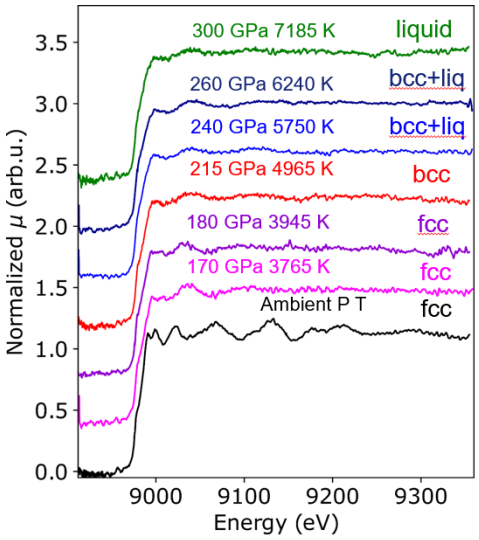
XAS provides local electronic and structural information around specific atoms whose core electrons are excited by the incident X-ray radiation. This technique is increasingly used in dynamic compression experiments [2, 3, 4] and offers complementary information to X-ray diffraction measurements. The element selectivity of XAS makes it well adapted to determine oxidation states and local ionic environment of both order and disordered systems.

ID24-ED offers time-resolved high-resolution X-ray Absorption Near Edge Spectroscopy (XANES) and Extended X-ray Absorption Fine Structure (EXAFS) measurements for materials with absorption edges between 5 and 28 keV.

The HPLF drive laser operates at 1053 nm wavelength and delivers 50 J in 4 to15 ns square pulses, producing ablation pressures up to 140 GPa in black Kapton, corresponding to around 300 GPa in 3d metals and 400 GPa in 4d metals. The facility is equipped with two line-imaging VISAR, one line-imaging streak optical pyrometry system for shot-to-shot characterization of the hydrodynamic conditions.

The science cases encompass fundamental science, Earth and planetary science and materials/industrial science. In this presentation I will provide an overview of the facility and focus on a selection of scientific results obtained during the first years of operation.





Left: photo of the shock event (curtesy of J-A Hernandez); right: XAS data of copper under shock compression up to 300 GPa [5]

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T5.1-O3 Instrumentation, Metrology and Techniques

MULTI-SCALE TRANSPARENT HIGH PRESSURE LABORATORY EXPERIMENTAL APPROACHES : APPLICATIONS IN DEEP ENVIRONMENTS STUDIES

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Abstract
Being able to investigate at lab scale the combined effects of thermodynamics, hydrodynamics, geo- and biochemical processes occurring in deep environment is still challenging. Over the last fifteen years, new types of HP transparent high-pressure micro- and millifluidics reactors (Figure 1) have been developed based on the idea of combining the advantages of small to medium scale process engineering (size reduction, fast screening, *in situ* analysis, reproducibility, control of hydrodynamics, improvement of thermal and material transfers, low consumption of reagents during optimization phases, etc.) with the properties of fluid systems used in high pressure and high temperature conditions (implementation of hydro- and solvothermal processes, studies of geofluid flows in model porous media, biology under extreme conditions, supercritical fluids, etc.). These tools allow to study more precisely the phenomena taking place at small scales and are complementary to the classical approaches using either macroscopic batch reactors or diamond anvil cells.

In this presentation, we will first detail the technologies available for the fabrication of high-pressure micro and millifluidics reactors, and then we will discuss their use in several applications related to the use of deep geological environments such as: (i) the geological storage of CO_2 (fluid flows, carbonation processes, solubility measurements, etc.), (ii) the production of hydrogen from iron and iron-bearing minerals in link with CO_2 capture and utilization topics and (iii) the effect of the deep biosphere on gas storage (CO_2, H_2) along with possible biochemical reactions (in particular methanogenesis).

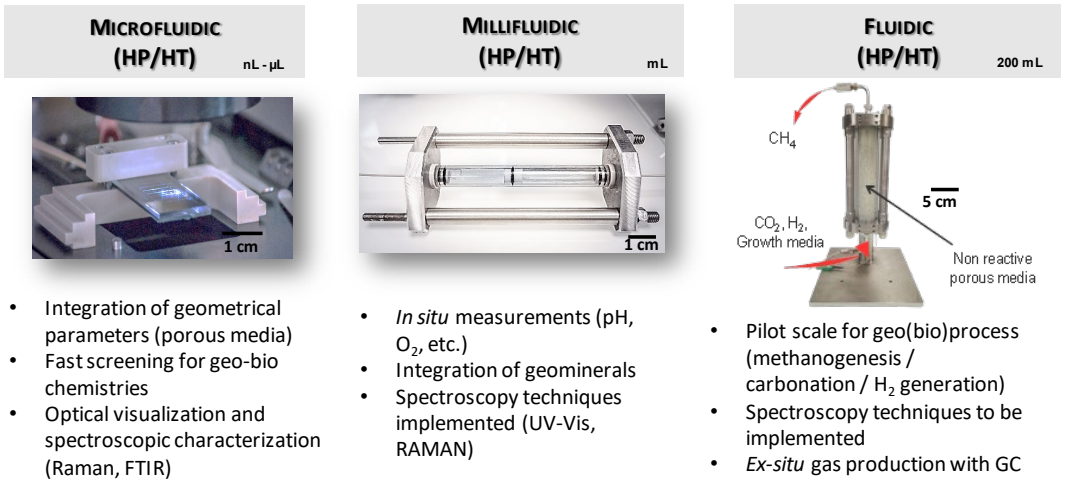

Figure 1: *Example of HP multiscale transparent reactors developed at ICMCB.*

Structural transformations under coupled extremes of pressure and swift heavy ion irradiation

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Abstract

The response of materials to the simultaneous application of high pressure and intense ionizing radiation remains largely unexplored, despite its relevance for functionality in extreme environments and for non-equilibrium materials synthesis [1]. This unique combination of extremes is accessible using the high-pressure irradiation platform installed in Cave A at the heavy-ion synchrotron SIS18 (GSI, Darmstadt, Germany) [2].

Micrometer-sized samples are compressed in diamond anvil cells (DACs) and irradiated with 200–480 MeV/u uranium ions. In-situ Raman spectroscopy and optical microscopy enable real-time tracking of structural and optical modifications as a function of accumulated fluence.

In this contribution, we present recent results on ion-induced transformations in various materials under high pressure, including molecular compounds such as carbon monoxide (CO) and sulfur (S), the inorganic compound sodium azide (NaN_3), and selected nanomaterials [3]. Effects identified by Raman spectroscopy and synchrotron X-ray diffraction include polymerisation, decomposition, bond rearrangement, and phase transformations, highlighting the rich landscape of radiation–pressure–coupled processes.

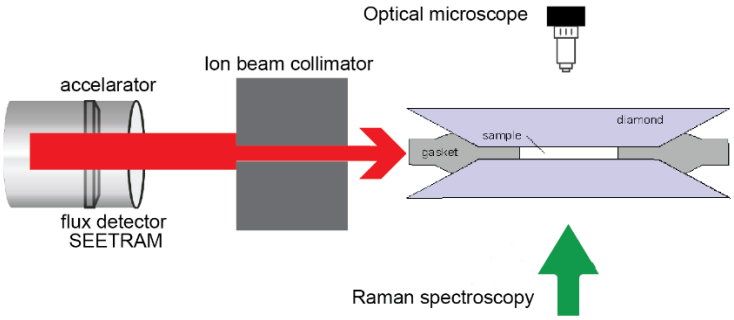

Figure 1. Schematic (not to scale) of the high-pressure irradiation platform at GSI. A pulsed ion beam exits the vacuum beamline through an Al window, is collimated, and passes through the gasket of a diamond anvil cell to reach the chamber.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T5.1-O5 Instrumentation, Metrology and Techniques

P61B LVP: The Large Volume Press station for in-situ X-ray diffraction and imaging on materials at HPHT

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Abstract

The 'Aster-15' LVP at the Wiggler beamline station P61B1 can routinely generate high pressure (ca. 30 GPa) and temperature (ca. 3000 K) HPHT environments on samples. Investigations using energy-dispersive X-ray diffraction (ED-XRD) and absorption-contrast imaging in the high-energy range 30 – 160 KeV reveal in-situ processes in near-real time. The type of experiments possible at P61B are summarized in Figure 1. The station provides two highly positional Ge-detectors for XRD acquisition at user-defined pre-calibrated diffraction angles (3° < 2θ < 10°), including vertical positioning (3° < 2θ < 20°) for cubic compression. These geometries are useful for e.g. tracking solid-state phase transformations and unit cell volume measurements for equations of state. For controlled sample deformation (< 15 GPa) using X-ray transmissive cBN/sintered-diamond anvils, stresses from lattice strains can be estimated with both detectors at the same 2θ (≥ 5°) and at 0° and 90° azimuthal positions. A beamstop is used to reduce background scattering and nearly eliminate Pb fluorescence (from detector shielding) in the diffraction patterns. Furthermore, we offer additional in-situ techniques, such as 1) acoustic emissions detection with 6 sensors (one on each anvil) combined with high-P deformation to study the physics of rock failure and earthquakes, 2) ultrasonic wave speed measurements using a $LiNbO_3$ transducer and a signal amplification system to study the elastic properties of materials and seismic structure of the Earth (to 38 GPa), and 3) electrical conductivity experiments on solid-state and partially molten systems to interpret magnetotelluric measurements e.g. of subduction zones. Imaging experiments, such as falling sphere viscosimetry, are enhanced with an extremely bright scintillator GAGG:Ce, for high-frame rate (150 fps) acquisitions. The in-situ LVP experiments are supported by an in-house suite of data processing software found on the beamline website. To apply for access, proposals can be submitted to P61B during regular calls for beam time, and we offer rolling access for LVP proposals (e.g. synthesis runs) that do not require X-rays. Details on the current status and development of a monochromator for angle-dispersive XRD will be presented, as well as information about the future in-situ LVP beamline at PETRA IV.

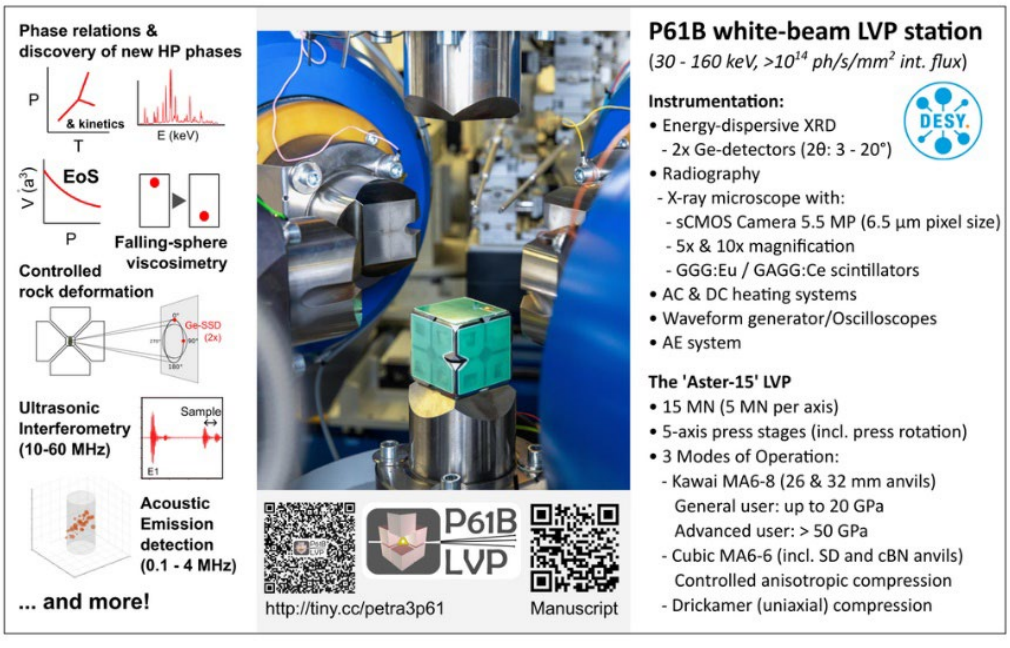

Figure 1. Overview of the capabilities of the P61B LVP beamline station.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T5.2-O1 Instrumentation, Metrology and Techniques

Benchmark melting behavior of rhodium under megabar pressures

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Leonid BURAKOVSKY (Los Alamos National Laboratory, United States of America)
Pablo BOTELLA (University of Valencia, Spain)
Anna PAKHOMOVA (European Synchrotron Radiation Facility, France)
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Abstract

Transition metals occupy a central role in condensed-matter physics and planetary sciences due to their distinctive electronic configurations, characterized by partially filled d-electron shells. The systematic trends governing the structural stability, cohesive energy, and extreme-conditions phase diagrams of transition metals are fundamentally driven by the degree of d-band filling [1], making their study essential for constraining the internal structures of terrestrial planets and exoplanets [2]. Rhodium (Rh), a chemically inert 4d transition metal within the platinum-group metals (PGMs), lies at the intersection of fundamental physics and technological relevance. Together with Ru, Pd, Os, and Ir, PGMs play key roles in catalytic processes, electronics, and extreme-environment applications [3]. Rhodium itself is widely used in high-temperature thermocouples [4], alloy hardening, and nuclear-related technologies [5,6], owing to its high melting point, low resistivity, and exceptional chemical stability. A precise understanding of its high-pressure behavior is essential for both applied performance and fundamental materials physics. Moreover transition-metal melting at extreme pressure remains one of the least constrained problems in condensed-matter physics, with theoretical predictions often differing by several thousand kelvin. Rhodium provides an ideal benchmark for testing finite-temperature electronic structure calculations. However, its high-pressure–high-temperature phase diagram has remained largely unexplored, with experimental melting data previously limited to pressures below 10 GPa [7].

Here we determine the high-pressure–high-temperature phase diagram and melting behavior of rhodium up to 100 GPa and 5000 K using *in situ* synchrotron X-ray diffraction in laser-heated diamond anvil cell, complemented by first-principles simulations. We show that rhodium retains its face-centered cubic structure throughout the investigated range and melts at temperatures systematically lower than predicted by most theoretical approaches. Analysis of the liquid diffraction patterns reveals that molten rhodium remains only 2–5% less dense than the corresponding solid at megabar pressures, indicating a substantial reduction of the solid–liquid volume change upon compression and placing new constraints on the thermodynamics of transition-metal melting. By combining static-compression, resistive-heating, and laser-heating measurements, we additionally establish a thermal equation of state spanning 0–100 GPa and 300–4500 K.

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Keywords: Melting, Extreme Conditions, Transition Metals, Laser-heating
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T5.2-O2 Instrumentation, Metrology and Techniques

Simple measurement of the hardness of C_{60} samples recovered after compression to 75 GPa.

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Hendrik HEIMES (Research School of Physics, Australian National University, Australia),

Abstract

Hardness, unlike elastic modulus, is not a fundamental material property [1]. Whereas elastic modulus is governed by interatomic bond stiffness and crystalline structure, hardness reflects how a material responds to localised stress, depending on a combination of yield strength, work hardening, and fracture behaviour. Because different indentation methods probe different combinations of these properties, a hardness value should be considered in the context of how it was measured.

For materials recovered after compression in a diamond anvil cell (DAC), conventional macro-scale methods such as Vickers indentation are impractical as this requires optical imaging of the residual indent which typically demands loads incompatible with the small DAC samples. Nanoindentation, as the name suggests, is more suited to such small samples and measures hardness using a combination of a well-characterized indenter tip with continuous in situ load and displacement measurements. Previous attempts to use nanoindentation to measure the hardness of materials created via DAC experiments have required extracting, mounting, and polishing the recovered sample, a process that is time-consuming and risks introducing artefacts including epoxy contamination and compliant substrate effects [2-3]. Here we describe a simpler alternative using direct nanoindentation on the sample still attached to the diamond culet itself, with no additional sample preparation.

In this technique the top anvil of a plate cell is carefully removed, and the sample and gasket are left in place on the bottom anvil. This is placed directly in a Hysitron nanoindentation system and indented using a Berkovich tip to loads up to 10 mN. Samples of compressed C_{60} fullerene to pressures up to 75 GPa were studied. A range of different hardnesses for the recovered samples was found, broadly consistent with our previous transmission electron microscopy studies [4].

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T5.2-O3 Instrumentation, Metrology and Techniques

In situ Raman thermometry for temperature determination in externally heated diamond anvil cells?

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Abstract

Externally heated diamond anvil cells (DAC) are widely employed in high-pressure and high-temperature experiments. They allow a precise and stable control of the temperature inside the sample chamber, unlike the laser heating DACs, but can only reach lower temperatures, usually limited to ~1000 K. In HP-HT experiments, temperature measurement is mainly performed using a thermocouple fixed to the diamond table, or through radiothermometry, though the latter method requires a higher temperature range and is affected by the emissivity problem. While the thermocouple method is precise, the geometry of the cell can significantly alter the result, either through direct heater-thermocouple interaction or suboptimal thermocouple positioning, leading to high discrepancies between the measured and the sample temperatures.

This study employs a Helios DAC from Almax easyLab with a resistive heating and a gas-membrane drive for pressure control, all enclosed in a vacuum chamber made by BETSA to prevent oxidation and minimize heat loss. Temperature is monitored by in situ Raman thermometry[1] through analysis of the Stokes and anti-Stokes Raman signals collected from both the DAC diamond cullet and a cubic boron nitride (c-BN) crystal enclosed in the sample chamber. c-BN exhibits no known reactivity with water below 1300 K, making it ideal for hydrothermal studies[2]. Pressure is simultaneously measured via ruby fluorescence shift[3], diamond Raman shift[4] and c-BN Raman shift[5].

The reliability of the Raman thermometry method is first validated in an Linkam setup at atmospheric pressure, using the spectra of c-BN, quartz and GeO_2. The α-β quartz phase transformation and the GeO_2 melting point, both observable through Raman spectroscopy, serve as fixed reference points. A maximum temperature of 1600 K is reached under nitrogen atmosphere, limited by the c-BN → phase transition to h-BN. C-BN is then used inside the DAC at temperatures up to 850 K and pressures up to 15 GPa, with argon and nitrogen as pressure-transmitting media. The melting curves of argon and nitrogen serve as fixed reference points[6], with the transition observed optically and via Raman spectroscopy for nitrogen at pressure higher than 7 GPa[7].

Linkam experiments demonstrate a temperature precision of ±50 K up to 1300 K for Raman thermometry. Initial DAC results evidenced a temperature gradient between the thermocouple and the sample of up to 400 K. This difference in temperature arises from the cell geometry, which heats the thermocouple primarily through conduction while the sample is heated through radiation. The deposition of graphite ink between the heater and the diamond reduces the gradient to a maximum of 200 K, enabling temperatures up to 850 K to be reached. The results also reveal a homogeneous temperature within the sample chamber and the diamonds, with diamonds, c-BN and ruby all remaining within a 50 K range, indicating that the diamond temperature effectively matches the sample temperature, and that temperature can be accurately measured via Raman thermometry on the diamonds alone.

This method offers a simple and precise temperature detection approach that overcomes the limitations of traditional measurements in externally heated DACs. Using the diamonds themselves eliminates the need for additional sensors inside the sample chamber, it allows reducing experimental complexity while maintaining accuracy (±50 K).

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T5.2-O4 Instrumentation, Metrology and Techniques

New X-ray Light Sources, Innovative Pressure Platforms, and Advances in AI: Opportunities for High-Pressure Research

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Abstract

Large Large-scale X-ray light sources have long been integral to high-pressure research, and major upgrades and new facilities are currently being developed and commissioned around the world. Over the last four years, the Advanced Photon Source (APS) has undergone a transformative upgrade, delivering a state-of-the-art storage ring with significantly increased brightness and improved beam coherence. Concurrently, the High Pressure Collaborative Access Team (HPCAT), a dedicated high-pressure research facility at APS, has implemented substantial upgrades and introduced new experimental capabilities.

HPCAT has also developed and deployed a range of advanced pressure platforms that expand accessible pressure-temperature conditions, enable a broader range of compression rates, and provide opportunities for complex loading paths that can be coupled with cutting-edge X-ray characterization techniques. At the same time, the rapid emergence of artificial intelligence is beginning to transform many aspects of scientific research, from experiment design and autonomous data collection to analysis, interpretation, and discovery.

This presentation will provide an overview of recent developments at APS and HPCAT, highlight selected scientific achievements enabled by these new capabilities, and discuss emerging opportunities and strategic directions for the high-pressure research (at HPCAT and across the broader community) in the coming decade.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T5.2-O5 Instrumentation, Metrology and Techniques

Lattice Dynamics from X-Ray Thermal Diffuse Scattering under High Pressure

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Abstract

Between the Bragg reflections in the X-ray diffraction pattern of any single crystal there exists a weak, continuous, diffuse pattern created by scattering of the X-rays by phonons (Fig. 1, left). This thermal diffuse scattering (TDS) pattern contains information about the lattice dynamics of the crystal. Technological advancements in the past 25 years have sparked renewed interest in TDS as an alternative to inelastic neutron and X-ray scattering techniques for studying the lattice dynamics of crystals [1, 2]. The principal advantage of using TDS is its far shorter data collection times when compared with inelastic scattering techniques. These short data collection times allow for more detailed studies of the lattice dynamics in crystalline systems as a function of pressure, temperature and/or other parameters. However, the data analysis involved with this technique is significantly more demanding.

We have been developing experimental and computational methods for the novel approach of collecting and analysing TDS data from single crystals inside diamond anvil cells (DACs) under compression. We have been taking advantage of the fast data collection associated with TDS techniques to determine full sets of phonon dispersion relations (Fig. 1, right) for a material at numerous different pressures with data collection times of the order of hours instead of days. Extensive model fitting is required to extract lattice dynamical information from the experimental data. In addition to the scattering from the sample, there are numerous sources of background signal, and particular attention must be paid to the Compton scattering and TDS signal from the diamond anvils in the DAC. We have found that modern, multi-panel phonon-counting detectors demand extra attention to the flat-field correction. Here we discuss experimental and data-analysis aspects of the TDS technique, and present first results on the lattice dynamics and pressure-induced anomalies in caesium metal and caesium iodide at pressures up to 10 GPa.

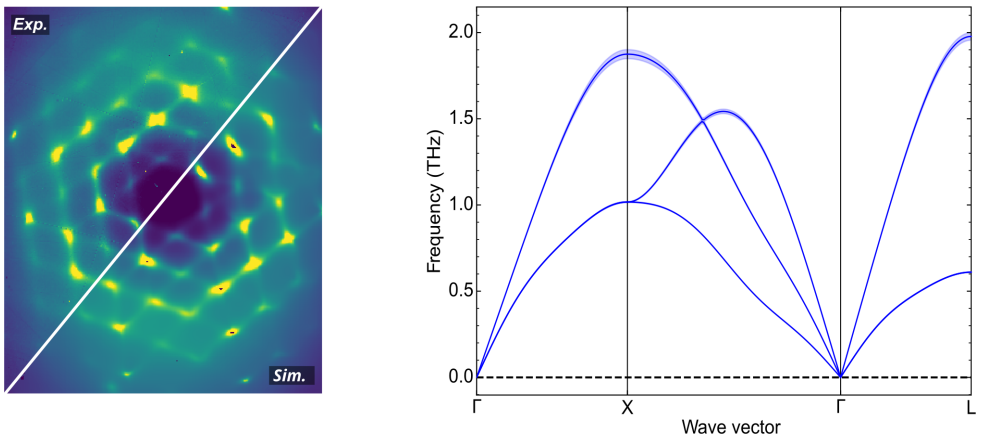

Fig. 1: (Left) Experimental and simulated TDS image of the high-pressure phase fcc caesium at 2.6 GPa and (right) the corresponding extracted phonon dispersion relations. The shaded bands indicate the numerical uncertainty of the phonon frequencies obtained.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T5.2-O6 Instrumentation, Metrology and Techniques

Determining thermal conductivity at extremes using X-ray Free Electron Lasers

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Abstract

The determination of thermal conductivity at extreme pressure and temperature conditions is a main branch of high pressure experiments and has various outputs for planetary science. Thermal conductivity at extremes determines planetary evolution as well as current dynamics. While there exists a variety of techniques already employed for thermal conductivity determination, a number of discrepancies persist for some of the key materials present in terrestrial planets. One of the most striking cases is Fe alloys at Earth's core conditions. A convincing assessment of such quantities requires new techniques benchmarked at very extreme conditions. Here, we present three recent developments based on a combination of X-ray Free Electron lasers, high-pressure diamond anvil cell (DAC) experiments, and numerical modeling that can be used to constrain thermal conductivity at extremes. We show how adjusting numerical models to match experimental x-ray diffraction data, optical temperature measurements, or post-mortem micro-analysis of recovered samples all offer novel solutions to assessing extreme thermal conductivity, reaching into high pressure liquid states.

Our first approach presents DAC experiments where volumetric x-ray heating was employed to bring metallic samples up to several thousands of K [Husband et al. 2021]. Using Finite Element Modelling (FEM), the time-dependent volume evolution of the crystal lattices upon heating can be reproduced [Edmund et al. 2024]. Model adjustments benefit from the thermal conductivity dependence of that evolution.

In a second approach, we demonstrate how measured temperature oscillations resulting from serial XFEL irradiation can allow fitting of the sample thermal conductivity. We characterize temperature oscillations measured on very short timescales with streak optical pyrometry and show how solid and liquid thermal conductivities can be determined from these data.

Finally, we introduce a melt volume-based analysis of thermal conductivity in X-ray heated samples, using recovered sample textures in cross-sectional measurements to establish melting extent. Simulations of the melt extent show that, for equal temperatures, the melt extent depends on the thermal conductivity of the sample predominantly for insulating pressure media. In particular, this technique is sensitive to the thermal conductivity of the liquid volume.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T6.1-O1 High-Pressure Crystallography

Clathrate hydrates at high pressure: The cases of methanol enclathration

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Tiziana BOFFA BALLARAN (Bayerisches Geoinstitut, Germany)
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Abstract

Clathrate hydrates are host–guest crystalline compounds: hydrogen-bonded water molecules form cage-like structures that encapsulate guest molecules. Their ability to accommodate a wide variety of guests has attracted strong interdisciplinary interest over the past decades. Clathrate hydrates are studied as functional materials for energy storage [1], CO_2 sequestration [2], and other technological applications [3], while also being recognized as important geomaterials that influence climate regulation and the evolution of organic matter on Earth [4] and on outer Solar System bodies [5]. The need to understand chemistry-structure-property relationships and the role of clathrate hydrates in the transport of volatiles within planetary interiors has driven the development of high-pressure hydrate research as a prominent field of study.

In this contribution, we will (1) provide an overview of the current state of knowledge on high-pressure clathrate hydrates; (2) discuss the effects of pressure on host-guest interactions and the structural evolution of clathrate hydrates; (3) present case studies demonstrating different mechanisms of pressure-induced methanol enclathration in the tetrahydrofuran (THF)-CH_3OH-H_2O [6] and CO_2-CH_3OH-H_2O systems, highlighting methanol's unexpected incorporation despite its well-known role as an antifreeze agent; and (4) discuss open questions and ongoing research activities in the field.

Financial support provided by the Agence Nationale de la Recherche (ANR) through the project CAGES ("High pressure clathrate hydrates in large ocean worlds", ANR-23-CE49-0002, PI A. Pakhomova) is acknowledged.

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Theory-guided discovery of pressure-induced transitions in the fast-ion conductor $BaSnF_4$

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Abstract

Fast-ion conductors such as $BaSnF_4$ are of significant interest for next-generation solid-state battery technologies due to their high ionic conductivity and chemical stability. However, the behavior of these materials under extreme conditions remains poorly understood, despite the relevance of pressure-induced modifications for tuning functional properties. In this study, we combine density functional theory (DFT) calculations with high-pressure experiments to investigate the structural evolution of $BaSnF_4$ up to 40 GPa [1]. As shown in Figure 1, DFT predicts two pressure-induced phase transitions: from the ambient-pressure tetragonal $P4/nmm$ phase to a monoclinic $P2_1/m$-I structure at 10 GPa, and subsequently to a denser monoclinic $P2_1/m$-II phase at 32 GPa. The first transition is experimentally confirmed via angle-dispersive X-ray diffraction (carried out using a diamond-anvil cell at ALBA synchrotron), Raman spectroscopy, and electrical resistivity measurements, all performed at ambient temperature. The second transition is supported by distinct changes in high-pressure Raman modes and resistivity behavior, consistent with a further structural reorganization. These findings not only clarify the high-pressure phase diagram of $BaSnF_4$ but also shed light on the potential for pressure-tuned ionic transport in fluorostannate-based solid electrolytes.

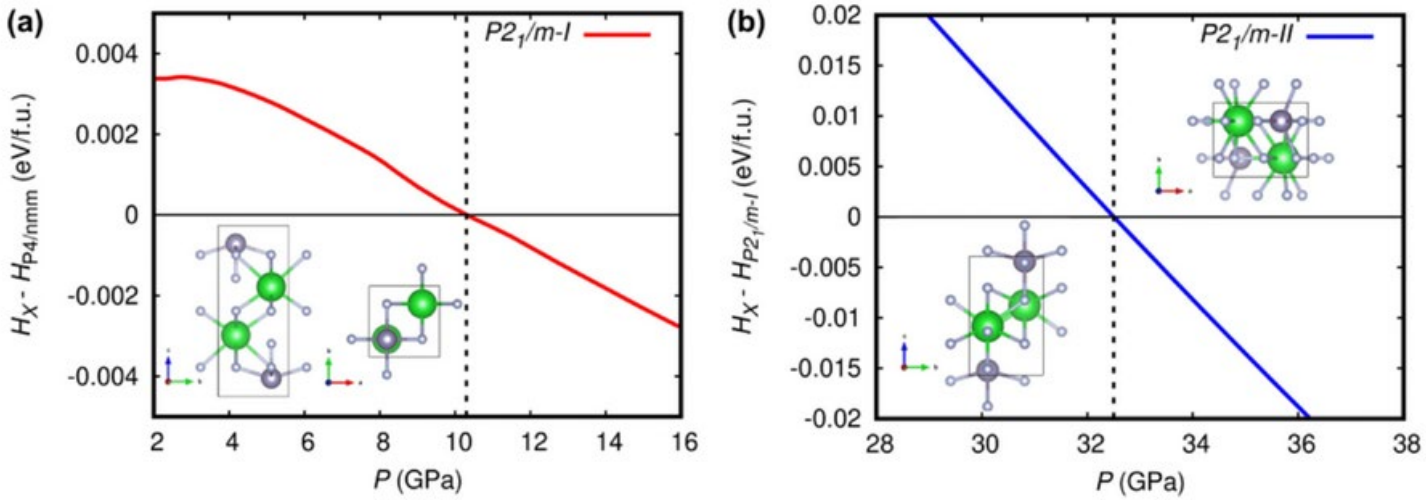

Figure 1: (a) Calculated enthalpy of the high-pressure monoclinic ($P2_1$/m-I) $BaSnF_4$structure relative to the ambient-pressure fluorite-type tetragonal structure ($P4/nmm$). (b) Calculated enthalpy of the higher-pressure monoclinic ($P2_1$/m-II) $BaSnF_4$structure relative to the lower-pressure monoclinic ($P2_1$/m-I) $BaSnF_4$structure. The overall sequence of phase transitions predicted by DFT is $P4/nmm$ (ambient pressure) → $P2_1$/m-I (>10 GPa) → $P2_1/m$-II (>32 GPa).

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High Pressure and High Temperature polymorphism of Na_2CO_3 up to 10 GPa

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Abstract

Sodium carbonate (Na_2CO_3) is a model system for studying complex polymorphism, owing to its rich sequence of temperature-driven phase transitions [1] and the presence of an incommensurately modulated structure at ambient conditions [2,3,4]. Despite extensive crystallographic investigations, its behavior under high-pressure and high-temperature (HP-HT) conditions remains only partially constrained, particularly in the 0-10 GPa range.

In this study, we present an in-situ investigation of Na_2CO_3 combining single-crystal X-ray diffraction and large-volume press (LVP) experiments to explore its thermoelastic properties and phase stability up to 10 GPa. We identify two previously unreported high-pressure polymorphs, ε and ε-II. The ε phase, stable above ~2 GPa, crystallizes in the monoclinic space group Cc and is characterized by a doubling of the c unit-cell parameter relative to the γ and β polymorphs. Its bulk modulus (47.6(8) GPa) is comparable to that of the γ phase, indicating similar compressibility. The ε-II phase, observed at higher pressures (~11 GPa), likely represents a metastable distorted variant of the ε structure.

By mapping phase transitions across a wide pressure-temperature range and assessing their reversibility, we refine the topology of the Na_2CO_3 phase diagram. Integration of high-precision single-crystal data with LVP constraints allows us to propose an updated phase diagram (Figure 1) featuring an expanded stability field for the incommensurate γ phase and a broad stability region for the ε polymorph under high-pressure conditions.

These findings provide new experimental constraints on the high-pressure behavior of sodium carbonate, improving the reliability of its phase diagram and offering a robust framework for future crystallographic, computational, and high-pressure studies.

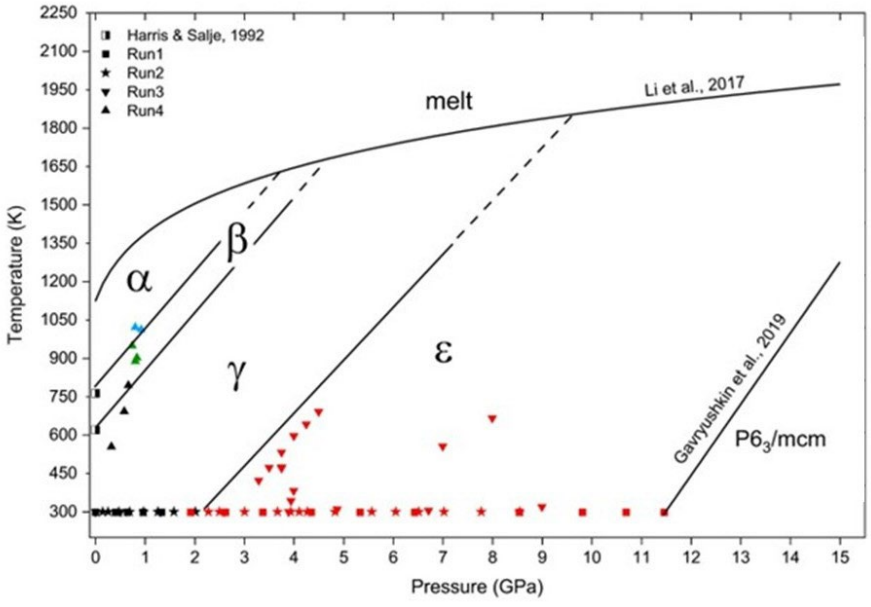

Figure 1: Phase diagram of sodium carbonate obtained from experimental data.

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T6.1-O4 High-Pressure Crystallography

ID15b and Hydrated borates at High-pressure

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Abstract

Hydrated borates, such as colemanite, kernite, ulexite, and borax, represent the primary ore minerals of boron—a critical geochemical marker for petrogenetic processes and a strategic resource for advanced technological applications. Classified as critical raw materials by the EU in 2017[1], these minerals are increasingly investigated as aggregates in neutron-shielding concretes due to their high thermal neutron absorption capacity, stemming from their elevated H and ^{10}B content. Structurally, hydrated borates consist of $B\varphi_x$ units (tetrahedra and trigonal planes), where φ represents an oxygen atom or a OH^- group or a H_2O molecule, organized into polyion clusters, which are linked to alkali or alkaline-earth polyhedra (*e.g.*, Na^+, $Ca2^+$, Mg^{2+}). Within these frameworks, H_2O molecules and OH^- groups form an extensive hydrogen-bond network that is fundamental to the stability of the crystalline edifice [2, 3]. This contribution explores the high-pressure deformation mechanisms and structural evolution of various hydrated borates, investigated via synchrotron X-ray diffraction at the ID15b beamline (ESRF). Our results show that these minerals undergo several high-pressure phase transitions. These involve the conversion of trigonal $B\varphi_3$ units into $B\varphi_4$ tetrahedra through the formation of additional B-φ bonds, or the rearrangement of the coordination spheres surrounding the divalent/trivalent cations (*e.g.*, Fig. 1). Interestingly, a recurrent structural pattern appears to emerge, potentially providing a basis for a predictive framework regarding the high-pressure stability of this mineral class (Fig. 2).

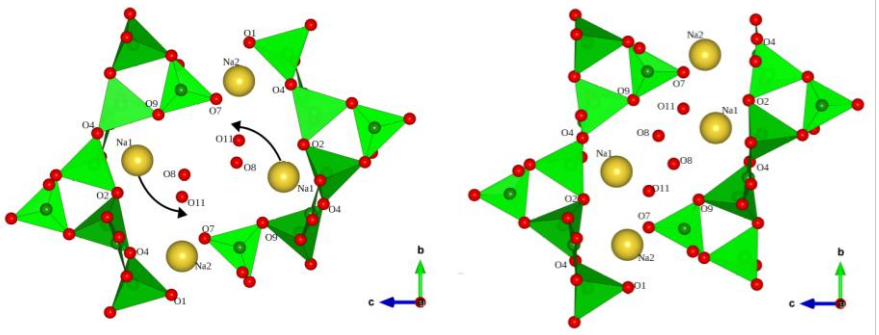

Fig.1: difference between the structures of kernite (left) and kernite-II (right)

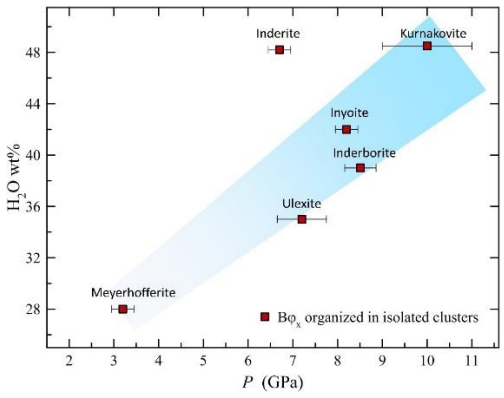

Fig.2: H_2O wt% *vs* $P_{(phase\ transition)}$ in a number of hydrated borate structures

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T6.1-O5 High-Pressure Crystallography

Cryogenic stabilization of molecular hydrogen in dense cubic ice

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Abstract

Hydrogen storage remains a central challenge for the deployment of hydrogen-based energy technologies, particularly due to the lack of safe and efficient solid-state storage materials operating near ambient conditions. While most strategies rely on porous frameworks or chemically reactive hosts, dense molecular solids have remained largely unexplored. In this work, we demonstrate that cubic ice (I_c), obtained from high-pressure hydrogen hydrates, can retain molecular hydrogen as an interstitial guest upon decompression, establishing a new paradigm for hydrogen storage in non-porous crystalline materials.

Hydrogen hydrates were synthesized at pressures above 3-4 GPa, where water and hydrogen form the fully occupied cubic C2 phase (H_2:H_2O ≈ 1:1). This phase represents a dense, hydrogen-rich structure stabilized by pressure-induced incorporation of H_2 within a hydrogen-bonded framework. Upon rapid cooling and decompression to ambient pressure, C2 transforms topotactically into fully crystalline cubic ice I_c, preserving the parent symmetry (*Fd*-3*m*). This structural continuity enables direct investigation of hydrogen retention mechanisms following release from high-pressure conditions.

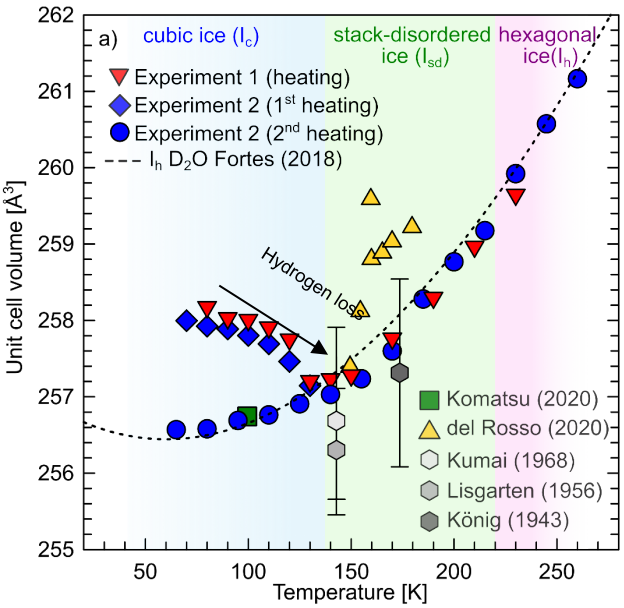

Figure 1. Unit cell volume evolution of cubic ice produced by decompression (to 0.1 MPa) of C2 hydrogen hydrate at low temperature (red and blue symbols) determined *via* neutron diffraction.

Using neutron diffraction, synchrotron X-ray diffraction, and Raman spectroscopy, we observe that the recovered I_c exhibits a reproducible lattice expansion (~0.6% at 80 K) relative to hydrogen-free ice, providing clear evidence for residual hydrogen trapped within the lattice. This expansion progressively vanishes upon heating to ~130 K, indicating gradual hydrogen release. Spectroscopic measurements further confirm the presence of molecular H_2 through characteristic roton and vibron modes, consistent with weakly bound, interstitial hydrogen occupying multiple local environments.

Importantly, moderate pressures (~0.18 GPa) significantly enhance hydrogen stability and reversibility. Under these conditions, remnants of the C2 phase persist up to 90 K, demonstrating that hydrogen-rich hydrate structures can survive far below their nominal stability fields. Moreover, cubic ice can be partially refilled with hydrogen at the same pressure, leading to lattice expansions exceeding 1.5% and confirming pressure-driven re-incorporation of H_2. The hydrogen content retained in I_c corresponds to several percent of the parent hydrate composition, with estimated storage densities comparable to interstitial hydrogen in metals.

These results reveal that pressure not only stabilizes hydrogen-rich hydrate phases but also enables metastable trapping and reinsertion of hydrogen in dense, non-porous crystalline ice. This behavior challenges the conventional view that hydrogen storage requires permanent porosity or strong chemical bonding. Instead, weak host-guest interactions within a dense hydrogen-bonded lattice can sustain significant hydrogen uptake under cryogenic conditions.

Beyond energy applications, these findings have implications for planetary and astrophysical environments, where pressure-temperature cycling and radiation processes may generate similar metastable hydrogen-bearing ice phases. Cubic ice may thus act as a transient hydrogen reservoir in icy moons, comets, and interstellar grains.

Overall, cubic ice emerges as a minimal model system for studying hydrogen-lattice interactions under pressure, highlighting dense hydrogen-bonded solids as a previously unrecognized class of materials for hydrogen storage physics.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T6.2-O1 High-Pressure Crystallography

From Intermolecular Interactions to Functional Properties: Pressure-Tuned Behavior of π-Conjugated Molecular Crystals

Anna KRAWCZUK (University of Goettingen, Germany),
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Abstract

Molecular crystals provide a unique platform for investigating the effects of compression on intermolecular interactions, as non-covalent contacts are generally far more responsive to pressure than covalent bonds. As a result, pressure offers an exceptional opportunity to continuously modify crystal packing and electronic structure, enabling direct observation of how structural changes translate into chemical and physical properties.

This talk addresses how high-pressure single-crystal X-ray diffraction, combined with optical spectroscopy, can be used to follow the evolution of intermolecular interactions in π-conjugated molecular crystals and correlate structural changes with their physical properties.

Particular attention is devoted to anthracene- and heptazine-based systems. In anthracene derivatives, compression progressively alters intermolecular π···π interactions and molecular packing, resulting in significant modifications of optical behavior. High-pressure crystallographic studies reveal the structural origins of these effects and provide insight into how subtle changes in intermolecular geometry influence the electronic structure of the crystal. In the most extreme cases, continued compression drives the system towards intermolecular bond formation, illustrating the intimate connection between non-covalent interactions and chemical reactivity in the solid state.

Complementary studies on heptazine-based materials demonstrate how pressure-induced modifications of crystal packing and supramolecular organization influence the response of π-conjugated chromophores. Particular emphasis is placed on the role of the crystal environment and co-crystallized species in governing structural adaptation under compression and shaping the resulting physical properties.

Together, these examples highlight how pressure can be employed to systematically manipulate intermolecular interactions in molecular crystals and establish direct links between crystal structure, electronic behavior, and functionality. The presented studies demonstrate the unique capabilities of high-pressure crystallography for understanding and ultimately controlling the properties of responsive organic materials.

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T6.2-O2 High-Pressure Crystallography

How subtle differences in organic molecular crystals influence their structural evolution in compression

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Samuele FANETTI (ICCOM, LENS, Italy)
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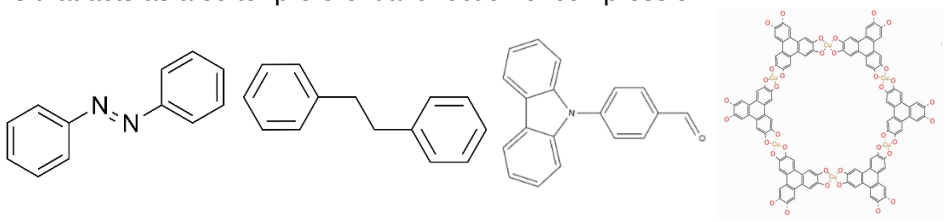
Abstract

Organic molecular crystals are an incredibly interesting class of materials to be studied in compression. Structural evolution under pressure depends on two different contributions: one that comes from the entire molecular unit moving within the unit cell, and the other instead that derives from intra-molecular changes. The most direct approach to observe these changes under pressure is synchrotron powder and single crystal X-ray diffraction, while fine variations in molecular structure and interactions can be complemented with spectroscopic techniques such as IR, Raman, UV-Vis and XAS spectroscopy. Simple molecular systems will be presented to showcase how small differences in chemical formula and conformations can result in very different structural evolution in compression, but also how distinct compounds can have similar features that can dictate how the system ultimately reacts to high pressure. Azobenzene/stilbene and bibenzyl are two closely related molecules differing only in the central chemical bond that links the two phenyl groups. This however makes azobenzene more rigid than bibenzyl, which has instead an additional degree of freedom in the torsional movement of the central bond. This difference plays a huge role in influencing the phase transition path that both undergo around 14 GPa: azobenzene exhibit a more drastic phase transition that needs to involve a greater molecular rearrangement in the structure [1], while bibenzyl is able to release the accumulated stress with molecular distortions that have a much smaller effect on the symmetry and unit cell [2]. N-(4-Formylphenyl)carbazole shares a similar torsional degree of freedom to bibenzyl and as such they share a comparable low pressure behavior where tortional motion provides access to a much softer preferred crystallographic direction of compression. However, an overall lower flexibility leads to rupture of the unit cell symmetry along a specific direction rather than the point group symmetry of the molecule. Lastly, the structural evolution in compression of novel 2D-MOFs composed by metal centers and hexahydroxytriphenylene (HHTP) units is showcased. These MOFs are gaining interest due to their straightforward synthesis procedure and semiconducting properties which arise from intermolecular interactions of stacked two-dimensional extended metal-organic molecules [3]. The nature of these compounds allows for compressions to higher pressure than usual MOFs thanks to the available space between layers that acts as a softer preferential direction of compression.



Left to right: azobenzene, bibenzyl, N-(4-Formylphenyl)carbazole, CuHHTP 2D-MOF

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T6.2-O3 High-Pressure Crystallography

Putting Pressure on Multicomponent Crystals: Tuning Single-Crystal-to-Single-Crystal Transformations via Compositional Engineering

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Abstract

Tailoring the chemical composition through the design and synthesis of multicomponent crystals allows for the modification of crystalline solid properties via control over the intermolecular interaction landscape and aggregation preferences [1]. This can directly affect a crystal's response to external stimuli, such as high pressure, enabling access to single-crystal-to-single-crystal (SCSC) transformations not observed in the monocomponent crystals of pure coformers. In this context, the formation of multicomponent crystals can be presented as a relatively straightforward method for the synthesis of stimuli-responsive crystalline materials.

Among pressure-induced SCSC transformations reported for multicomponent crystals are phase transitions and solid-state reactions. Significant elastic deformations can also be regarded as continuous SCSC transformations if the crystallinity of the material is preserved. While physical changes observed upon compression provide insight into the effect of chemical diversification on phase stability and mechanical response, the research area concerning topochemical reactions is especially compelling. In these cases, not only does the molecular arrangement change, but the chemical nature of the components is altered. The aggregation of different chemical units within a crystal lattice allows for regio-selective reactions to take place [2] without the need for solvents, making such processes an environmentally friendly alternative to traditional synthesis [2]. Pressure is a powerful stimulus for inducing reactions in crystals [3], as lowering interatomic distances directly affects the energy barriers of chemical processes. It must be noted, however, that not all solid-state reactions are SCSC transformations, as they often lead to the loss of crystallinity or require additional stimuli like UV irradiation.

This presentation focuses on recent high-pressure investigations of multicomponent crystals, specifically highlighting observed SCSC transformations. These include phase transitions [4], cocrystals exhibiting significant negative linear compressibility over a wide range of pressure [5,6], and chemical reactions between coformers, such as proton transfer or the formation of new covalent bonds [4,7,8].

Acknowledgment

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T6.2-O4 High-Pressure Crystallography

Pushing the 10 GPa Pressure Boundary for Organic Solids: Crystal Structure Determination of α-Glycine Above a Megabar

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Abstract

Survey of the Cambridge Structural Database (CSD) shows almost 93% of high-pressure depositions (only accounting for 0.36% of the database) to be reported at pressures below 10 GPa.[1] The range of molecular solids studied under pressure encompass not only incredibly common chemical reagents and solvents, but also classes of biomolecules that make up the fundamental building blocks of life. These organic molecular crystals often have extensive networks of non-covalent intermolecular interactions, which play a significant role in the relative arrangement of molecules to form the overall crystal packing.

It is hypothesised that past the 10 GPa (equivalent to 100,000 bar) pressure, intermolecular void space in organic molecular crystals approaches zero, requiring modifications in the network of intra and intermolecular bonding interactions to accommodate for further compression.[2] The lack of single-crystal X-ray diffraction (SCXRD) data on such solids past this pressure threshold presents a clear gap in our understanding of the impact of pressure on interactions that govern the formation of molecular crystals and contribute to the structure-function relationship in biological macromolecules.

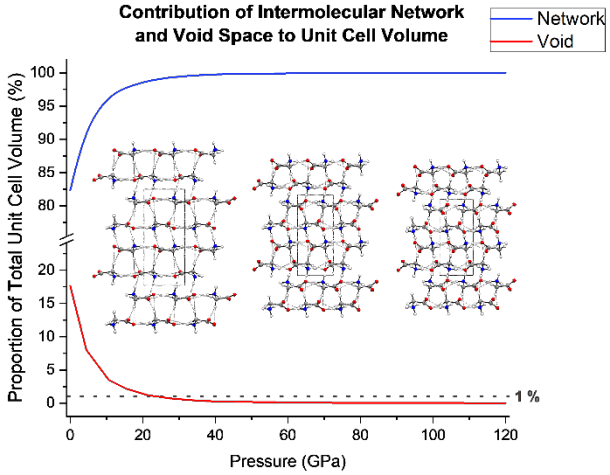

Figure 1. Plot of the contribution of the intermolecular network and void space to the total unit cell volume of α-glycine with increasing pressure. Marked by the grey dashed line is the point at which the proportion of total unit cell volume corresponding to void space is less than 1%. A section of the crystal structure of α-glycine at increasing pressure intervals is shown in the centre of the plot (from left to right: 0.0 GPa, 60.0 GPa, and 120.0 GPa).

Here we will present the results of SCXRD experiments at pressures in excess of a megabar, surpassing the so-called '10 GPa pressure boundary' by over tenfold. The simplest proteinogenic amino acid, glycine, was chosen for the incredible robustness of the α-phase at high pressures. Our SCXRD experiments yielded high quality diffraction data allowing the structure of α glycine to be fully solved and refined up to 120.0 GPa. This far exceeds both the previous highest pressure single crystal structure of α glycine, and the typical pressure range for organic molecular crystals. From these data, the evolution of the intermolecular hydrogen bonding network as a response to pressure has been tracked, and calculations of geometric and energetic data will be presented. Of particular note is the remarkable ability of this crystal structure to accommodate pressure even after the point where void space accounts for less than 1% of the total unit cell volume, found to occur after 21.5 GPa. The data presented will provide insight into the structural modifications undergone by the intermolecular bonding network as a direct response to compression, and highlight the value of studying molecular solids up to this new 1.2 megabar threshold.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T6.2-O5 Simple Systems and Experiments at extreme conditions

The crystal structure of ruby up to 170 GPa

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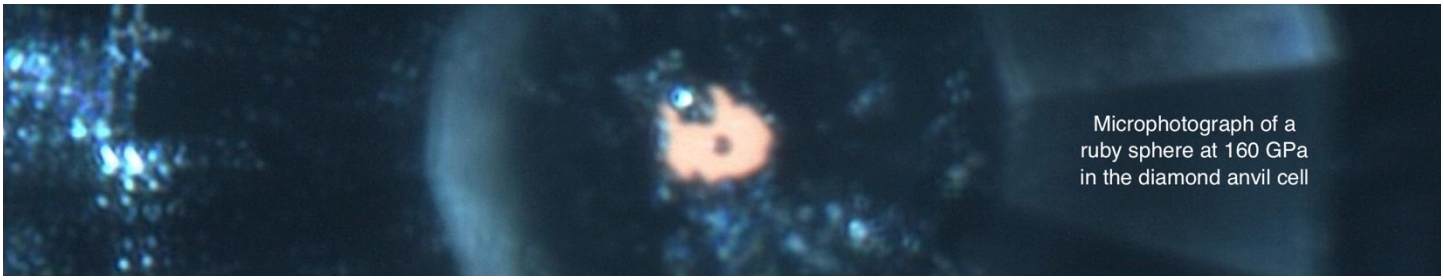
Abstract ()

Ruby, chromium-doped corundum, might very well be the second most critical material in high-pressure experimental science after diamond. The pressure and temperature dependence of its fluorescence is indeed the most widely used pressure gauge [1,2], it is also used as window material in shock compression, as medium and insulator in micro fabricated sample chambers and so on. Corundum is a prototypical structure - common to many sesquioxides and 2:3 compounds; AlO_6 octahedra are common building blocks of minerals. It is therefore important to determine precisely the deformation mechanisms of Al_2O_3. Indeed, a great deal of work has been performed in determining experimentally and computationally its properties under pressure with the greatest accuracy possible (see [3] and references therein).



We obtained an accurate assessment of the behavior of the material at ambient temperature in its metastable pressure range, above 80 GPa. A small ruby sphere was compressed in helium in a diamond anvil cell, and its long-range ordering was probed using synchrotron single-crystal micro-diffraction. We improved greatly from previous analogous measurements [4] with higher resolution and better sampling of the reciprocal space.

We will compare bulk and axial compressibility data with the literature. Robust single-crystal structural refinements were obtained at about 80 and 127 GPa, settling any lingering controversy on the bonding response of ruby under pressure.
These results represent a reference experimental structural observations to understand and model ruby's behavior under very high pressures.

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New look at phase diagram of cuprite under pressure

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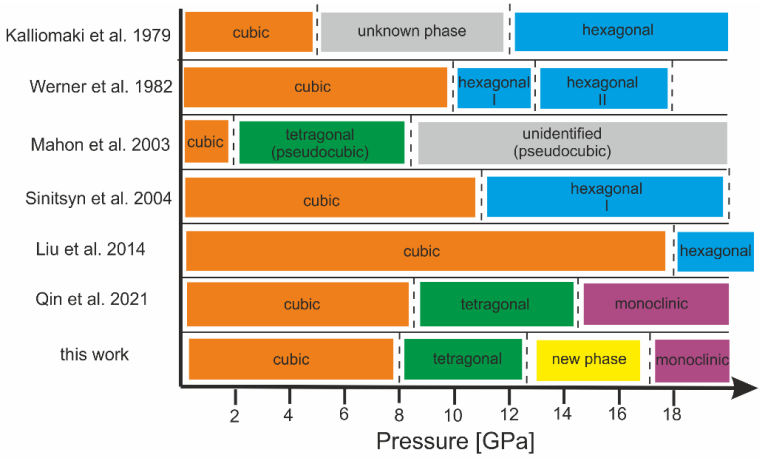
Abstract

Although the scientific literature presenting researches of cuprite under pressure already covers several papers, the real appearance of its phase diagram still remains unclear. On one hand cuprite is pretty simple compound which crystallizes at cubic crystal system, Pn-3m, at ambient pressure. On the other hand, when external pressure is applied, cuprite undergoes many phase transitions.

One of the first extensive studies were conducted by Kalliomaki et al..[1] In this paper researches claimed that cuprite under pressure undergoes two phase transitions, firstly at ca 5 GPa to some unknown structure and then at 12 GPa to some hexagonal structure. Werner and Hochheimer came to different conclusions.[2] They claim that first phase transition to unknown hexagonal structure occurs at 10 GPa and the second to another hexagonal at 18 GPa. These results were based on X-ray powder experiment. Mahon et al.[3] repeated the high-pressure, powder X-ray experiments. Authors revealed that firstly cubic structure undergoes transition to tetragonal phase, between 0.7 and 2.2 GPa, and later to some unidentified pseudo-cubic phase at 8.5 GPa. Results of applying high-pressure and heating the sample of cuprite were investigated by Sinitsyn et al..[4] First transition, at room temperature, to a hexagonal phase II occurred at ca. 11 GPa and another one to different hexagonal phase III at 21 GPa. There were performed also multiple DFT calculations. Liu et co-workers[5] showed that cubic Cu_2O under pressure should transforms to the metastable hexagonal phase between 18 and 20 GPa. The most recent experimental data based on single-crystal X-ray diffraction measurements conducted by Qin and co-workers,[6] confirmed existence of cubic to tetragonal phase transition at 10.4 GPa (from Pn-3m space group to $P4_2/nnm$ space group) and revealed novel monoclinic phase which appears at 16.1 GPa (space group P1a or P12/a1).

On the basis of our experiments it seems that the situation is even more complicated. The hexagonal phase does not exists, but we understand why many scientists believed in its existence. Also, we suspect that a new phase may exist, but interpretation may change as a fact of developing techniques and access to them. It could be just a question of interpretation based on data of insufficient quality. For better understanding the situation we present these information as a simplified chart below.



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T6.3-O1 High-Pressure Crystallography

Phase transition mechanism of the pressure-induced $\beta \leftrightarrow \gamma$ transformations in tin

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Agnès DEWAELE (CEA, DAM, DIF France)
Nicolas BRUZY (CEA, DAM, DIF France)
Nicolas GUIGNOT (Synchrotron Soleil, France)
Gaston GARBARINO (European Synchrotron Radiation Facility, France)

Abstract

Solid-solid phase transformation mechanisms need to be understood to establish suitable kinetic laws. Two classes of solid-solid phase transformations are described in the literature. Martensitic transformations have a 'military' displacive atomic mechanism that produces a new phase seed with a time scale that can be as low as sub-ns; however, they induce elastic stresses that need to be relaxed, which is a phenomenon at the microstructure scale. Reconstructive transformations, with nucleation and diffusional growth steps, sometimes massive, are thermally activated and slower but produce a microstructure at mechanical equilibrium. The understanding of the transformation mechanism is necessary to establish suitable kinetic laws for each transformation.

Sn (tin) exhibits a rich polymorphism under high pressure and varying temperatures that has been studied with different techniques and platforms. This makes it an archetypal system to study phase transformations in metals and their mechanisms. Here, we investigate the β-Sn $\leftrightarrow$ γ-Sn phase transformations occurring at ~10 GPa at room temperature.

Single crystals have been statically compressed and characterized using in situ x-ray diffraction. Multiple transformation cycles were performed in diamond anvil cells to measure their conditions and the associated microstructures. The crystal orientation of the child phase can be deduced from the orientation of its parent, which characterizes a martensitic mechanism: $(101)_\beta$ || $(110)_\gamma$ and $\left[10\bar{1}\right]_\beta$ || $\left[1\bar{1}1\right]_\gamma$ orientation relationships (OR) between β-Sn and γ-Sn, never reported before, are repeatedly observed. An atomic pathway to account for these observations will be discussed.

New insight into the transformation mechanism can now be obtained with a micrometer resolution 2D XRD method, which reveals the full microstructure of the compressed sample.

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T6.3-O2 High-Pressure Crystallography

Na-Si phase diagram at HPHT

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Abstract

To construct an experimental phase diagram of the Na-Si system, it is important to emphasize that the compounds participating in the equilibria, i.e., Na_4Si_4, Na_8Si_{46} (sI) are stoichiometric. At the same time, non-stoichiometric phase is possible for $Na_{30.5}Si_{136}$ (sII-HP). Na_xSi_{136} is non-stoichiometric compound, “ideal” stoichiometry at x = 24 (for clathrate we adopt the coefficients in chemical formula corresponding to unit cell composition); x superior to 24 up to 30.5 correspond to high-pressure phase denoted as HP-sII (Yamanaka *et al.*, 2014), while at ambient pressure of Ar or in vacuum sII with x from 0 to 24 forms (Cros & Pouchard, 2009, Kasper *et al.*, 1965).

sII-HP coexists with Si-I at low temperatures, while sI becomes more stable at higher temperatures in the case of excess Si. Excess Na makes sII-HP stable up to the melting temperature. Previous reports suggest that ΔV of melting be close to 0 (Courac *et al.*, 2019), thus with weak slope dT/dp of melting curve. Rapid quenching of a stoichiometric liquid results in the crystallization of sII-HP, indicating that the melting of this phase is congruent. Some experiments show the coexistence of sI and sII-HP with the absence of Si-I. Figure represents the tentative phase diagram at 5 GPa compatible with all available experimental observations.

At pressures above 8 GPa, channel clathrate structure of Na_xSi_{24}, only phases with stoichiometries x = 4 or x ~0 are known (Guerette et al., 2018, Kim et al., 2015, Kurakevych et al., 2013). Long keeping of Na_4Si_{24} leads to sodium escape from the lattice, and its hydrolysis on the surface with air humidity. Anyway, heating in vacuum remains a method of choice to produce best samples of Si_{24} (Kim et al., 2015).

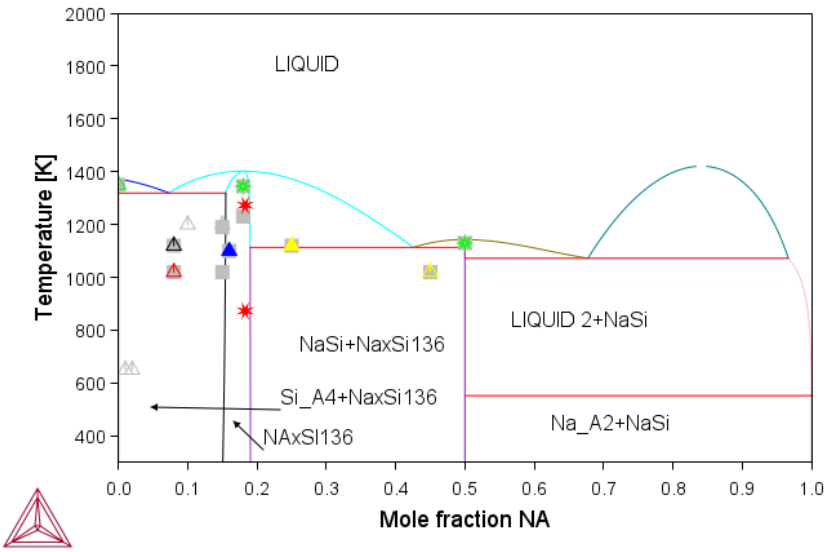

Figure. Phase diagram of Na-Si system at 5 GPa: experimental data vs CALPHAD simulation using ThermoCalc software.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T6.3-O3 High-Pressure Crystallography

Is gold really stiffer at the nanoscale?

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Thomas BÜRGI (University of Geneva, Switzerland),

Abstract

The elastic properties of metallic nanostructures have been a subject of intense debate, often clouded by a lack of distinction between isolated nanoparticles and nanocrystalline solids. While the latter frequently exhibit size-dependent compressibility due to grain boundary effects and inter-crystallite constraints, the intrinsic elasticity of individual, ligand-protected nanoparticles remains an open question. Among these, gold stands out as a paradigmatic case where the literature remains divided; previous studies on Au nanoparticles report a chaotic landscape of bulk modulus K_0 values, with discrepancies of up to 70%—ranging from 133 to 290 GPa [1-3]—compared to the well-established bulk value of 167 GPa [4].

In this work, we demonstrate that these variations are largely experimental artifacts rather than intrinsic size effects. We present a systematic study using high-pressure synchrotron X-ray diffraction on a diverse library of Au nanostructures in colloidal dispersions: from single-crystalline spheres and rods [5] to penta-twinned decahedra and rods with tetragonal and orthorhombic symmetries [6]. By ensuring strictly hydrostatic conditions, we eliminate the deviatoric stresses that typically render diffraction data unreliable and lead to artificial overestimations of K_0. Our results reveal a remarkably consistent bulk modulus of $K_0 \sim 170$ GPa across all shapes, symmetries, and sizes (10–50 nm), echoing the behavior of bulk gold.

To push the limits of this invariance, we extended our research to the molecular regime by performing high-pressure single-crystal X-ray diffraction on the atomically precise $Au_{25}(PET)_{18}$ cluster. By successfully solving the complete crystal structure under pressure and tracking the individual inter-atomic Au-Au distances within the 13-atom gold core of the cluster, we provide direct evidence that, within our experimental accuracy, the Au-Au bond remains as compressible as in the macroscale. This work offers a consistent framework to reconcile previous discrepancies: once experimental artifacts and grain boundary effects are decoupled, gold's elasticity appears as an intrinsic property of the metallic bond, showing a remarkable size-independence from the macroscale down to the atomic cluster.

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T6.3-O4 High-Pressure Crystallography

Surfing Between Structure and Spin State: High-Pressure Studies of Spin Crossover Compound

Benjamin BERTIN, Almudena INCHAUSTI, Elodie TAILLIEUR, Elen DUVERGER-NEDELLEC, Nathalie DARO, Patrick ROSA, Guillaume CHASTANET, Mathieu MARCHIVIE, Philippe GUIONNEAU (*Université de Bordeaux, CNRS, Bordeaux INP, ICMCB, UMR5026, 33600 Pessac, France)*

Abstract

Spin crossover (SCO) materials are attracting growing interest for many applications due to their ability to switch reversibly between high spin (HS) and low spin (LS) states under numerous external stimuli such as temperature, light or pressure. According to this last stimulus and due to their ability to switch reversibly between HS and LS associated with a high entropy variation, SCO complexes have been recently identified as potential candidates for solid-state barocaloric refrigerant[1,2] (for the cooling systems of the future). Within this context, designing molecular-based spin transition materials that are optimal for barocaloric application requires a thorough understanding of SCO behavior under extreme conditions.

In this work, we investigate a spin-crossover material as a model system to better understand the effects of pressure on functional materials. Our study focuses on its thermodynamic behavior though the construction of a pressure-temperature phase diagram. To achieve this, we employ advanced X-Ray diffraction or absorption techniques, which enable us to probe structural changes associated with spin transition under pressure and temperature. By systematically exploring a wide range of pressures and temperatures with small steps, we identify phase boundaries and characterize the coexistence of distinct spin states. The resulting phase diagram contributes to a deeper understanding of how external pressure influences phase stability and transition mechanisms in such systems, offering a broader perspective on their physical properties and potential technological relevance.

Beyond the targeted SCO properties (such as $T_{1/2}$ and transition abruptness), identifying suitable candidates for barocaloric application requires a thorough understanding of the properties and stability of the different phases under pressure. The results presented here therefore illustrate one of the essential steps that must be undertaken before considering a spin crossover material for barocaloric applications.

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From $[CO_3]$ towards $[CO_4]$: a high-pressure study of two novel hydrous carbonates

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Abstract

Carbonates are ionic compounds that are typically known to feature $[CO_3]^{2-}$ groups, in which the sp^2 hybridization of the orbitals of carbon leads to a trigonal planar geometry of the carbonate anions. Many examples of metal carbonates with the general chemical formula $MeCO_3$ (Me = Ca, Fe, Mg, etc.) have been reported at ambient conditions. Owing to the rotations of the carbonate anions $[CO_3]^{2-}$, such sp^2 carbonates exhibit a wide range of polymorphs even at pressures below 20 GPa.

At pressures higher than 20 GPa, the definition of carbonates has been expanded to include compounds based on $[CO_4]^{4-}$ tetrahedra, where the central carbon atoms form sp^3 hybridized orbitals with their four neighboring oxygen atoms. These compounds become more common at pressures above 50 GPa with examples[1, 2] exhibiting a wealth of structural diversity due to tetrahedra polymerizing via common vertices. Alike the chemistry of silicates[3, 4], this results in the formation of various structural units of various dimensionalities. The dominance of the sp^3 hybridization for carbonates above 50 GPa was predicted by calculations[5, 6] and has been experimentally well-documented [7].

However, the mechanisms that lead to this transition are still not fully understood. Merlini at al. [8] have demonstrated that $CaCO_3$-II begins to exhibit an intermediate state of the carbonate anions between 40 and 60 GPa, with the carbon atoms gradually moving away from the plane of the $[CO_3]^{2-}$. Another factor that affects the displacement of carbon from the ideal trigonal configuration is the hydrogen interactions in the structure. This effect was demonstrated in nuclear magnetic resonance spectroscopy[9] studies of monohydrocalcite and ikaite, two naturally occurring calcium carbonate hydrates.

To further study the effect of pressure and hydrogen on the structural evolution of carbonates, we performed high-pressure, high-temperature experiments on the $CaCO_3(s) + H_2O(l)$ system at 38(2) GPa and 2000(200) K using a laser-heated diamond anvil cell. Usage of multi-grain, single crystal X-Ray diffraction at ID27 and ID11 beamlines of European Synchrotron Radiation Facility allowed us to identify new hydroxide and hydroxy-hydrate carbonates, namely tR45 $Ca_3(CO_3)_2(OH)_2$ and mP104 $Ca_4(CO_3)_3(H_2O)_2(OH)_2$, as products of the reaction. Compression of the discovered phases up to 74 GPa revealed a gradual evolution of the central carbon from trigonal to tetrahedral, a change that is more pronounced for tR45 $Ca_3(CO_3)_2(OH)_2$ (Figure 1). In the current contribution we will present the pressure-induced evolution of both phases and discuss the mechanism of this structural change enhanced by the presence of OH^- groups interacting with the carbonate anions.

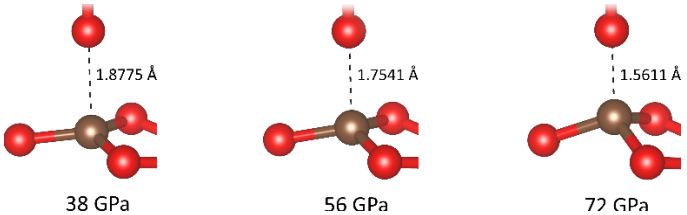

Figure 1: Schematic representation of the effect of compression on the geometry of CO_3 triangular units in tR45 $Ca_3(CO_3)_2(OH)_2$, showing the gradual evolution of the geometry of central carbon position.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T6.3-O6 High-Pressure Crystallography

Assessing Synthesis Pathways to Superconducting Mg_2IrH_6

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Abstract
Hydrogen-rich binary compounds have enabled superconductivity at unprecedented temperatures (>150 K), establishing hydrides as a central platform for exploring phonon-mediated high-T_c superconductivity [1]. However, due to the prohibitively high pressures required to stabilise these phases (>~150 GPa), research has now turned to ternary hydride compositions, with multiple computational studies indicating that the incorporation of a second host element may help to stabilise superconducting states to significantly lower pressures; opening the possibility of practical applications of these materials.

Of such predicted structures, cubic Mg_2IrH_6 has been proposed as one of the most exciting candidates, with an ambient pressure superconducting transition between 80-160 K [2,3]. In this work, various synthesis pathways to the proposed superconducting structure have been explored utilising X-ray diffraction crystallography, Raman spectroscopy and electrical transport measurements, supported by ab-initio calculations, mapping the thermodynamic landscape of the Mg-Ir-H system.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T6.4-O2 High-Pressure Crystallography

Shear-driven formation of diamond during cold compression of graphite and glassy carbon

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Abstract

Carbon's exceptional versatility in forming diverse phases makes it important across modern applications, ranging from energy storage to industrial cutting tools. Significant scientific interest remains in exploring the mechanisms governing carbon phase formation, particularly diamond which has outstanding properties. Previous work has demonstrated that cold-compressed graphite can transform into metastable, high-density exotic structures under elevated pressure including M-carbon, W-carbon, and Z-carbon [1-3]. However, none of these phases have proven recoverable at ambient conditions. Understanding the pathways leading to diamond formation carries considerable importance, as diamonds serve as mineralogical markers of impact events and high-pressure metamorphism in meteorites and planetary crusts. Beyond pressure and temperature, shear stress has emerged as an additional critical variable governing whether diamond or other dense, diamond-like phases will nucleate [4-5].

This study examines the formation of high-density carbon phases from highly oriented pyrolytic graphite (HOPG) and glassy carbon precursors subjected to room-temperature compression under non-hydrostatic, high-shear conditions. Samples were processed in both conventional and rotational diamond anvil cells (DACs) to vary the compression environment. Recovered samples were sectioned into lamellae by focused ion beam (FIB) milling and subsequently characterized by transmission electron microscopy (TEM). Using electron energy loss spectroscopy (EELS) spectrum imaging, we demonstrate that high-density diamond phases are recoverable from both precursor materials without sample heating and at lower pressures than generally required. Microstructural analysis revealed clear signatures of shear-driven deformation, including shear bands and associated defects, while diffraction analysis identified a range of phases beyond conventional diamond: amorphous diamond, nanocrystalline lonsdaleite, and mixed cubic/hexagonal diamond stackings. The diversity of recovered phases is attributed to the heterogeneous stress conditions present within the sample chamber. Collectively, these findings establish that elevated temperatures are not a prerequisite for diamond-like phase formation, implying that diamond can arise across a broader range of geological and synthetic environments than previously recognized.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T6.4-O3 High-Pressure Crystallography

Understanding quartz polymorphs' formation during impact events using dynamic compression

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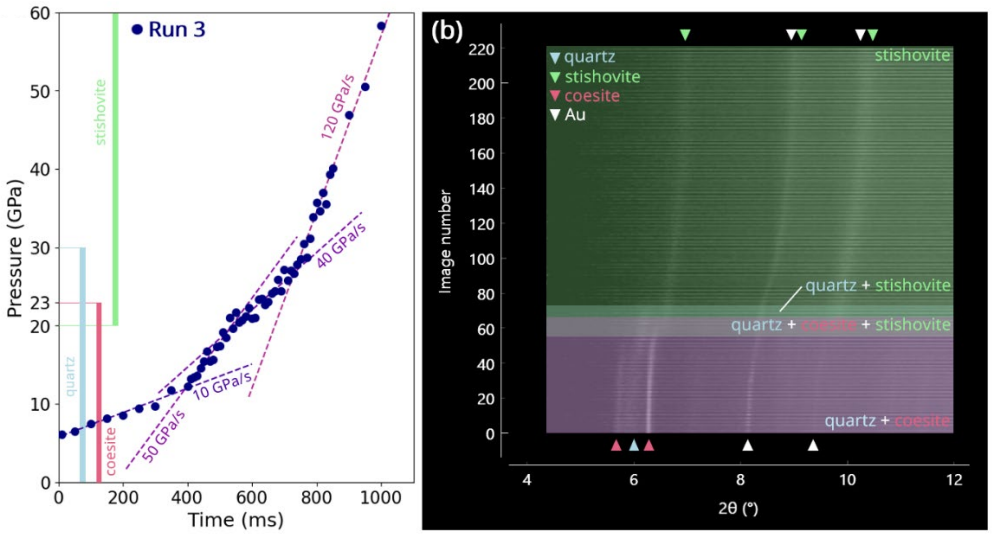
Abstract

Asteroid impacts are known to have played a crucial role in the early stages of our planet, being involved in the formation of the Earth – Moon system and in the delivery of water. Therefore, the study of the remaining traces of such events on the Earth's surface is a key to understand its evolution to the present day. Since quartz (SiO_2) is an abundant component of the Earth's lithosphere, fingerprints of shock in its crystallographic structure are nowadays routinely used as impact barometer, by comparing the composition of the shocked sample with SiO_2 polymorphs stable at extreme pressure and temperature conditions.

Upon compression, quartz undergoes solid – solid phase transitions into a wide variety of polymorphs. Among them, *coesite* is stable in the range 2 – 10 GPa, while *stishovite*, is stable in the span 10 – 80 GPa. In natural shocked silica samples, high contents of coesite and stishovite can be found, but the way they form under such conditions remains to this day elusive and cannot be fully explained experimentally. Investigating the behaviour of quartz upon fast compression is therefore essential to understand the presence of these polymorphs in natural shocked samples.

In our work we performed isothermal, rapid compression ramps in the range 10 – 1000 GPa/s with m-DACs, to bridge the gap between the low and the ultrafast compression rates investigated so far, and to reach timescales comparable to those of natural impacts. Using time-resolved X-ray diffraction (XRD), we were able to follow the structural changes in the sample throughout the compression ramp.
Our results show direct transformation of quartz into stishovite, by-passing coesite, alongside clear extension of metastability of quartz toward higher pressures (Fig. **1**). It is at odds with the composition of natural shocked silica sample showing high contents of coesite and it rules out the direct transformation of quartz into coesite upon compression during the impact. Possible explanations may involve amorphization and back-transformation into coesite on pressure release, and post-shock temperature increase.



1. Left : pressure vs. time curve during an experimental run. Vertical rods represent the metastability domains of the SiO_2 polymorphs upon compression. Right : Colormap of XRD patterns collected along the experimental run. Coloured areas represent the metastability domains of the SiO_2 polymorphs.

Experimental X-ray Studies of Liquid Polymorphism

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Max GERIN (ESRF,FR),
Laura HENRY (SOLEIL, FR),
Martin DEMOUCRON (ESRF, FR),
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Ciprian G. PRUTEANU (Edinburgh Univ, UK).

Abstract

The liquid-liquid transition (LLT) is a rare and intriguing phenomenon is which a single-component liquid transforms into another one via a first-order transition. Due to their counterintuitive nature, LLTs have intrigued scientists for many years and challenged our perception of the liquid state, for which the notion of polymorphism was long considered impossible. Since the early 1970's, LLTs have been predicted from computer simulations of several systems, and heavily debated in the case of water. So far though, experimental evidence remain scarce and often controversial as they mostly concern supercooled, i.e. metastable, liquids. Meanwhile, our understanding of the LLT remains quite primitive, and there is no theory able to predict whether a given system will exhibit this phenomenon.

Clear, in situ evidence of a LLT in the stable liquid domain have so far been obtained in two cases, phosphorus [1-3] and sulfur [4]. In both cases, this was established by investigating the high-pressure, high temperature liquids using synchrotron x-ray sources. By combining several x-ray-based techniques, important information may be accessed, such as the liquid structure, its density and density-contrast images of phase coexistence which can firmly establish the occurrence of a LLT.

In this talk, I will present results obtained by our consortium from recent experiments at the ID27 beamline of ESRF and PSICHE beamline of SOLEIL. Both beamlines have made large efforts to develop and implement instrumental and analytical tools for the investigation of disordered systems under high pressure [5,6]. After reviewing these techniques, I will present and discuss our experimental data obtained on two systems, realgar (As_4S_4) [7] and As-P alloys.

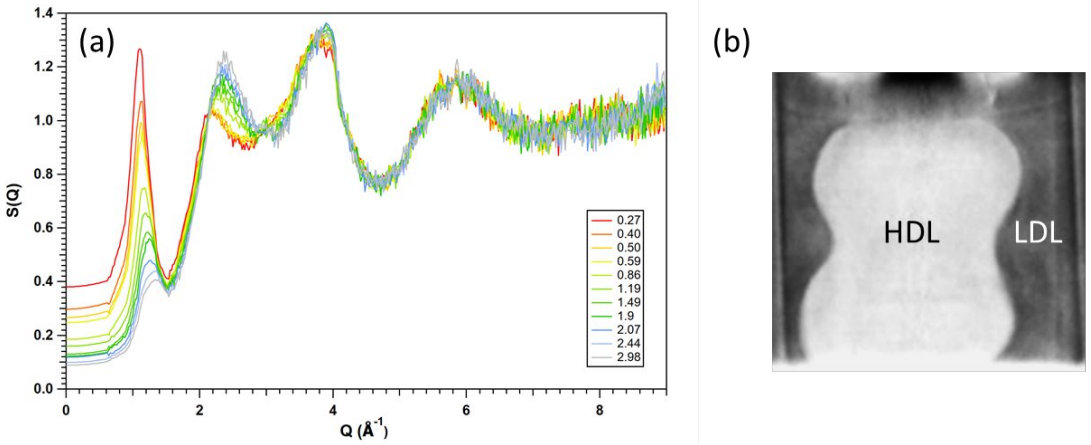

Figure 1: (a) Structure factor of liquid As_4S_4 as a function of pressure extracted from x-ray diffraction data collected at ESRF ID27. (b) Slice of a 3D tomography made at SOLEIL PSICHE, of a As-P liquid sample inside the Paris-Edinburg press, showing the coexistence of two liquids with low (LDL) and high (HDL) densities.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T7.1-O2 Simple Systems and Experiments at extreme conditions

Raman fingerprint of high-temperature superconductivity in compressed hydrides

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Lara BENFATTO (La Sapienza university, Italy)
Gaston GARBARINO (ESRF, France)
Francesco MAURI (La Sapienza university, Italy)
Federico Aiace GORELLI (HPSTAR and SHARPS, China)

Abstract (do not remove this word, but do remove all text between parentheses)

The discovery of high-temperature superconductivity in hydrogen-rich compounds under extreme

pressures [1, 2] has prompted great excitement, intense research, but also debate over the past decade. Electrical transport has been the primary diagnostic tool for identifying superconductivity in these systems, whereas complementary probes, including magnetic, spectroscopic, tunnelling and ultrafast methods, can be qualitative due to experimental constraints and sample heterogeneity [3–7]. Recent concerns over their reliability have fuelled controversy, leading to scepticism [8, 9] and pointing out the need for alternative, quantitative approaches [10, 11]. In this study, we acquired unprecedented high-quality Raman spectra of hexagonal LaH10 at approximately 145 GPa and low temperatures, in conjunction with electrical transport measurements. Upon cooling, we observe a drop of resistivity and simultaneous remarkable variations of phonon frequencies and linewidths. These effects are interpreted and well reproduced by the Migdal–Eliashberg theory, providing strong evidences of phonon-mediated superconductivity and enabling a quantitative determination of the superconducting energy gap. Our results establish Raman spectroscopy as a robust, contact-free probe with micrometric resolution for studying high temperature superconductivity, opening a powerful route to its discovery and characterization.

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Probing superconductivity at very low temperature and high pressure using NV centers in diamond

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Abstract

High pressure enhances quantum properties of materials such as the superconductivity of cuprates[1], nickelates[2] and superhydrides[3]. The diamond anvil cell (DAC) is a tool that allows to create pressure comparable to those existing in the Earth core, above the megabar range (100 GPa). However, it sets heavy constraints on the methods available for in-situ characterization. By implanting nitrogen-vacancy (NV) centers on the tip of a diamond anvil, we demonstrated that it is possible to study high pressure magnetic or superconducting phase transitions with high sensitivity and micrometer spatial resolution. In the case of superconductivity, we can probe and map the expulsion of an external magnetic field when the temperature decreases below the critical temperature, also called Meissner effect[4].

In collaboration with Attocube Systems AG (Germany), we have developed an original, high-performance and versatile experimental platform for studying superconductivity of materials at high pressure and very low temperature (starting at 4K). The platform is an optical, closed-cycle Helium cryostat compatible with membrane DACs, providing a precise and independent control of pressure and temperature. Moreover, it is equipped with a 500 mT vector superconducting magnet.

We present critical temperature measurements performed on a MgB_2 powder at high pressure using this platform. We observe a linear decrease of the critical temperature with pressure from 35 K at 0 GPa down to 14 K at 25 GPa, in agreement with the literature[5]. Above 25 GPa, the superconducting phase of MgB_2 seems to disappear, according to our current measurements. Further measurements will be performed to study in detail this process.

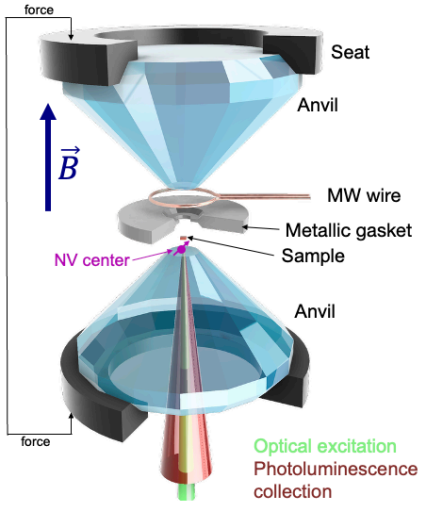

Figure 1. Scheme of the DAC, showing the main components and sample configuration.

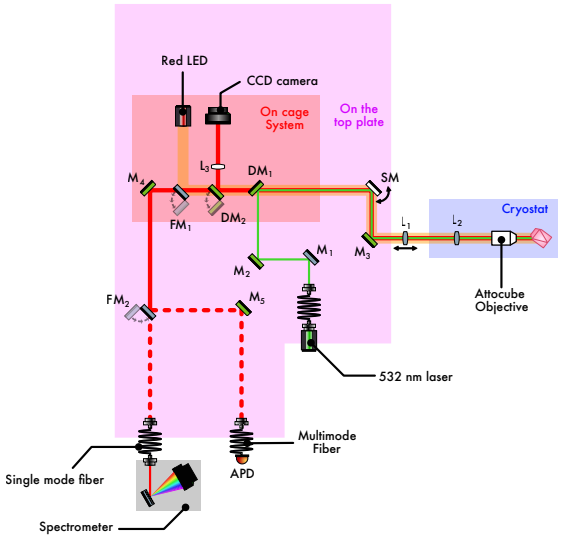

Figure 2. Scheme of the experimental setup.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T7.1-O4 Simple Systems and Experiments at extreme conditions

From diamond to BC8 to simple cubic and back: Kinetic pathways to post-diamond carbon phases from metadynamics

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Abstract

Understanding the kinetic pathways connecting carbon polymorphs at multimegabar pressures remains a major unsolved problem in high-pressure physics. Here, we provide insights into the long-standing question of BC8 formation and stability by combining a state-of-the-art SNAP machine-learning interatomic potential with enhanced sampling via metadynamics, enabling direct access to transition mechanisms far beyond the reach of standard molecular dynamics. Our simulations show that carbon phase transformations are intrinsically complex, proceeding through multiple intermediate disordered and crystalline states governed by nontrivial kinetic ordering. We determine the upper pressure limit for BC8 formation and reveal that hexagonal diamond transforms to BC8 faster than cubic diamond—an unexpected and experimentally testable prediction. We also identify a *P*222 carbon phase that becomes competitive with diamond and simple cubic above 1.8 TPa, and we demonstrate that BC8 may be quenched to ambient conditions at moderate temperatures. Together, these results establish a general and transferable framework for resolving kinetic pathways in solid-solid phase transitions and provide physical insights into carbon's complex high-pressure landscape.

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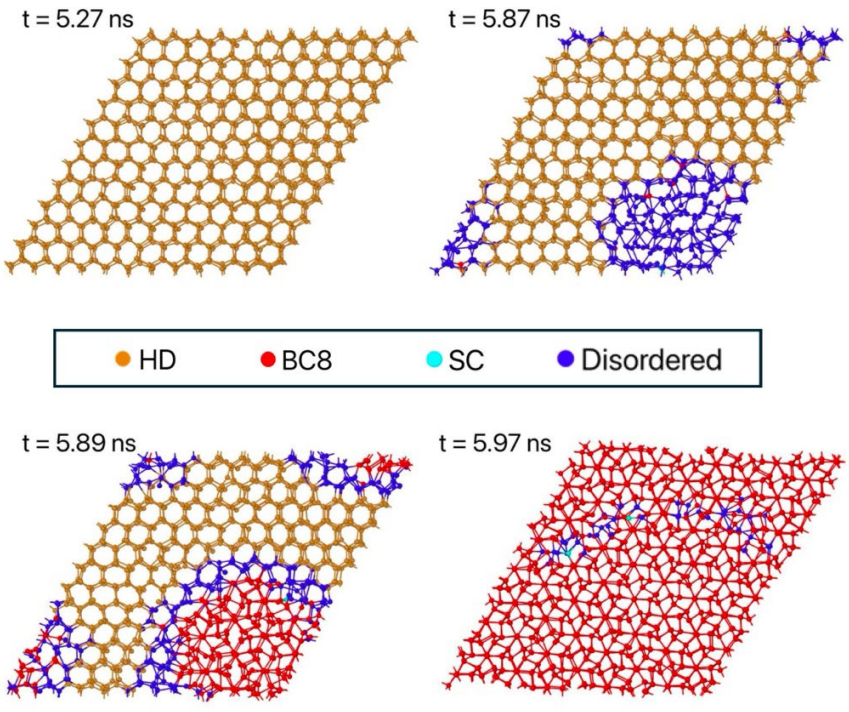

Transition from hexagonal diamond to BC8.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T7.1-O5 Simple Systems and Experiments at extreme conditions

High pressure studies of dense oxygen and nitrogen binary mixtures

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Abstract

Through a series of high-pressure Raman scattering and x-ray diffraction experiments on N_2-O_2 binary mixtures with oxygen concentrations varying from 10% to 77%, we systematically explore the molecular interactions of the mixtures. Our study widely extended the room-temperature phase diagram for the N_2-O_2 system from 12 GPa to ~60 GPa for all concentrations and up to ~160 GPa for 28% of oxygen.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T7.2-O1 Simple Systems and Experiments at extreme conditions

MICROSCOPIC INVESTIGATION OF LASER SHOCKED GLASSY GEO_2

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J.A. Hernandez Colonna (ESRF, FR),
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T. Vinci (Ecole Polytechnique, FR),
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Abstract
Germanium dioxide (GeO_2) is an important structural and chemical analogue of SiO_2. Investigating GeO_2 can be advantageous thanks to its simple phase diagram under moderate (<100 GPa) static P, T conditions[1] and being more accessible to hard X-rays synchrotron techniques.
However, the analogy between GeO_2 and SiO_2 is still not fully established at more extreme and dynamic conditions. In particular, none of the GeO2 polymorphs – quartz, rutile and glass – has been investigated under dynamic P, T conditions using X-rays microprobes.
In this study, we have explored the structural and electronic evolution of glassy GeO_2 under laser-driven shock compression at High Power Laser Facility (HPLF) of the ESRF[2], up to 200GPa and 15000K, by ultrafast (100 ps) X-ray Absorption (XAS) measurements.
Online VISAR diagnostics and hydrodynamic simulations using the MULTI code, provide the pressure–temperature conditions reached along the Hugoniot and along release states. The XAS spectra reveal clear modifications of the local atomic structure, consistent with an increase in Ge coordination under compression. In parallel, we observe marked changes in the electronic structure and optical properties, indicating a progressive closure of the band gap.
These observations are supported by Principal Component Analysis (PCA), used to identify distinct structural regimes along the compression path, Fig. 1, and DFT-MD simulations, which reproduce the evolution of the electronic density of states and provide insight into the microscopic mechanisms driving the gap closure.
Our results provide the first direct microstructural constraints on glassy GeO_2 under dynamic compression up to 200GPa and establish ultrafast XAS as a powerful tool to probe structural and electronic evolution under extreme conditions.

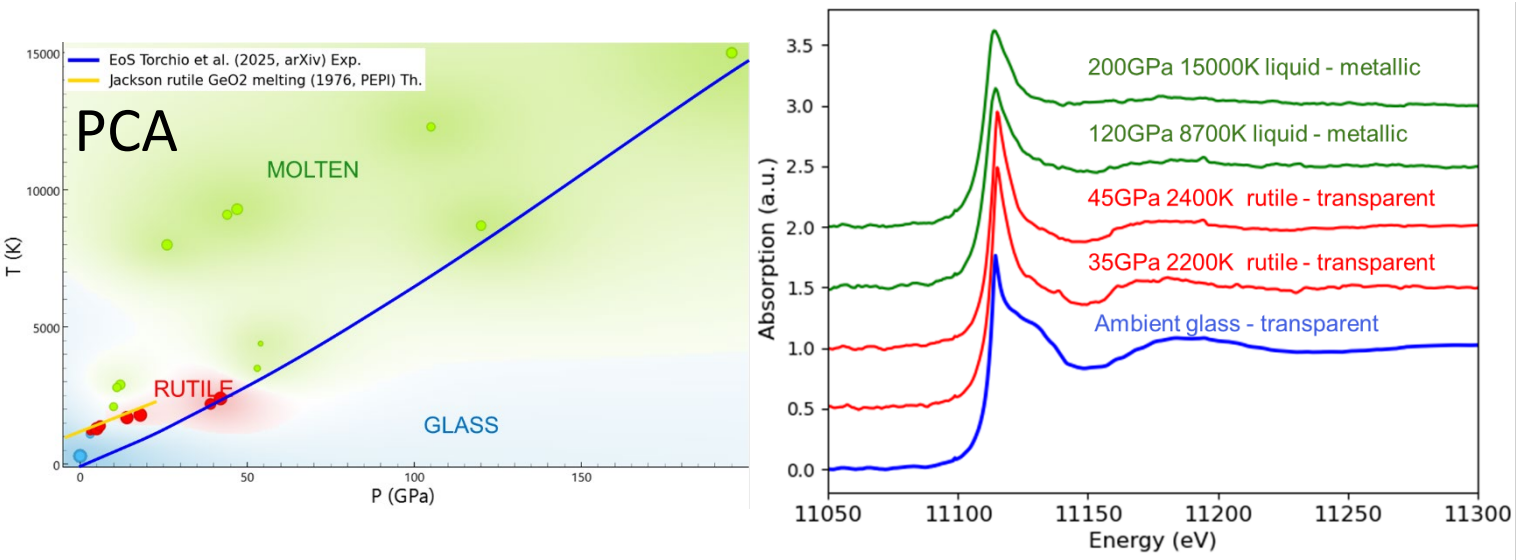

Fig. 1

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Nanosecond timescale plasticity in shock-compressed polycrystalline MgO up to pressures above 100 GPa

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, 110 participants involved in HIBEF Priority access granted beamtime #6659 [3)],

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Abstract

MgO is an important industrial ceramic and serves as a model for experimental and computational studies of mechanical behaviour. At very low strain rates (10^{-16} /s) and high pressures, the slow diffusion of oxygen impedes dislocation recovery and strengthens MgO dramatically [1]. At high pressures above 50 GPa, a change in deformation mechanism is also predicted where the slip system changes from [110](110) to [110](100) [2]. Here, we focus on the mechanical behaviour of dynamically compressed MgO at conditions up to 150 (20) GPa and 2000 (300)K. We use laser shock compression along with ultra-fast diagnostics at the HED sector of the European XFEL to probe how the rapidly changing pressure-temperature conditions affect microstructures in shock-compressed polycrystalline MgO. These observations, coupled with elasto-viscoplastic self-consistent (EVPSC) simulations, unequivocally prove that MgO attains plastic regime in the nano-seconds scale which we successfully study and model in terms of strength and deformation mechanisms. The experiments point to a rich intricate mechanical behaviour in shocked polycrystalline ceramics for the first time based on in-situ XRD measurements at the nanosecond timescale. The method may have profound impact on studies of plastic behavior of ceramics under high P/T conditions, including the viscosity and rheological behaviour of Earth and Earth-like exo-planets.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T7.2-O3 Simple Systems and Experiments at extreme conditions

Combined Strain- and Stress-Induced Phase Transformations and Microstructure Evolution under High Pressure

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Abstract

Phase transformations (PTs) under plastic compression and compression and torsion, using metallic or ceramic anvils (which are traditional for high-pressure torsion) or a diamond anvil cell (DAC) and a rotational DAC (RDAC), are referred to as plastic strain-induced PTs under high pressure [1]. They require completely different thermodynamic and kinetic descriptions and experimental characterization than pressure-induced PTs (under hydrostatic loading) and stress-induced PTs (with external stresses below the yield strength). Since strain-induced PTs stop when plastic straining stops, it is generally accepted that their kinetics is determined by plastic strain rather than time; time is not an important parameter [1].

However, recently, the *time dependence of strain-induced PT* in DAC at constant plastic strain was revealed with in situ x-ray diffraction studies on α-ω PT in Zr at room temperature [2]. After nucleation, the high-pressure phase grows over the next hour until reaching a steady state. This was formalized via two similar strain-controlled kinetic equations for the instantaneous and steady-state volume fractions of the high-pressure phase *c*, connected by Arrhenius-type thermally activated growth kinetics.

Also, during torsion in dynamic RDAC of Fe-7%Mn alloy at 1,000 and 1,500 RPM (strain rate up to $2 \cdot 10^3$/s), which causes BCC→HCP PT, the volume fraction of the HCP phase *c* does not change. After torsion stops, *c* increases by 30% within a few minutes after 1,000 RPM and *c*→0 after 1,500 RPM [3]. Thus, nuclei of the HCP phase are generated during straining at high strain rate, but growth or disappearance occurs on a few-minute time scale under stress, depending on the local pressure. Crystallite size, microstrain, and dislocation density also continue to evolve after torsion stops.

These results imply that a combined theory of plastic strain- and stress-induced PTs and microstructure evolution under high pressure, accounting for the effect of plastic strain rate, must be developed. Phase-field simulations also show that, after nucleation of a high-pressure phase at the tip of a strain-induced dislocation pileup, high-pressure regions grow and coalesce at a fixed plastic shear [4]. Also, steady state *c* and phase microstructure for almost every interface and for the entire polycrystalline sample are determined by the phase equilibrium criterion for stress-induced PTs, i.e., by stresses or (in the simplest case) applied pressure instead of plastic strains. This suggests an important hint and imposes a strong constraint on the future general theory for combined plastic strain- and stress-induced PTs. In fact, phase-field theory and simulations in [4] are an example of such a theory at the microscale, but macroscale thermodynamic and kinetic approaches, generalizing those in [1], are to be developed.

Independently, plastic straining has a strong effect on both direct and reverse BCC↔HCP PT in Fe-7%Mn alloy, which leads to the simultaneous occurrence of the direct and reverse PTs in the pressure range 3.20 GPa < p < 6.17 GPa. The kinetic equation for strain-induced PTs, which takes into account both direct and reverse PTs, admits a steady solution depending on pressure. It describes well the experimental results for the BCC↔HCP PT in the Fe-7%Mn alloy, which allows the determination of the material parameters in this equation.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T7.2-O4 Simple Systems and Experiments at extreme conditions

Compositions, structures, and properties of chlorides system under high pressure

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Xiao DONG (Nankai University, China)

Abstract

With the rapid development of high-pressure techniques and computational methods, research on chloride systems has expanded to unconventional stoichiometries, leading to new materials with novel electronic properties. This work employs high-pressure techniques to investigate the composition, structure, and properties of several representative chloride systems. (I) The Grüneisen parameter (γ), a key thermodynamic quantity describing anharmonic effects, connects different equations of state (isotherms, isentropes, Hugoniots). In view of slow progress in high-pressure γ measurements, we developed a technique using a dynamic diamond anvil cell (dDAC) combined with a fast signal acquisition system. Using this method, we determined γ of NaCl at room temperature over a broad pressure range (3.80–21.33 GPa) for the first time and successfully derived its Hugoniot curve. (II) Calcium–chlorine system under high pressure (0–100 GPa) was investigated by theoretical simulations and experiments. Calculations show that CaCl, Ca_5Cl_6 and Ca_3Cl_4 are stable under high pressure and contain monovalent calcium ions. Using a laser-heated diamond anvil cell, we synthesized CaCl and obtained its high-pressure isothermal compression curve. (III) We identified a stable chlorine-rich compound, $CaCl_3$, which exhibits a Rubik's cube-like Fermi surface and quasi-flat bands in its band structure. Using a tight-binding model, we show that the unique electronic properties originate from intrachain (nearest-neighbor) interactions within one-dimensional chlorine chains.

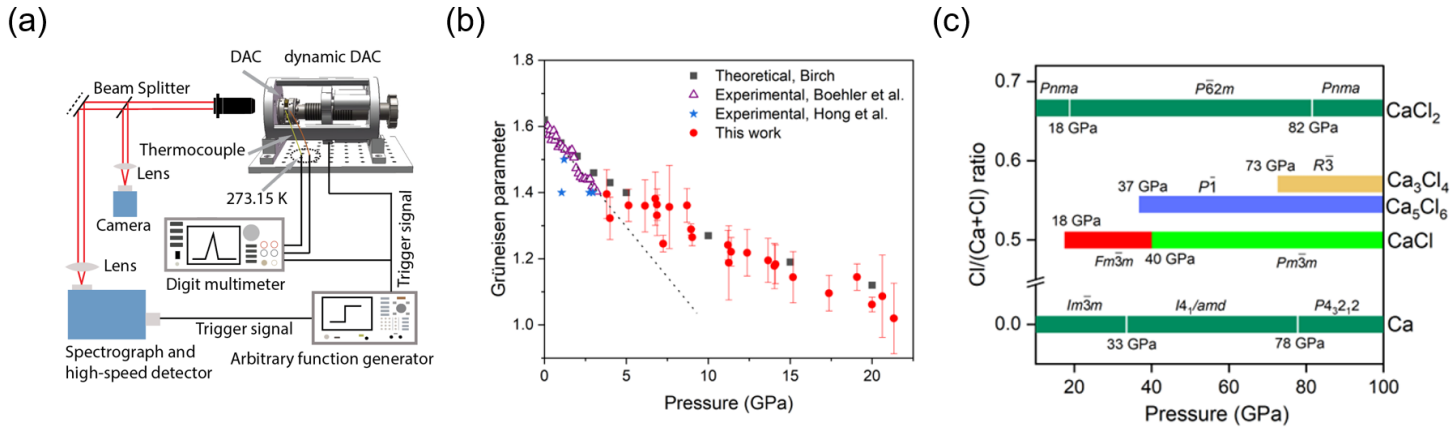

Figure1 (a) Schematic illustration of the programmable automatic high pressure jump and temperature detection apparatus. (b) Grüneisen parameter vs. pressure for sodium chloride from our data and previously published data. We measured the Grüneisen parameters in a wide pressure range. The dashed line is the extrapolation from the previous experimental data. (c) Phase diagram of calcium-chlorine system.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T7.2-O5 Simple Systems and Experiments at extreme conditions

Phosphorus-Doped N-Type Diamond Semiconductors through High-Pressure Thermal Diffusion

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Abstract

Diamond is known as the ultimate semiconductor due to its outstanding physical properties. However, the dense carbon atomic arrangement in its lattice and the relatively large doping atom radius make n-type doping highly challenging and result in poor electrical performance, which remains a major technical bottleneck for the application of diamond semiconductor materials. The report will introduce the high-pressure thermal diffusion method for n-type doping of diamond single crystals, which employs a high-pressure environment to significantly reduce the volume difference between phosphorus atoms and carbon atoms in the diamond lattice. The proposed high-pressure thermal diffusion method can achieve effective doping and ionization of phosphorus atoms in the lattice of diamond. The prepared phosphorus doped diamond exhibits the lowest resistivity (2 Ω.cm) and highest electron concentration (2.3×10^{18} cm^{-3}) observed in any known phosphorus doped diamond single crystal at room temperature. The high-pressure thermal diffusion method will provide an effective new technology for n-type doping of diamond, which is expected to play an important role in the design and preparation of diamond based semiconductor devices in the future.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T7.2-O6 Simple Systems and Experiments at extreme conditions

Thermoelastic properties of liquid Bi determined by picosecond acoustics

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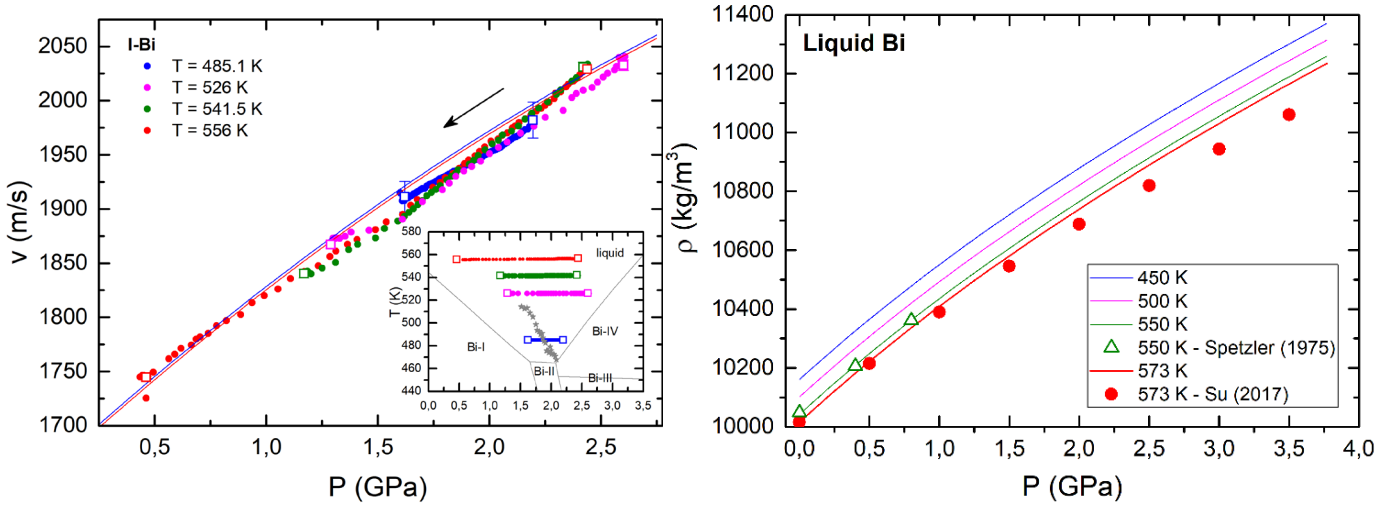
Abstract

Bismuth (Bi) has attracted considerable attention over the years due to its unique properties at high pressure and temperature. Among these, abnormal behaviour has been observed in the liquid state, possibly linked to a reversible liquid-liquid transition (LLT) [1]. To investigate this transition, picosecond acoustics measurements were performed on liquid Bi confined in diamond anvil cell [2, 3], up to 4 GPa and in the range of 450-600 K. Sound velocity measurements in the liquid state were extended in the metastable regime, several tens of K below the melting line. From these sound velocity data, we derived the equation of state of the liquid ρ(p,T) and other thermodynamic quantities such as the bulk modulus B_T or the isobaric specific heat C_p. Our experimental results reveal no significant anomalies in the thermo-elastic properties of liquid Bi across the investigated $p-T$ range. Specifically, our findings do not support the existence of a liquid-liquid structural transition, either above or below the melting line.



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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T8.1-O1 Spectroscopic and Structural studies

Infrared spectroscopy studies of perovskite oxides at high pressures

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Abstract

Phonon studies are fundamental to the understanding of the physics at play in perovskite oxides. In the laboratory, Raman and infrared spectroscopies are the most commonly implemented techniques for that purpose; they are now routinely carried out as a function of temperature with (nearly) equal ease. When it comes to high-pressure studies however, they are still unequal. Raman spectroscopy has been overall more easily implemented with diamond-anvil cells and is now routinely performed in the lab or at large facilities up to the Mbar and beyond. In contrast, measuring infrared spectra under pressure *in the phonon range* has been more challenging for a number of reasons, some rather mundane – such as the need for proper references, and some more fundamental – such as the diffraction limit that sets a minimum size for samples and therefore caps the maximum pressure reasonably achievable.

In this contribution, I will provide a summary of several infrared spectroscopy studies at high pressures performed by our group on the AILES beamline at the SOLEIL synchrotron source. Our original motivation, the direct observation of polar soft modes at high pressures has been challenging. However, along the way through many experiments carried out on a number of classical perovskite oxides, ferroelectric or not ($BaZrO_3$, $PbTiO_3$, $KNbO_3$), and other compounds up to a maximum pressure of 70 GPa, we have learnt a number of useful lessons. The antiferrodistortive transition Pm-3m → I4mcm common to so many perovskites and the associated mode activations will be given a particular focus.

Re-emergence of a polar instability at high pressure in $KNbO_3$

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Pierre RODIERE, Pierre BOUVIER (Institut Néel CNRS/UGA, Grenoble, France),
Björn WEHINGER, Gaston GARBARINO, Mohamed MEZOUAR (ESRF, Grenoble, France),
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Mael GUENNOU (University of Luxembourg, Luxembourg)

Abstract

Ferroelectricity in perovskites is generally suppressed under moderate hydrostatic pressure, yet first-principles calculations have long predicted a re-emergence of the polar instability at higher pressures. Experimental confirmation of this prediction has remained elusive. Here, we investigate the high-pressure behaviour of the lead-free ferroelectric perovskite $KNbO_3$ up to 63 GPa using single-crystal X-ray diffraction at the ESRF and SOLEIL synchrotron sources, complemented by Raman and infrared spectroscopy and second-harmonic generation (SHG) imaging. Following the known ferroelectric-to-cubic transition near 14 GPa, we identify two further high-pressure phase transitions. At 37 GPa, the emergence of superlattice reflections at the R point signals a transition to a tetragonal I4/mcm phase with anti-phase octahedral tilts. At 44.6 GPa, incommensurate satellite reflections appear, and structural refinements in superspace reveal a monoclinic modulated phase I2/c(0σ1σ2)0s combining displacements of both K and Nb cations with additional octahedral tilts. Soft modes associated with the tilt instability and the incommensurate modulation are clearly observed in Raman spectra, alongside persistent order-disorder signatures consistent with the known character of $KNbO_3$. SHG measurements confirm that the incommensurate phase remains centrosymmetric, indicating that the re-emergent polar instability does not lead to a macroscopically ferroelectric state but is instead frustrated by competition with the tilt instability. This work provides direct experimental evidence for the theoretically predicted high-pressure polar instability in a lead-free perovskite and highlights the role of order-disorder character and tolerance factor in enabling such a coexistence of competing structural instabilities.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T8.1-O3 Spectroscopic and Structural studies

Probing pressure-induced structural evolution and its impact on the optical behavior of the vacancy-ordered halide double perovskite Rb_2TeBr_6

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Goutam Dev MUKHERJEE (IISER Kolkata, India)

Abstract

We investigate the pressure-induced structural and optical evolution of Rb_2TeBr_6, a lead-free halide perovskite derivative, using synchrotron X-ray diffraction, Raman spectroscopy, photoluminescence (PL), and optical absorption measurements. At ambient conditions, Rb_2TeBr_6 crystallizes in a cubic Fm-3m structure that remains stable below 8.0 GPa. Within this pressure range, subtle inter-octahedral rotations emerge, leading to localized deviations from the ideal cubic framework. This pressure-induced octahedral reorientation enhances radiative recombination, resulting in a pronounced increase in PL intensity up to 2.4 GPa, followed by gradual PL quenching due to the activation of nonradiative relaxation pathways at higher pressures. Upon further compression, Rb_2TeBr_6 undergoes a structural transition to an orthorhombic Pnnm phase near 8.0 GPa, followed by a lower symmetry phase above 10.7 GPa and eventual amorphization beyond 25.5 GPa. Optical absorption measurements reveal continuous band-gap narrowing with increasing pressure. These results demonstrate a strong interplay between lattice dynamics, electronic structure, and optical properties in Rb_2TeBr_6, highlighting its potential as a pressure-tunable material for advanced optoelectronic applications.

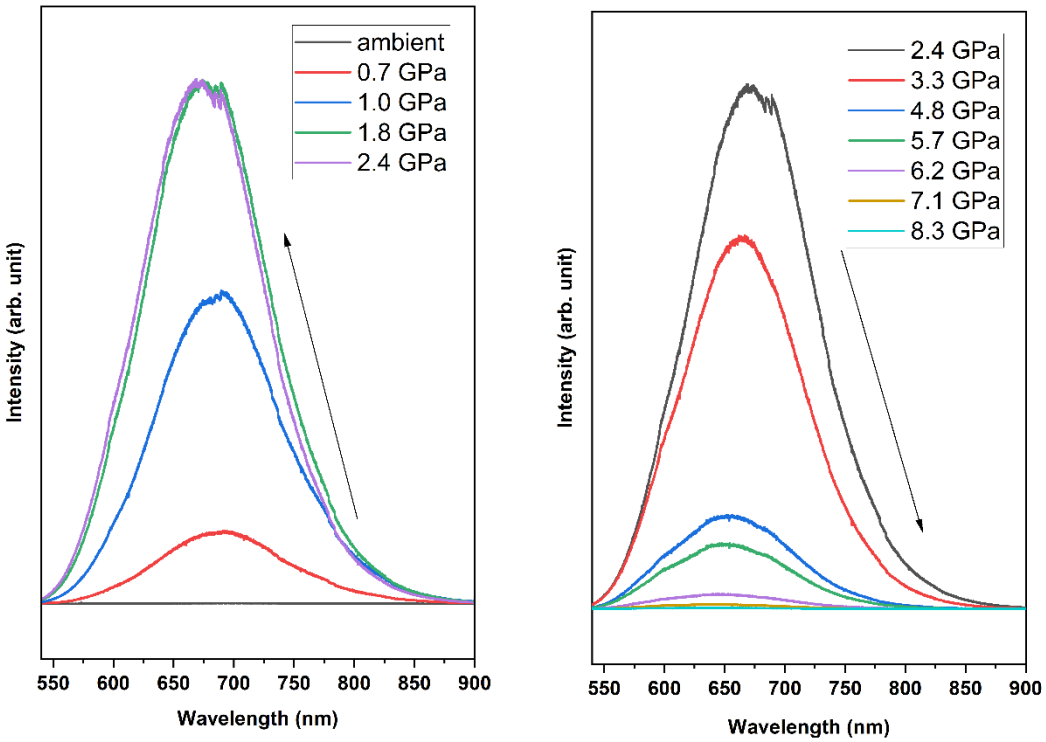

Figure: Photoluminescence (PL) spectra of Rb_2TeBr_6 at selected pressures, showing PL enhancement up to ~2.4 GPa followed by gradual quenching with further compression.

Pressure-enhanced ferromagnetism in Cs_2CrCl_4 studied by optical spectroscopy

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Abstract

Cs_2CrCl_4 is a rare transparent ferromagnet (T_C = 52 K)[1] whose magnetic ordering arises from a cooperative Jahn-Teller (JT) effect. This effect stabilizes an in-plane antiferrodistortive (AFD) Ruddlesden−Popper-type perovskite structure (*Cmca*)[2]. Within this structure, Cr^{2+} ($3d^4$) ions exhibit a strong JT distortion, forming $CrCl_6^{4-}$ octahedra with alternating short (R_s = 2.39 Å) and long (R_l = 2.79 Å) Cr-Cl bonds in the plane (Figure 1). This configuration leads to orbital ordering that maximizes ferromagnetic (FM) Cr^{2+}–Cr^{2+} superexchange coupling by directing the half-occupied dz^2 orbitals of each ion toward the empty dx^2-y^2 orbitals of its neighboring Cr^{2+} ions.

Despite early optical studies on A_2CrCl_4 (*A*: K, Rb), their pressure-dependent behavior remains entirely unexplored. Pressure offers a clean tuning parameter to modify the in-plane JT distortion or to induce octahedral tilting–the former favoring FM coupling, the latter AFM coupling.[3,4] We present the first high-pressure optical absorption study on Cs_2CrCl_4.

Two spin-flip transitions ($^5B_{1g}(^5D) \rightarrow {}^3B_{1g}(^3G)$ and $^3A_{1g}(^3H)$), both parity- and spin-forbidden electric dipole transitions in the isolated ion, become weakly allowed via spin-dependent exchange mechanism[5], making their intensity a sensitive probe of magnetic exchange. These transitions show a strong temperature dependence with associated oscillator strengths increasing from $f \sim 10^{-8}$ at 4.2 K to $f \sim 10^{-5}$ at room temperature. In Cs_2CrCl_4, pressure increases the intensity of these peaks, consistent with DFT simulations showing enhanced exchange interaction upon compression. This behavior **contrasts sharply** with isostructural Mn^{3+} layered perovskites ($AMnF_4$, *A*: Na, Cs), where analogous spin-flip peaks decrease in intensity with pressure due to pressure-induced tilting of the JT-distorted MnF_6^{3-} octahedra reducing the exchange mechanism.

Our results establish a direct magneto-optical correlation under high pressure and highlight optical spectroscopy as a powerful tool for probing pressure-driven magnetic transitions in JT-distorted layered perovskites. A full account will be presented at the EHPRG Meeting.

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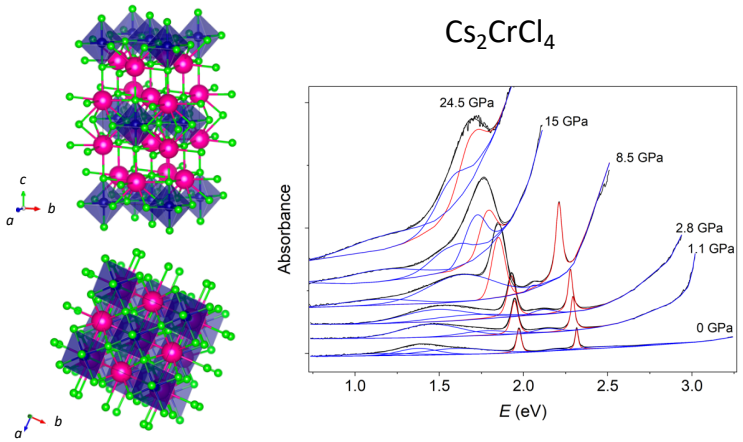

Figure 1.
(Left side) Orthorhombic crystal structure of the layered perovskite Cs_2CrCl_4 (*Pbca*) showing the antiferrodistortive Jahn-Teller-distorted $CrCl_6^{4-}$ octahedra.
(Right side) Pressure dependence of the optical absorption spectrum at room temperature. The spin-flip peaks (in red) increase their intensity with pressure, together with the progressive reduction in charge-transfer band gap energy.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T8.1-O5 Spectroscopic and Structural studies

Pressure-Induced Structural and Optoelectronic Modulations in 2D Dion-Jacobson Hybrid Lead Iodide Perovskites with a Rigid Spacer

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Abstract

Two-dimensional hybrid organic-inorganic perovskites (HOIPs) are known for their enhanced chemical and thermal stability relative to three-dimensional variants, positioning them as promising materials for advanced optoelectronic applications. External pressure provides an effective route to modify their structures and tune their optoelectronic responses. This study examines the high-pressure behavior of the Dion-Jacobson 2D HOIP DPDAPbI□, which incorporates the rigid organic spacer N,N-dimethylphenylene-p-diammonium (DPDA). Combining photoluminescence, UV-visible absorption, vibrational spectroscopy, and in situ synchrotron powder X-ray diffraction, we identify an isostructural phase transition near 1.5 GPa, marked by a pronounced change in photoluminescence intensity linked to free-exciton emission. Synchrotron X-ray diffraction reveals significant anisotropic compression along the c-axis, while structural analysis indicates the rare occurrence of reduced lead-iodide octahedral distortion below 2 GPa, contrasting with the increased octahedral distortion commonly reported in lead-based 2D HOIPs. Density functional theory calculations elucidate the structural origins and mechanisms driving the pressure-induced phase transition and optoelectronic tuning. These findings highlight the critical interplay between rigid organic spacers and inorganic octahedra in modulating high-pressure optoelectronic properties, offering design insights for future 2D HOIPs with tailored functionalities.

Keywords: 2D hybrid organic-inorganic perovskites; Dion-Jacobson; high pressure; photoluminescence; UV-visible absorption; octahedral distortion; bandgap

X-Ray Pump-Probe Study of Diamond Formation with and without Color Centers

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Abstract

Renowned for its exceptional hardness and unique properties, diamond holds immense promise for diverse technological applications spanning mechanics, electronics, and photonics. Color centers, impurities formed by vacancies in the diamond lattice, introduce additional electronic states within the wide bandgap, making diamond suitable for quantum technology applications. In particular, with negatively charged silicon-vacancy (SiV) centers are emerging as promising single-photon emitters due to their narrow zero-phonon line transition at 738 nm. [1] An efficient method to synthesize diamond, with or without SiV centers, is the high-pressure high-temperature (HPHT) method. Identifying ideal precursors and understanding the kinetics of the phase transitions and the Si incorporation mechanism in the lattice are essential to fully exploit this method. [2] Diamondoids, consisting of hydrogen-terminated carbon cages superimposable on the diamond lattice, emerge as promising candidates for synthesizing high-quality diamond and exhibit lower pressure–temperature (P–T) thresholds compared to other hydrocarbons for diamond formation. [3] Moreover, adamantane, the smallest diamondoid with the chemical formula $C_{10}H_{16}$, can be functionalized with Si atoms (AdaSi) and used as a precursor for SiV center formation. [4] Despite these advances, the time-resolved structural dynamics of diamond and color center formation remain underexplored.

We recently performed time-resolved X-ray pump–probe experiments on compressed diamondoids utilizing 2.2 MHz X-ray pulse trains at the High Energy Density (HED) instrument of the European X-ray Free-Electron Laser Facility (EuXFEL).[5] We heated pure diamondoids, including adamantane, and an Si-functionalized AdaSi sample in a diamond anvil cell using trains of 200 ultrashort X-ray pulses, each 25 fs in duration with a 443 ns interpulse spacing, delivering high pulse energy and brightness. Submicrosecond temporal resolution X-ray diffraction (XRD) patterns revealed the formation dynamics and conditions of diamond across five samples at high pressures ranging from 13 to 20 GPa. The fastest diamond nucleation was observed in pure triamantane, where diamond was detected at around 30 μs at 19 GPa. We also determined energy and energy-delivery-rate thresholds for SiV formation in AdaSi samples, which show a strong pressure dependence, requiring higher energies at lower pressures. Post-recovery XRD and Raman spectroscopy revealed various carbon-based products, including graphite and amorphous carbon, while photoluminescence confirmed the presence of SiV centers. This study provides an ultrafast, *in situ* perspective on diamondoid-to-diamond conversion and SiV center incorporation, offering insights for developing efficient synthesis routes for color centers targeting a wide range of technological applications.

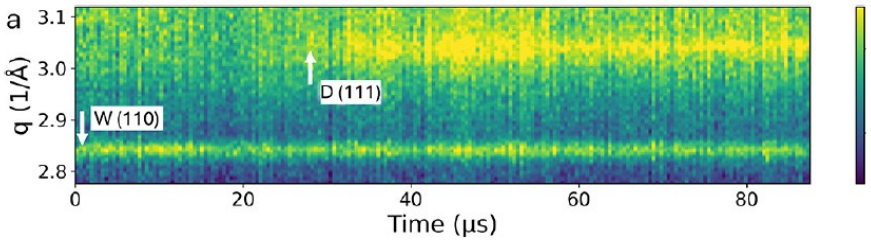

Figure 1. Batch view of 200 XRD patterns from the pulsed X-ray train with a 443 ns interpulse spacing, showing the emergence of the diamond (111) peak at approximately 27 μs (run 605). The onset of the diamond (111) peak is labeled “D (111)” and the tungsten (110) peak is labeled “W (110)”, with arrows indicating both. [5]

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T8.2-O1 Spectroscopic and Structural studies

Hydrated Carbonates under Pressure

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Abstract

Hydrated carbonates play an important role in the global carbon cycle and industrial carbon sequestration technologies. Understanding the fundamental crystallochemistry and mechanical properties of these minerals under different thermodynamic conditions is essential for predicting their phase stability. This work presents a comprehensive high-pressure investigation of two natural hydrated carbonates: the sodium sesquicarbonate trona ($Na_3H(CO_3)_2.2H_2O$) and the trihydrated magnesium carbonate nesquehonite ($MgCO_3.3H_2O$), and of a hydrated silicate-carbonate Y-kainosite ($Ca_2Y_2Si_4O_{12}(CO_3).H_2O$). Their high-pressure structural behavior was studied by a joint experimental and theoretical approach consisting of in-situ synchrotron single-crystal and powder X-ray diffraction (XRD) and complementary density functional theory (DFT) calculations.

Trona undergoes a phase transition at 12.8 GPa from its initial monoclinic structure to a dense triclinic polymorph. This phase transition was accompanied by an increase in the Sodium (Na) coordination number from 6 to 7–8. Nesquehonite, on the other hand, undergoes two pressure-induced phase transitions at the lower pressure thresholds of 2.4 GPa and 4 GPa, respectively. The transition to the second pressure-induced phase is marked by a distinctive coordination expansion of the Mg^{2+} cation from 6 to 7, forming distorted [MgO_7] pentagonal bipyramids. For Kainosite, the P-V data were fitted to the Birch–Murnaghan EOS to determine the bulk modulus: B_0 = 109.8(13) GPa. The effective coordination numbers of the Ca and Y atoms progressively increased with pressure, which entails the densification of the structure, due to the reorientation of [Si_2O_7] disilicate groups, the [CO_3] carbonate groups and the water molecules. The compressibility and anisotropy of low- and high-pressure phases were determined. Particularly interesting is the negative axial compressibility and negative thermal expansion observed in nesquehonite.

Across all the minerals, structural stability is observed to be heavily mediated by the dynamic reorganization of hydrogen-bonding networks. While trona exhibited 1D chain-like hydrogen bonding that reorganized into a localized 2D network at high pressure, nesquehonite's framework is sustained by highly directional 2D networks that accommodate significant polyhedral distortion. Together, these findings provide critical mechanistic insights into how pressure-induced coordination expansions and hydrogen-bond topologies dictate the stability of dense hydrated carbonate polymorphs in high-pressure environments.

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High-Pressure Multi-Probe Studies of Lithium-Ion Battery Materials

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Abstract

Recent advances in high-pressure and multi-probe characterization techniques offer new opportunities to investigate and engineer materials for next-generation lithium-based batteries. Pressure is a particularly powerful parameter because it can directly modify atomic arrangements, defect populations, microstructure, and transport properties, providing insight into structure–property relationships that are difficult to access under ambient conditions.

Our research employs a multiscale approach combining advanced synthesis, in situ high-pressure experiments, and complementary characterization methods to explore the response of battery materials under compression. Particular attention is given to understanding how pressure influences both structural order and functional properties in electrode and solid-electrolyte materials.

For the cathode material $LiNiO_2$, a promising cobalt-free positive electrode, in situ synchrotron X-ray diffraction and Raman spectroscopy measurements were performed in a diamond anvil cell up to 50 GPa. Compression induces significant modifications of the layered structure, including variations in Li/Ni cation mixing and local structural disorder. The results reveal a competition between pressure-induced ordering and disordering mechanisms: moderate compression stabilizes the layered framework, whereas higher pressures promote cation mixing and local distortions. These observations provide new insight into the structural stability of Ni-rich cathodes and the influence of lattice disorder on electrochemical performance.

Pressure also plays a key role in the processing and optimization of solid electrolytes for all-solid-state batteries. Using the UToPEc setup at the Psiché beamline of Synchrotron SOLEIL, we conducted in situ high-pressure sintering experiments on amorphous Li_3PS_4 and crystalline Li_6PS_5Cl under compressive stresses up to 3700 MPa (Thompson et al., Adv. Funct. Mater., 2026, DOI: 10.1002/adfm.75195). This unique platform enables the simultaneous acquisition of synchrotron X-ray diffraction, X-ray absorption tomography, density measurements, and electrochemical impedance spectroscopy. By correlating structural evolution, densification, and porosity changes with ionic conductivity, we identify the mechanisms governing pressure-assisted consolidation and ion transport.

Together, these studies demonstrate how pressure can be used both as a probe of fundamental structural behavior and as a processing tool for optimizing battery materials.

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135-kagome metals under pressure: Dimensionality crossover and Fermi surface reconstructions

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Abstract

Kagome metals provide a unique platform where nontrivial band topology (Dirac crossings, flat bands, and van Hove singularities) give rise to density-wave order and superconductivity [1,2]. The strong tunability of these electronic states by external parameters opens new perspectives to explore correlated and topological quantum phenomena. In this talk, I will compare the pressure evolution of three isostructural kagome metals, CsV_3Sb_5, $CsCr_3Sb_5$, and $CsTi_3Bi_5$, combining high-pressure single-crystal X-ray diffraction (XRD) with density functional theory calculations to establish a direct link between lattice evolution and electronic structure.

Despite sharing the same crystal structure, these compounds exhibit very different electronic behaviors that manifest distinctly under pressure. Transport studies reveal rich temperature–pressure phase diagrams. In CsV_3Sb_5, van Hove singularities near the Fermi energy drive a charge-density-wave (CDW) instability coexisting with superconductivity at ambient pressure. Upon compression, suppression of the CDW gives rise to a superconducting dome, followed by a reentrant superconducting phase at higher pressures, forming a characteristic double-dome structure [3]. In contrast, $CsTi_3Bi_5$ lacks both CDW and superconductivity at ambient pressure due to van Hove singularities being located well above the Fermi level; nevertheless, superconductivity emerges under pressure with a similar double-dome profile [4]. In the case of $CsCr_3Sb_5$, flat bands lie closer to the Fermi level, stabilizing a density-wave state at ambient pressure, while superconductivity only appears above ~3 GPa and peaks near 5 GPa [5].

Our high-pressure single-crystal XRD measurements, performed up to 20–25 GPa, reveal a universal yet anisotropic lattice response across all three systems. Owing to the 2D nature of these materials, compression along the *c*-axis is significantly stronger than within the kagome planes. This anisotropic compression drives a pressure-induced dimensional crossover, occurring near ~5 GPa for CsV_3Sb_5 and $CsCr_3Sb_5$, and at a lower pressure of ~3 GPa for $CsTi_3Bi_5$. Concomitantly, we observe a systematic evolution in in-plane stiffness, increasing from CsV_3Sb_5 to $CsCr_3Sb_5$ to $CsTi_3Bi_5$, indicating progressively stronger kagome-plane bonding. In contrast, the *c*-axis compressibility is reduced in $CsTi_3Bi_5$, resulting in a lower overall compressibility anisotropy.

Combined with our previous spectroscopic results on CsV_3Sb_5 [6,7], these findings suggest that pressure-induced interlayer bonding shifts the Sb/Bi *p*-states toward higher energies. This leads to a reconstruction of the Fermi surface and provides a unifying mechanism for the emergence and reentrance of superconductivity. Our results highlight the central role of lattice-controlled dimensional crossover in tuning electronic topology and superconducting instabilities in kagome metals.

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Pressure-triggered molecular organization in tsaregorodtsevite, a natural TMA-sodalite zeolite

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Abstract

Understanding the mechanical response and host–guest interactions in porous materials is critical for unraveling their structural flexibility, functional behavior, and technological potential. Tsaregorodtsevite, $[N(CH_3)_4][Si_2(Si_{0.5}Al_{0.5})O_6]_2$, represents a rare natural zeolite in which tetramethylammonium (TMA^+) cations are encapsulated within an ordered sodalite-like orthorhombic (*I*222) framework under ambient conditions [1]. While its thermally driven phase behavior has been previously explored [2], its structural evolution under compression has remained entirely unexplored.

Elucidating the host–guest interplay in tsaregorodtsevite under pressure is essential not only for understanding its intrinsic structural and mechanical properties but also for establishing a model framework applicable to related zeolitic systems. In this work [3], we systematically investigate its mechanical behavior and pressure-induced structural evolution, with particular emphasis on framework deformation mechanisms and the dynamic response of the guest TMA^+ species. High-pressure in situ single-crystal X-ray diffraction combined with Raman spectroscopy reveals that tsaregorodtsevite remains remarkably robust, exhibiting no evidence of pressure-induced amorphization up to 16 GPa. The observed reversible compressibility is governed predominantly by cooperative tilting of relatively rigid $(Si/Al)O_4$ tetrahedra about shared oxygen hinges, rather than bond compression. Strikingly, the compression mechanism is strongly mediated by the steric constraints and positional rearrangements of the extra-framework TMA^+ cations, which actively regulate cavity deformation and framework flexibility. First-principles total-energy calculations corroborate these findings, providing atomistic insight into the energetics and stability of the compressed structures. Importantly, pressure induces a continuous disorder-to-order transition of the TMA^+ species, highlighting the decisive role of guest accommodation in controlling the compressibility and structural response of the framework. These results establish tsaregorodtsevite as a compelling model system for understanding pressure-driven host–guest coupling in porous materials.

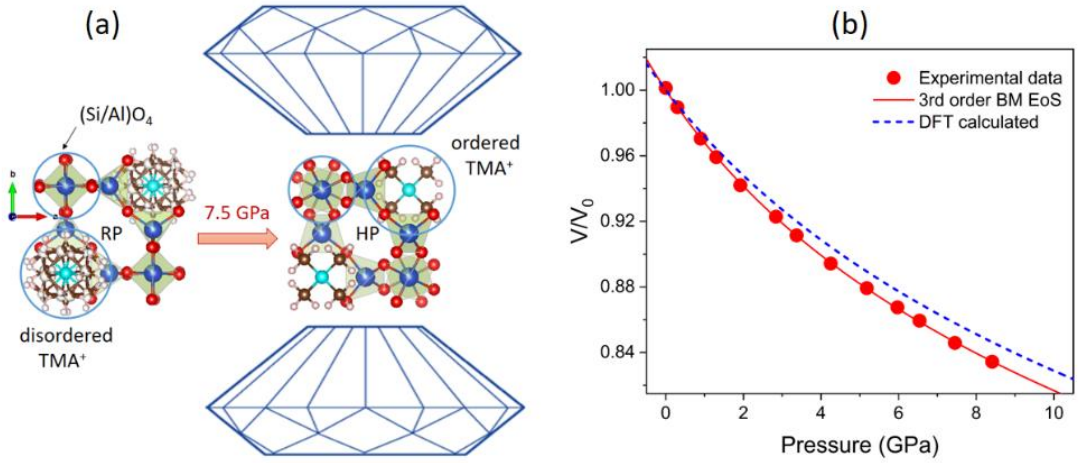

Figure 1: (a) Pressure-induced molecular ordering within crystal structure of tsaregorodtsevite, and (b) its equation of state (EoS).

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T8.2-O5 Spectroscopic and Structural studies

Pressure–Temperature Phase Diagram of Diglycine Perchlorate

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Abstract

Perchlorates (-ClO_4^-) are widely recognized for their strong oxidizing nature and diverse structural chemistry. Organic perchlorates exhibit weak intermolecular interactions that play a decisive role in modulating their physical properties and energetics, often contributing to exothermic behavior during synthesis, handling, and applications. This necessitates a detailed understanding of their dissociation mechanism and phase behaviour, which is still a gap area in this class of materials. Here we present our studies on diglycine perchlorate (DGPCl), a model organic perchlorate, carried out in two steps. First, the complete thermal dissociation mechanism of DGPCl was understood using a variety of techniques including vibrational spectroscopy, mass spectrometery (MS), differential scanning calorimetry and synchrotron XRD. Subsequently, using simultaneous high-pressure–high-temperature (HP-HT) investigations, we could successfully construct its PT-phase diagram, providing a comprehensive understanding of the phase behavior of this model compound. For these systematic studies in the range 1atm – 20 GPa and 30 – 400°C, a resistive heated symmetric diamond anvil cell, with type IIa diamond anvils was used to measure infrared and Raman spectra.

At ambient conditions, DGPCl crystallizes in a triclinic lattice (phase I), stabilized by O-H---O and N-H---O H-bonds, with significant ambiguity in the reported thermal behaviour [1, 2]. Our studies show a reversible melting transition near 130°C (phase II), followed by an irreversible transition at 170°C forming colored intermediate liquid phase (phase III). Above 220°C, it decomposes via evolution of gases, namely H_2O, CO_2, HCN, HCl, CO, CH_4, N_2O and NO. The gases have been identified using high-resolution rotational-vibrational spectroscopy and MS [3]. Our studies further reveal that the remnant residue (phase IV) comprises of ammonium perchlorate (AP- a highly potent oxidizer) along with carbon (a potential fuel), leading to an exothermic dissociation enthalpy of ~405 kJ mol^{-1} above 260°C. Using room temperature (RT)- HP studies, we further note that DGPCl shows multiple phase transitions leading to the formation of AP above 6 GPa without heating.

The PT – phase diagram of DGPCl, being reported for the first time for this class of compounds, constructed using HP-HT spectroscopic studies is shown in Fig.1a. For visual interpretation and to monitor gas evolution, we repeated the HP-HT studies under an optical microscope (see Fig.1b). DGPCl shows a sluggish melting behaviour, with completion shown by the melting line. The H-bonds get strengthened in the melt phase, as infered from CH, OH, NH vibrational modes. Unlike RT-HP studies, heating at HP reveals the formation of an unique combination of AP and AN in the intermediate phase in addition to an imine complex, just prior to dissociation, as shown in Fig.1c. We find that all the DGPCl modes are replaced by new ClO_4, NH_4, NO_3 modes and entirely different lattice region for temperatures higher than 240°C. Complete details of various phases of DGPCl and its energetics under varying P-T conditions, and comparison of its phase diagram with the most widely used oxidizer- AP, will be discussed.

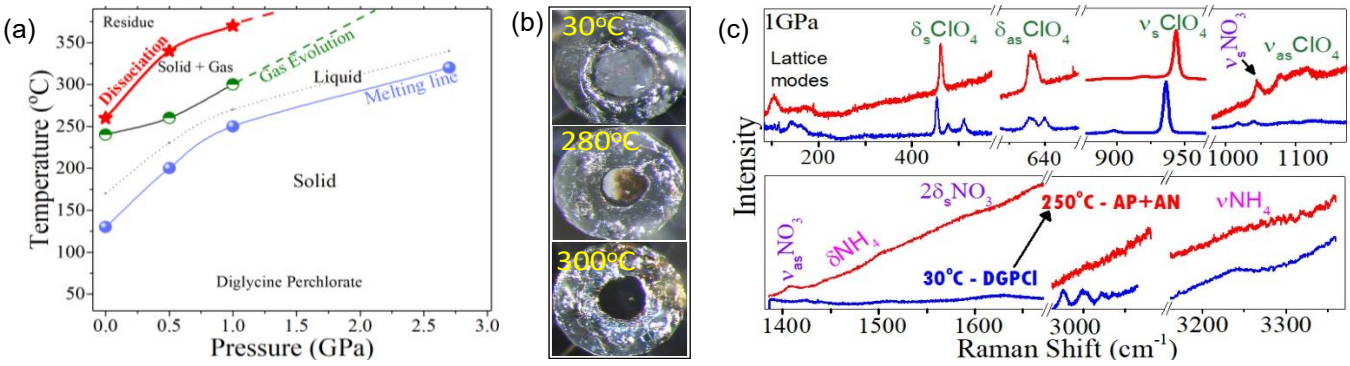

Fig.1(a) Constructed P-T phase diagram of DGPCl, (b) Micro-photgraphic images at 1GPa, (c) Raman spectra at 1GPa-30°C & 250 °C, changes in baseline and vibrational modes suggest melting and conversion to AP – AN complex, respectively.

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Red-to-NIR Optical Tuning in Rhodium(I) Complexes

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Abstract

Piezochromic materials (PCMs) exhibiting large, reversible spectral modulation are highly desirable for applications in pressure sensing, anti-counterfeiting, optical switching, and smart photonics [1,2]. However, most molecular PCMs display relatively modest emission shifts (≈100–150 nm), and fully reversible visible to near infrared (NIR) transitions remain rare [3,4].

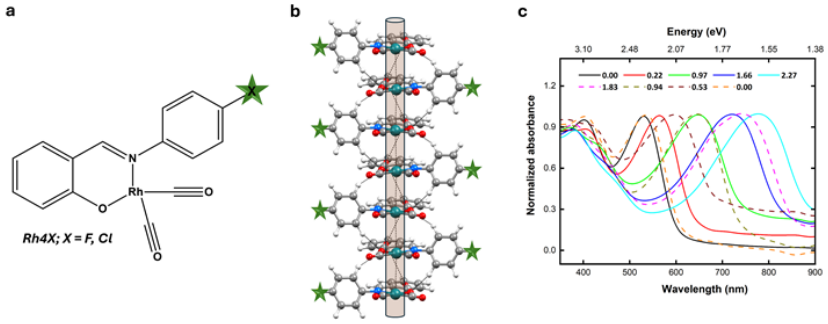

Fig. 1. (a) Molecular structure of **Rh4X** (X = F, Cl, Br), (b) 1D chains formed via Rh···Rh metallophilic interaction, highlighted within a cylindrical surface, and (c) reversible piezochromic shift (absorption spectra) seen in **Rh4F** from ambient pressure to 2.27(5) GPa.

In this contribution investigations on three square-planar rhodium(I) dicarbonyl Schiff-base complexes (**Rh4X**, X = F, Cl, Br; **Fig. 1a**) will be presented and discussed. The **Rh4Br** derivative was studied first both photocrystallographically and under high pressure since it formed best quality and most stable crystals out of the series [5,6]. This was due to a distinct crystal packing featuring with discrete Rh···Rh-stabilised dimer motifs in contrast to the **Rh4F** and **Rh4Cl** analogues forming isostructural crystals with metal···metal interactions stabilising the nearly linear 1-dimensional chains along the crystallographic *Z*-axis (**Fig. 1b**). As expected the spectroscopic properties of **Rh4Br** in a crystalline state are governed mainly by the metalophillic interactions which is supported by the observation of transient Rh···Rh excimer formation in a single crystal. Application of high pressure leads to strengthening of the metallophilic interaction and influences molecular orbitals contributing to the lowest-energy electronic transitions. Consequently, a reversible piezochromism (yellow-to-orange-to-red) under compression–decompression cycles with a bathochromic shift of ≈75 nm in emission maxima (up to 7 GPa) is observed. The piezochromic effect appeared to be much stronger in the case of the two other systems characterised by columnar architecture. High-pressure structural studies reveal anisotropic unit-cell compression dominated by contraction along the *Z*-axis, leading to significant strengthening of Rh···Rh interactions. Under moderate compression (< 5 GPa), both complexes display giant, continuous, and largely reversible bathochromic shifts spanning the visible to deep NIR region, reaching ≈245 nm in absorption and ≈388 nm in emission, with pressure sensitivities up to ≈106 nm GPa^{-1} (**Fig. 1c**). TD-DFT calculations reproduce the experimental observations and establish metallophilicity-assisted HOMO-LUMO gap narrowing as the origin of the giant piezochromism

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T8.3-O2 Spectroscopic and Structural studies

High-Pressure study of wurtzite InP nanowires

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Abstract

In this project we have studied the structural behaviour of wurtzite-phase (WZ) InP nanowires (NW) containing InAs quantum dots and coated with Sb_2S_3 phase change material (PCM) [Fig. 1a] under high pressure (HP) using a diamond anvil cell, Raman spectroscopy and synchrotron techniques. These hybrid nano-devices hold significant potential as wide-range wavelength-tunable single-photon sources (SPS) in the telecom band. HP Raman spectroscopy [Fig. 1b] and synchrotron XRD measurements performed at ID27 beamline, ESRF, suggest changes in the electronic structure around 3-5 GPa [Fig. 1c] and a wurtzite to rock-salt phase transition of InP in the region of 11-14 GPa, supplementing scarce low pressure measurements [1] and simulations [2]. For the first time, we were able to experimentally determine the bulk modulus of the hexagonal wurtzite phase of InP. Ultimately, these findings will support the development of a wavelength-tunable SPS for quantum technologies based on locally strained PCM.

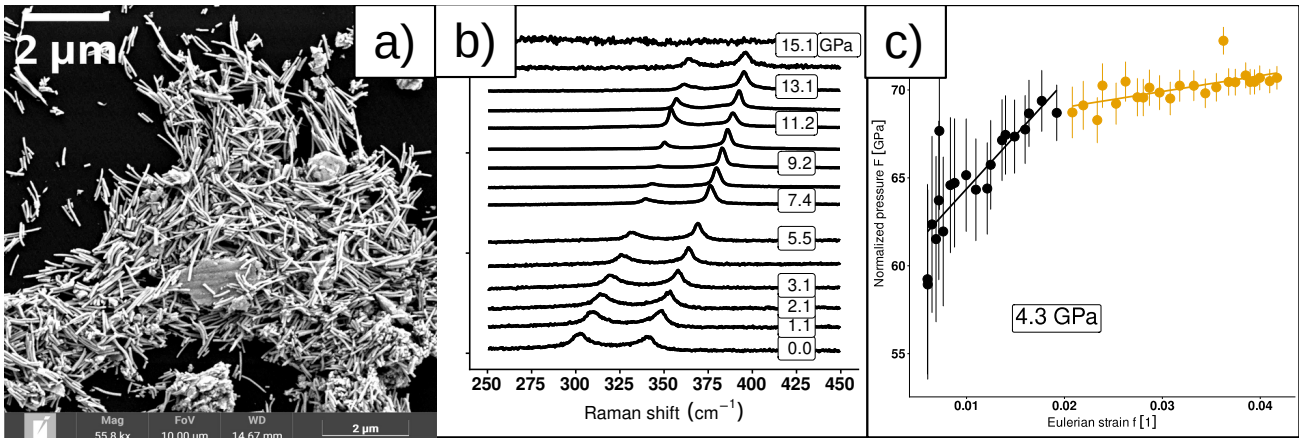

Fig. 1: a) SEM image of WZ InP NWs on a diamond anvil. b) Raman spectra at different pressures. c) Normalized pressure (F) - Eulerian strain variable (f) plot.

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High-pressure study of ferroelectric SbSI: from long-range order to local probes

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Abstract

Ferroelectric materials with intrinsic spontaneous polarization are of broad interest due to their rich fundamental physics and their potential for applications in advanced sensors, memory devices, energy conversion, and photovoltaics [1]. In these systems, the coupling between crystal structure and electronic properties is often correlated with lone-pair formation. Due to their stereochemical activity, lone pairs promote structural distortions that can drive ferroic behavior. Among the most promising classes of materials, van der Waals antimony-based chalcohalides have recently attracted attention as potential solar absorbers [2]. In particular, antimony sulfoiodide (SbSI) exhibits a spontaneous polarization below the transition temperature close to room temperature, arising from a displacive structural transition from the orthorhombic Pnam to $Pna2_1$ space group, together with a suitable band gap for photovoltaic applications [3]. However, the underlying physics of this material is not yet fully understood. For instance, at low temperature a negative thermal expansion is observed along the crystallographic c-axis, which can be associated with a larger Sb displacement along z position and plays a key role in the emergence of spontaneous polarization.

Applying external pressure provides an additional powerful and clean way to modify local structure and atomic coordination, offering direct insight into the mechanisms that govern ferroelectricity and phase stability [4].

In this work, we investigate the high-pressure behavior of SbSI using a combination of complementary synchrotron techniques, including X-ray Diffraction, X-ray Absorption Spectroscopy (XAS), and Nuclear Forward Scattering (NFS) on ^{121}Sb. Under compression, SbSI exhibits very subtle structural modifications, consistent with those observed as a function of temperature [5]. While diffraction probes the average crystal structure, XAS and NFS provide direct access to the local environment of Sb, which is believed to play a central role in driving the ferroelectric state through its lone-pair activity. Focusing on the local response of antimony reveals signatures of distortions and electronic rearrangements that cannot be unambiguously identified using a single technique. This multi-scale approach is essential for disentangling the complex coupling between structure and ferroelectricity in SbSI.

Based on these results, we propose a pressure-temperature (P-T) phase diagram of SbSI, highlighting the presence of a low-temperature high-pressure phase, characterized by a structural transition from the orthorhombic to a monoclinic crystal structure. Particular emphasis is placed on the unique sensitivity of ^{121}Sb NFS, technique available at the ID14 Nuclear Resonance beamline of the ESRF, to the local electronic and structural environment of antimony. This local probe approach is further supported by complementary studies on elemental Sb under high pressure, illustrating the broader applicability of NFS to Sb-based systems and its ability to reveal subtle changes which are difficult to access with other techniques.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T8.3-O4 Spectroscopic and Structural studies

Application of high-pressure spectroscopy to identify the UV color center in 2D boron nitride

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Abstract

Layered boron nitride is one of the key two-dimensional (2D) materials and is the subject of intensive research, both due to numerous new physical phenomena and advanced applications. It comprises boron and nitrogen ions forming flat sp^2 covalent bonds with a honeycomb structure inside the layers and weak van der Waals bonds between the layers, creating a three-dimensional crystal with a wide indirect bandgap of ~6 eV [1]. This bandgap accommodates numerous optically active electronic states of structural defects and impurities that are abundant in currently grown crystals and epitaxial layers. They can act as bright single photon sources with various photon energies or as efficient light emitters with extreme thermal stability [2-5]. One of the brightest emissions at ~4 eV originates most likely from a carbon dimer-related defect [3,4,6,7]. To fully control and develop unique BN applications on demand, both the nature and electronic structure of color centers should be identified.

The most common 2D BN is centrosymmetric hexagonal BN (hBN), but the BN atomic planes can also be arranged in non-centrosymmetric configurations like rhombohedral (rBN) or Bernal (bBN). Different layer stacking sequences influence the UV emission of color centers in the BN host [7]. In this work, we used the diamond anvil cell technique to perform high hydrostatic pressure studies of the low-temperature photoluminescence (PL) of hBN, rBN, and bBN in the 3 – 4.2 eV spectral region. The results showed that the PL energy (E_{PL}) decreased with pressure less sensitively than the bandgap, and the observed pressure coefficients of E_{PL} depend strongly on the BN polytype. Theoretical calculations of pressure dependencies of various defect levels in BN polytypes confirmed that the observed emission was associated with carbon-related defects. Our results show that tuning the stacking sequence in various polytypes of a given crystal provides unique “fingerprints” contributing to identifying defects in 2D materials [8].

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Unlocking hidden phases in Fe(II) spin crossover complexes under pressure

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Abstract

Spin crossover (SCO) is typically described, in its simplest form, as a two-state electronic equilibrium between high-spin (HS) and low-spin (LS) configurations. Within this framework, temperature and pressure are often treated as equivalent thermodynamic variables capable of shifting the same underlying equilibrium. However, in the solid state, the spin transition is intrinsically coupled to a deformable and cooperative lattice, whose collective response can significantly influence not only the transition conditions but also the transformation pathway. In particular, phase transitions may lead to a substantial shift of the SCO regime towards significantly higher pressures than anticipated, [1] or even to the stabilisation of the HS state under conditions where a LS state would normally be expected. [2]

Among the most widely studied SCO compounds are Fe(II)-based systems (d^6) in octahedral coordination environments, which typically undergo switching between S = 2 and S = 0 spin states. These materials have attracted considerable attention for solid-state refrigeration applications, as some exhibit large to colossal barocaloric effects. [3,4] Consequently, there is growing interest in mapping their pressure–temperature (p,T) phase diagrams and understanding their behaviour under pressure.

In this contribution, we investigate a series of Fe(II) complexes exhibiting contrasting (p,T) responses. By comparing different structural motifs, we demonstrate that lattice topology plays a decisive role in governing how the electronic transition evolves under pressure. Depending on the system, the lattice may reorganise prior to spin switching, evolve cooperatively with the SCO, or become unstable upon compression, enabling structural rearrangements not observed along the thermal pathway.

A combination of high-pressure Raman spectroscopy, together with synchrotron single-crystal and powder X-ray diffraction and X-ray absorption spectroscopy, allows us to unravel the interplay between spin state and structure under different thermodynamic stimuli. Our results highlight how pressure can reveal hidden lattice instabilities and alternative transformation routes, and further emphasise that SCO in molecular solids arises from a delicate balance between electronic configuration and collective structural response.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T8.4-O2 Spectroscopic and Structural studies

Absence of charge density wave transition in $SnSe_2$ at extreme conditions

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Abstract

Transition Metal Dichalcogenides (TMDs) have attracted significant attention as their layered crystal structure results in anisotropic mechanical and electronic properties and into the quantum confinement of charges into single layers, making them prototypical two-dimensional (2D) materials [1, 2]. In recent years, high-pressure (HP) studies on TMDs showed that the pressure-induced enhancement of the weak inter-layer interaction among adjacent layers can strongly modify their structural and electronic properties [3-6], resulting in a rich phase diagram which can host a metallic transition in semiconducting TMDs [3- 5] or more exotic phenomena at high-pressure/low-temperature (LT) conditions, such as charge density waves (CDWs) or superconducting states [3, 6]. Among them, $SnSe_2$ has recently gained attention due to the unusual CDW-like phenomenology emerging during the metallization process, consisting of a periodic lattice distortion (PLD) witnessed by X-ray diffraction [6] and the high-pressure reorganisation of the band structure leading to the suppression of large parts of the Fermi surface suggested by Density Functional Theory calculations [7].

In our work, we seek experimental evidence of a CDW-like ordering by investigating the evolution of the inter-band electronic transitions, the charge carriers, and the vibrational spectrum of $SnSe_2$ by synchrotron-based infrared transmission and reflectivity high-pressure measurements and by LT/HP Raman spectroscopy. By IR spectroscopy, we demonstrate a clear metallization above 16 GPa, with the closure of the bandgap and the subsequent increase in the Drude plasma frequency in the far-IR region. The metallization is accompanied by a change in the Raman spectrum ~16 GPa, in accordance with the literature [6]. On increasing pressure up to 27 GPa, we find no evidence for the presence of CDW neither in the IR spectra, displaying no signatures of Fermi-level gapping, nor in the LT/HP Raman measurements, lacking CDW-related spectral contributions, such as the amplitude mode.

Our IR and Raman spectroscopic studies of $SnSe_2$ provide an exhaustive picture of the electronic, optical and vibrational evolution of $SnSe_2$ under extreme pressure and temperature conditions, without finding clear evidence support for the formation of an unusual pressure-induced CDW in the investigated 0-27 GPa and 300-65 K ranges.

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High Pressure Raman Spectroscopy of $IrTe_2$ up to 25.9 GPa: Spectroscopic Mapping of Lattice Destabilization and Amorphization

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Abstract

The transition metal dichalcogenide $IrTe_2$ exhibits a fascinating, closely competing phase landscape governed by exotic charge-ordering, local structural dimerizations, and superconductivity. While macroscopic boundaries and long-range structural modifications have been previously mapped using X-ray diffraction techniques, a continuous, localized spectroscopic investigation under high static pressures remains essential to understanding local structural reconstructions and atomic-scale distortions. In this work, we present a detailed high-pressure Raman scattering study of single crystalline $IrTe_2$ executed continuously up to a maximum pressure of 25.9 GPa at room temperature using a diamond anvil cell (DAC).

At ambient conditions, the recorded spectra are dominated by two prominent, well resolved Raman active optical phonon modes located near 128 cm^{-1} and 165 cm^{-1}, assigned to the E_g in-plane shear and A_{1g} out-of-plane symmetric stretching modes, respectively. Under increasing pressure, the reduction of interatomic distances induces a primary blue shift in the peak positions (ω) toward higher wavenumbers. From 0.5 GPa up to approximately 3.3 GPa, both the E_g and A_{1g} modes exhibits a highly linear, tightly constrained pressure dependence (dω/dP). However, around 5.1 GPa, distinct anomalies emerge in the phonon frequency slopes and full width at half maximum (FWHM) profiles for both modes, providing clear spectroscopic confirmation of the macroscopic transition to the low symmetry dimerized phase.

Crucially, a severe structural destabilization is tracked between 10 GPa and 14 GPa. Within this regime, the crystal lattice undergoes an intense structural instability, where the stretching mode exhibits a massive broadening anomaly with the FWHM exceeding 128 cm^{-1} at 13.4 GPa accompanied by a sharp frequency softening beyond this point. Upon further pressure elevation above 17.4 GPa and extending up to 25.9 GPa, the sharp crystalline modes completely merge into a singular, highly diffuse, and heavily broadened multi-phonon band. This behavior provides direct spectroscopic evidence of an extreme, pressure induced lattice amorphization, which serves as a definitive experimental benchmark for the high pressure phase diagram of correlated 5d transition metal dichalcogenides.

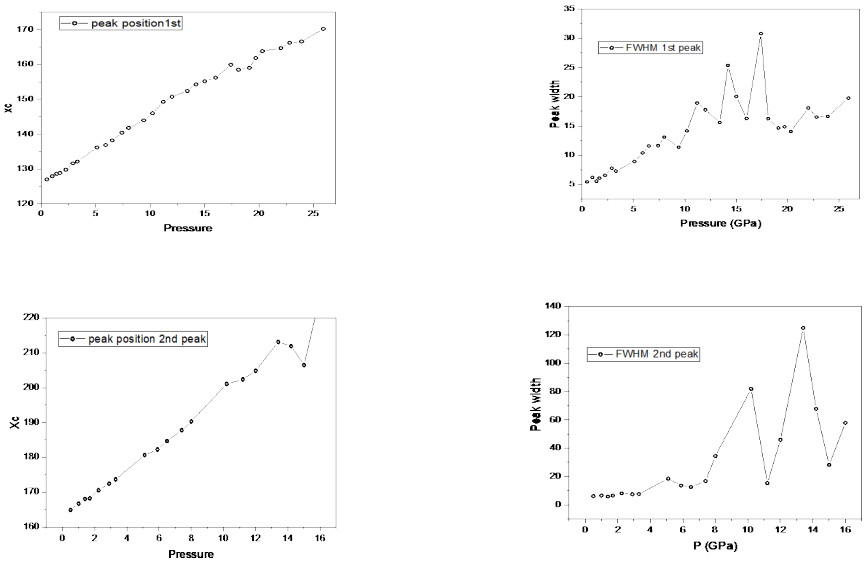

Figure 1: Pressure dependence of the phonon peak positions (wavenumbers) and full width at half maximum (FWHM) profiles for the Eg and A1g modes of single-crystalline IrTe2. The data clearly illustrates the initial linear regimes, the dimerization anomaly at 5.1 GPa, and the severe structural destabilization and softening tracking beyond 13.4 GPa.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T9.1-O1 Theoretical and Computational approaches

High Pressure Electrides and Core-Electron Chemistry

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Abstract

The theoretical prediction and experimental discovery of high-pressure electrides (HPEs), compounds assuming open structures where the valence electrons are localized in interstitial voids, was unexpected and paradigm-changing. We present the results of quantum chemical calculations on the iconic Na-hP4 HPE showing that increasing density causes a 3s → 3pd electronic transition due to Pauli repulsion between the 1s2s and 3s states, and orthogonality of the 3pd states to the core. The large lobes of the resulting Na-pd hybrid orbitals point towards the center of an 11-membered penta-capped trigonal prism forming multicentered bonds [1]. We introduce descriptors that can be obtained from the quantum mechanical electron density that can be used to characterize electrides, and illustrate how the multi-objective functionality in the XtalOpt evolutionary algorithm for crystal structure prediction can be used for HPE discovery [2]. We describe how quantum crystallography was employed in conjunction with single crystal X-ray diffraction to provide the first experimental signatures of the localized electrons within Na-hP4 at 223 GPa [3]. Finally, we show that core-electron bonding is key for the B1 → B2 pressure induced structural phase transition in alkali fluorides [4].

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T9.1-O2 Theoretical and Computational approaches

High Pressure Melting vs Decomposition of GaN: *ab initio* Molecular Dynamics Study and comparison to the experimental data

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Abstract ()

The technology of GaN is very much advanced due allowing for key applications like LEDs or high power-high frequency transistors. Nevertheless, GaN fundamental physical properties including phase diagram, are still not determined. In this work, simulations of GaN crystal behavior at heating to extremely high temperatures in a wide pressure range are reported. A*b initio* density functional theory (DFT) Molecular Dynamics extensive calculations were used to obtain the temporal change of the system. Heating of an initially perfect wurtzite GaN crystal to a temperature above 3500K resulted in destruction of the crystalline lattice and transition of the system to a perfectly disordered fluid. At the pressure of 7.1 GPa and below, the formation of N_2 molecules inside the cluster was detected, therefore the process was identified as the thermal decomposition of GaN. At pressures as high as 15 GPa, the formation of N_2 molecules was suppressed despite of total loss of the crystalline order. The system consisted of the single gallium and nitrogen atoms, so the high pressure process was identified as congruent melting of GaN.

An excellent agreement of the simulation results with well-established experimental data on GaN decomposition has been found. The absence of N_2 molecules in the fluid at high pressures indicates that the intersection of the decomposition line and the melting line occurs in the pressure range between 7 and 15 GPa. At pressure above the intersection point, gallium nitride can be congruently melted without decomposition in contrast to lower pressures where GaN decomposes before reaching the melting point. This is in agreement with the proposed melting model based on our earlier experiments, suggesting a reversal of the decomposition-melting sequence at heating, at 12 GPa.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T9.1-O3 Theoretical and Computational approaches

Atomistic Mechanisms of Shear-Induced LDA↔HDA Transformations and Shear Banding in Amorphous Silicon under High Pressures

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Abstract

Mechanisms of plastic deformations in amorphous solids, phase transformations (PTs) between different amorphous phases under hydrostatic loading, and PTs in crystalline materials under severe plastic deformations attract significant attention due to their great fundamental importance and applied potential. However, we are not aware of any publications on plastic shear-induced amorphous-amorphous PTs under pressure.

Here, we integrate sciences of severe plastic deformations of amorphous materials, strain-induced PTs in crystalline materials under high pressure, and sear banding, and extend them to study shear deformation under constant pressures in amorphous Si, shear-induced PTs from low-density amorphous (LDA) to high-density amorphous (HDA) Si, and mutual effects of PT and shear band formation using molecular dynamics simulations with the state-of-the-art Gaussian Approximation Potential. Shear deformation leads to the formation of a shear band, in which a dissipative structure of turbulent-like flow with swirls is revealed, followed by a reduction in the number of swirls via coalescence with further shearing. Increasing pressure results in LDA↔HDA PT with increasing atomic fraction of HDA due to pressure and shear, which in turn suppresses the shear banding, enabling the uniform deformation-PT at 9.8 GPa.

The simulations reveal that shear-induced LDA↔HDA PTs occur simultaneously until reaching steady state. Shear reduces the pressure for initiation and completion of LDA↔HDA PT by 4.3 and 5.1 GPa compared to hydrostatic loading, respectively. The atomic mechanism of PT differs fundamentally from that under hydrostatic loading. In bulk, Si deforms by atomic rearrangement in localized STZs with high nonaffine displacements, which trigger nucleation of HDA clusters within LDA and, concurrently, of LDA clusters within HDA, without their growth and coalescence. Despite the much larger shear and the expected atomic fraction of HDA in a shear band, a surprisingly sharp drop in atomic fraction of HDA within the shear band was discovered. It was found that this anomalous behavior is related to the change in deformation mechanism: swirls in a shear band promote reverse PT from HDA↔LDA more effectively than the direct PT. While a clear correlation between fields of the nonaffine squared displacement and the atomic coordination in the bulk is found, such a correlation in a shear band is lacking. There is no correlation between the atomic displacement and coordination number fields, both within and outside the shear band.

We developed a simple, mechanism-based analytical model that uses accumulated plastic strain rather than time, simultaneous direct-reverse PTs, pressure-dependent driving forces for both PTs, and different yield strengths of the phases. It possesses a steady-state solution depending on pressure. Both non-stationary and stationary solutions accurately describe the MD simulation results across all pressures, allowing us to determine all material parameters. A kinetic equation is also derived for pressure-induced LDA↔HDA PTs, and the stationary solution reproduces the MD simulation results correctly. Despite the large shear stresses, they surprisingly do not affect the PT kinetics. This happens because, according to atomic mechanisms, shear stresses simultaneously promote both direct and reverse PTs in different regions, resulting in negligible net effects.

Transformation-induced plasticity (TRIP) due to volume change during amorphous-to-amorphous PT is revealed. While for crystalline solids, temperature and/or stress hystereses require temperature and/or stress cycling to accumulate significant TRIP, LDA↔HDA PTs occur simultaneously, and each of them produces TRIP. Consequently, even for relatively low net atomic fraction of HDA, TRIP and stress relaxation can be significant due to a large number of back-and-forth events. An equation for the TRIP-induced deformation rate is proposed that accounts for the above results. Our findings provide deep atomistic and macroscopic insights into the coupled pressure-shear deformation and PT in amorphous Si, offering a crucial theoretical foundation for designing experiments and various engineering applications, including optimizing ultra-precision surface treatment by inducing ductile machining regimes and controlling failure in amorphous Si via pressure and PT.

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T9.1-O4 Theoretical and Computational approaches

Hydrogen bond disappearance and electron-deficient multicenter bond formation in compressed hydrogen halides

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Abstract

Pressure-induced hydrogen bond symmetrisation (PIHBS) has been thoroughly studied in hydrogen halides HX (X= F, Cl, Br), mostly in relation to the search for metallic hydrogen and the high-temperature superconductivity in hydrogen-related systems [1-3]. In these molecular systems, the PIHBS occurs due to the pressure-induced polymerization of the HX molecules. Using ab initio calculations, we demonstrate that the resulting symmetric X–H–X bonds in dense HX halides form through a gradual redistribution of electron density, evolving from localized two-center bonds into delocalized multicenter interactions. A systematic bonding analysis reveals that this process does not result in the formation of electron-rich multicenter bonds (ERMBs), or three-center four-electron (3c-4e) bonds, as might be expected for a hydrogen bond according to the IUPAC definition, and as occurs in the biflouride anion, HF_2^- (Fig. 1a). Instead, electron-deficient multicenter bonds (EDMBs), more specifically three-center two-electron (3c-2e) bonds concatenated in a zigzag arrangement, are formed in dense HX halides (Fig. 1b). The formation of EDMBs proceeds in several stages as already verified in other compounds, e.g. pnictogens and chalcogens [4], alkaline AX_3 halides [5], and AIO_3 perovskites [6], as proposed in the Unified Theory of Multicenter Bonding (UTMB) [7,8], which enables the characterization of bonding regimes that challenge classical definitions and expand our understanding of molecular and solid properties.

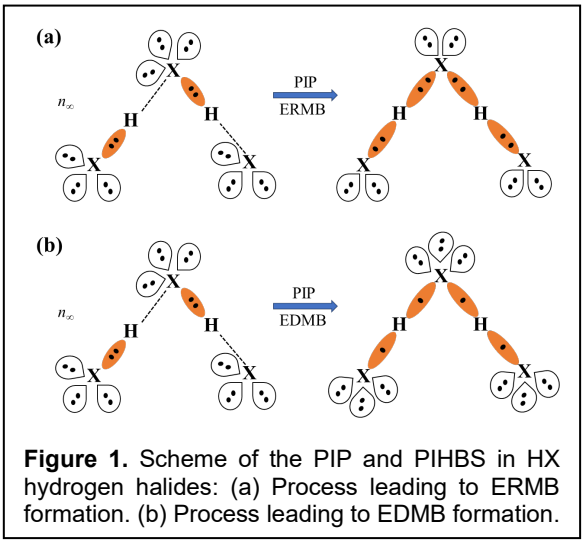

Figure 1. Scheme of the PIP and PIHBS in HX hydrogen halides: (a) Process leading to ERMB formation. (b) Process leading to EDMB formation.

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[2] S. Lu et al., Prediction of novel crystal structures and superconductivity of compressed HBr, RSC Adv. 5, 45812 (2015).

[3] Q. Gu et al., High-temperature superconducting phase of HBr under pressure predicted by first-principles calculations, Phys. Rev. B 96, 064517 (2017).

[4] H. H. Osman et al., Electron-deficient multicenter bonding in pnictogens and chalcogens: Mechanism of formation. J. Mater. Chem. C 12, 10447 (2024).

[5] E. Bandiello et al., From Polyanions to Infinite Chains: Chemical Bonding Evolution in AX3 Polyhalides under Pressure, J. Mater. Chem. C 13, 21936 (2025).

[6] H. H. Osman et al., Unconventional Electron-Deficient Multicenter Bonds in AIO3 Perovskites. Chem. Mat. 37, 4187 (2025).

[7] H. H. Osman et al., A Unified Theory of Electron-Rich and Electron-Deficient Multicenter Bonds in Molecules and Solids: A Change of Paradigms, J. Mater. Chem. C 13, 3774 (2025).

[8] F.J. Manjón et al., Introduction and Extension of the Unified Theory of Multicenter Bonding: The Role of the Charge-Shift Bonding, Molecules 31, 82 (2026).

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T9.1-O5 Theoretical and Computational approaches

Rapid Mechanical Property Prediction using Wyckoff Set Regression for Scalable Materials Exploration

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Florian TRYBEL (Linköping University, Sweden),
Rickard ARMIENTO (Linköping University, Sweden)

Abstract

Recent advances in machine learning have significantly accelerated materials discovery. Despite these advances, the space of all possible crystal structures and their properties is enormous, and full exploration is computationally infeasible. Exploring the combinatorial space of Wyckoff positions, capturing symmetrically inequivalent atomic positions, is a more tractable problem. The GPU-optimized transformer-based WREN (Wyckoff REpresentation regressioN) framework can be used to efficiently navigate this space. WREN has demonstrated to be highly effective in rapidly relating symmetry to formation energies on vast scales [1]. We extend its application by predicting the essential mechanical properties of bulk and shear modulus. These are necessary quantities to understand a materials behaviour and stability under high pressure. As WREN's descriptor is independent of atomic positions, this not only enables property prediction without realizing crystal structures but opens up the tantalizing prospects to rapidly screen phase competition at high pressure at an unpresented scale. I will present recent methodological developments and compare predictions with experiments, ab-initio and other machine learning approaches.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T9.2-O1 Theoretical and Computational approaches

Machine-Learned Electron Localization in Dense Hydrogen

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Julia CONTRERAS-GARCIA (Sorbonne Université)

Abstract

Machine learning offers a promising route to bypass the high computational cost associated with explicit electronic-structure calculations for real-space bonding descriptors. Here, we present a geometry-based machine-learning framework for predicting the electron localization function (ELF) of hydrides directly from atomic configurations, without requiring Kohn–Sham orbitals or kinetic-energy densities. The model is trained on first-principles datasets spanning multiple pressure regimes in random binary structures and achieves consistently high predictive accuracy, with coefficients of determination exceeding R^2>0.99. In addition to reproducing the global ELF distribution with high fidelity, the framework accurately captures the spatial organization of localization features relevant to hydrogen bonding and network formation.

To characterize the remaining discrepancies between predicted and reference ELF fields, we perform a combined real- and reciprocal-space analysis of the residual error. The residual is found to be highly structured rather than stochastic, being dominated by smooth, long-wavelength components whose correlation lengths exceed typical H–H bonding distances. The magnitude and spatial extent of these nonlocal contributions increase systematically with pressure, indicating that the most difficult aspects of ELF prediction arise from collective electronic responses extending beyond the local bonding environment. Despite representing only a small fraction of the total ELF amplitude, these components can be efficiently described using a band-limited Fourier correction formulated in the logit representation.

Importantly, ELF-derived topological descriptors remain robust against these structured residuals. In particular, networking characteristics, including connectivity patterns and critical-point topology, are preserved with high fidelity across a wide range of thermodynamic conditions, enabling the prediction of critical temperatures. Although the model is trained exclusively on binary systems, it transfers successfully to ternary hydrides.

Overall, this methodology allows rapid evaluation of ELF-derived descriptors, including networking values, bonding topology, and localization-driven structural motifs, without the need for explicit electronic-structure calculations. More broadly, these results suggest a viable path toward large-scale, geometry-based electronic-topology analysis for materials discovery and high-throughput exploration of bonding phenomena across diverse chemical environments.

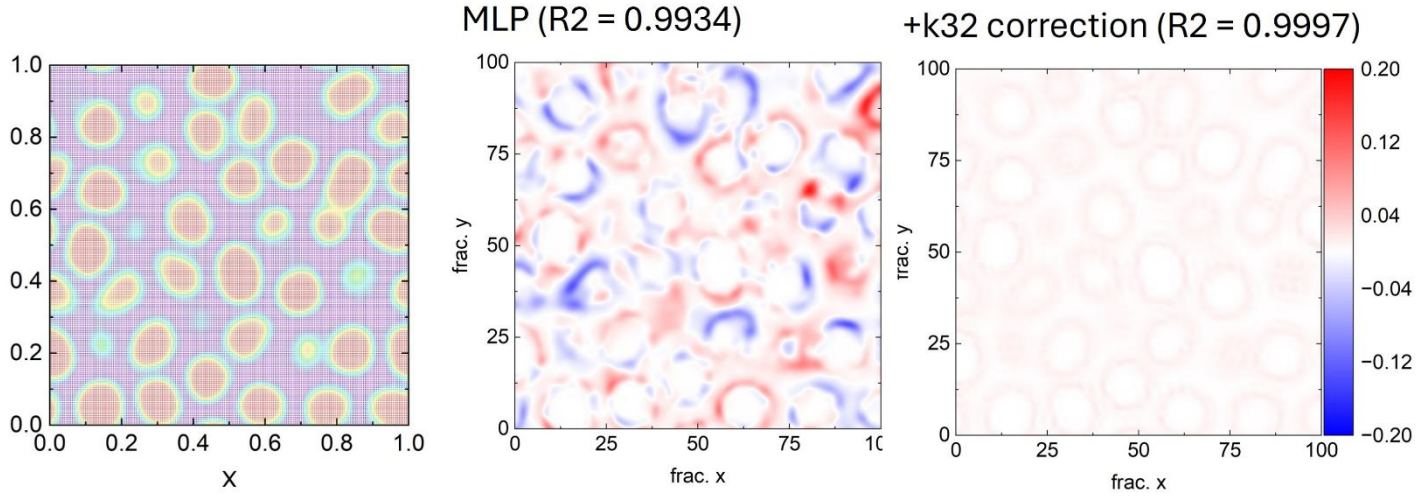

Figure 1. a) DFT-computed ELF in real space (color scale from 0 (blue) to 1 (red); fractional coordinates relative to 11~\AA, b) Real-space residual between predicted and DFT ELF with the real space predictor, c) Real-space residual between predicted and DFT ELF with the real+reciprocal space predictor.

Model for Equation of State and Solidus and Liquidus of a Mixture for Description of High-Entropy Alloys

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Dean PRESTON (Los Alamos National Laboratory, USA)

Abstract

Self-consistent thermodynamic description of a mixture (a compound, an alloy, etc.) including both its equation of state (EOS) and solidus and liquidus surfaces (lines in the case of a binary mixture) is a challenging problem. We review several standard approaches with the associated mixing rules and discuss their shortcomings. We propose a new thermodynamics-based analytic model for the EOS of a N-component mixture, N ≥ 2. The model uses N−1 free parameters the values of which can be easily determined from the available experimental data on the binary subsystems; examples of such subsystems are shown in Figures 1 and 2. The knowledge of these parameters is required for the construction of the EOS. However, the calculation of both the solidus and liquidus surfaces of a N-component mixture, which the model also suggests, requires the knowledge of the melting curves of each of the constituents of the mixture, but no other information such as their EOSs is really needed. We apply the new model to multi-component mixtures of transition metals, emphasizing its suitability for the description of high-entropy alloys (HEAs), a revolutionary class of materials that depart from traditional metallurgy — which uses one base metal with minor additions — by mixing five or more elements in nearly equal proportions. An example of a quinary A-B-C-D-E HEA is shown in Figure 3. This approach creates a "high-entropy" effect that stabilizes simple solid-solution crystalline structures, resulting in materials with exceptional strength, fracture toughness, and resistance to corrosion and high temperatures. Our examples of the application of the new model to real multi-component systems will include both the ternary Cu-Pd-Pt alloy and ThO_2-UO_2-PuO_2 mixed-oxides (MOX) fuel system, the quaternary U-Pu-Nb-Zr alloy, and the quinary V-Nb-Ta-Mo-W HEA.

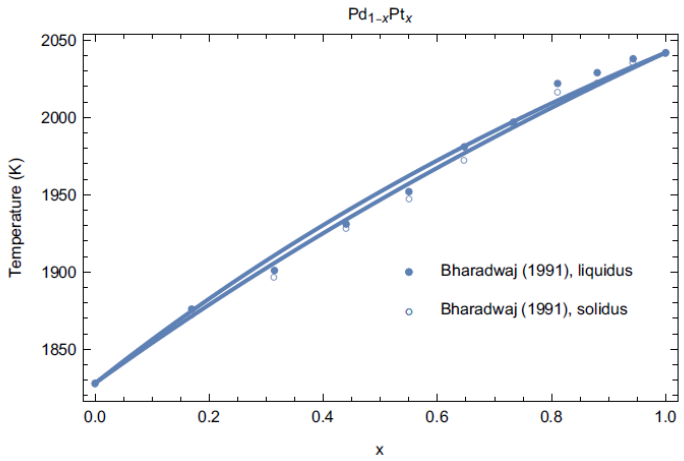

Figure 1. The high-T portion of the phase diagram of Pd-Pt system: Comparison of the new mixing model (lines) to the experimental data of Bharadwaj of 1991.

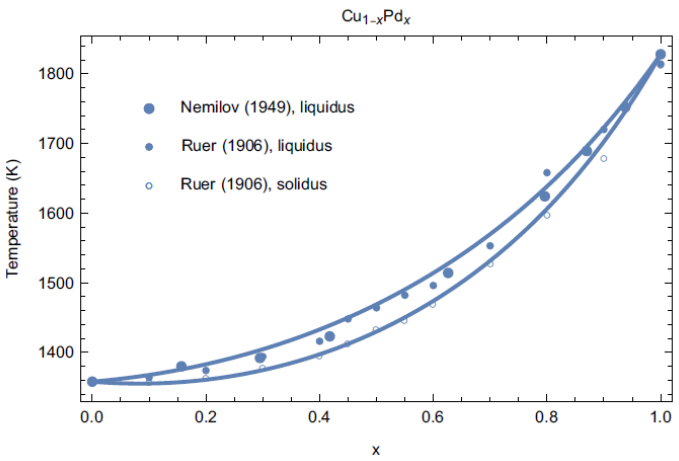

Figure 2. The high-T portion of the phase diagram of Cu-Pd system: Comparison of the new mixing model (lines) to the available experimental data from two sources.

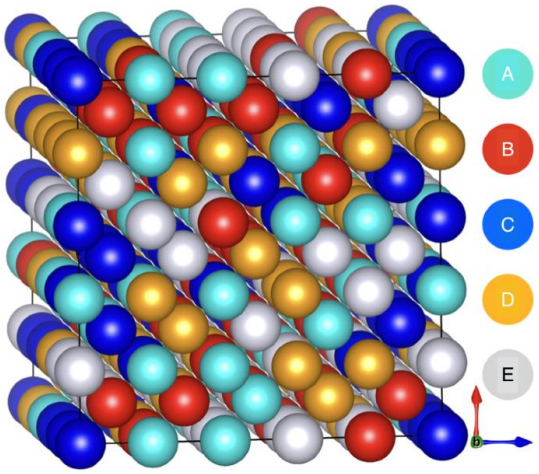

Figure 3. Example of HEA: a quinary A-B-C-D-E system; letters represent different transition metals.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T9.2-O3 Theoretical and Computational approaches

Machine-Learning Simulations Predict Phase Transformations of Fullerite in a Diamond-Anvil Cell

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Alan SALEK (Royal Melbourne Institute of Technology, Australia),
Dougal MCCULLOCH (Royal Melbourne Institute of Technology, Australia),
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Nigel MARKS (Curtin University, Australia)

Abstract

Fullerite is a molecular solid of C_{60} cages held together by van der Waals forces. Under ambient conditions the molecules sit on a face-centered cubic lattice and rotate freely. While the collapse of the C_{60} cages under high pressure and temperature is well established, the precise structural pathways under non-hydrostatic conditions remain incompletely characterized. Here we report the use of Molecular dynamics simulations with a Machine-Learning Interatomic Potential (MLIP) [1] to study phase changes in fullerite through a compression and decompression process. Both uniaxial and hydrostatic conditions are used to mimic diamond anvil cell (DAC) experiments using the stuffed cell and the gas-loaded cell respectively. All structures are compressed up to 100 GPa and decompressed to mimic sample recovery from a DAC.

Our simulation results quantitatively agree with experiment, reproducing the pressure threshold at which transformations are seen in the DAC [2] and provide an atomistic picture of the transformation mechanism of fullerite into higher-density carbon allotropes. Pressure-induced cross-linking of the fullerene molecules starts at 1.3 GPa for uniaxial conditions and 1.6 GPa under hydrostatic conditions. Collapse of the C_{60} cages into tetrahedral amorphous carbon occurs around 30 GPa under uniaxial load and 45 GPa under hydrostatic load in good agreement with experiments. The density and sp^3 fraction predicted by the MLIP also quantitatively agree with experimental electron energy loss spectroscopy measurements. In conclusion, our results confirm that MLIPs can capture the full pressure-driven transformation pathway of fullerite, from molecular cross-linking to the collapse into ultrahard amorphous carbon, with quantitative agreement to experiment, opening the door to new preparation protocols for the formation of dense carbon phases.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T9.3-O1 Theoretical and Computational approaches

Exploration of the Na-Si Phase Diagram and Theoretical Structure Prediction of a Layered Sodium Zintl Phase Na_2Si_3

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Sylvain PITIÉ (IC2MP, France)
Gilles FRAPPER (IC2MP, France)

Abstract

First-principles crystal structure prediction and density functional theory (DFT) calculations were employed to investigate the high-pressure behavior and electronic properties of the sodium silicide Na_2Si_3. Evolutionary structure searches identified a previously unknown tetragonal phase (space group *P*-42$_1$*m*, *Z* = 2) that becomes thermodynamically stable near 5 GPa and remains dynamically stable upon decompression to ambient pressure. The predicted structure consists of layered silicon slabs separated by sodium atoms and can be interpreted within the Zintl–Klemm framework through formal charge transfer from Na to the silicon network.

Electronic structure calculations indicate semiconducting behavior with an indirect band gap of approximately 1.14 eV at ambient pressure. Compression leads to a systematic increase in the band gap, demonstrating pressure-dependent electronic tunability. The calculated bonding characteristics and charge distribution support the ionic–covalent nature of the compound and the formation of a layered silicon framework. Analysis of the crystal topology highlights pentagonal motifs within the silicon sublattice, while lattice-dynamics and transport-related calculations suggest relatively low thermal conductivity. These computational results establish Na_2Si_3 as a pressure-stabilized Zintl phase with potentially attractive electronic and thermoelectric properties.

In addition to the Na_2Si_3 compound, the binary Na–Si phase diagram under pressure has been explored using a variable-composition evolutionary algorithm (XtalOpt) and *ab initio* random structure searching (AIRSS) combined with machine-learned interatomic potentials, such as EDDPs. New compositions and phases have been identified as not only dynamically stable but thermodynamically stable or metastable. Their structural and electronic properties will be presented and discussed.

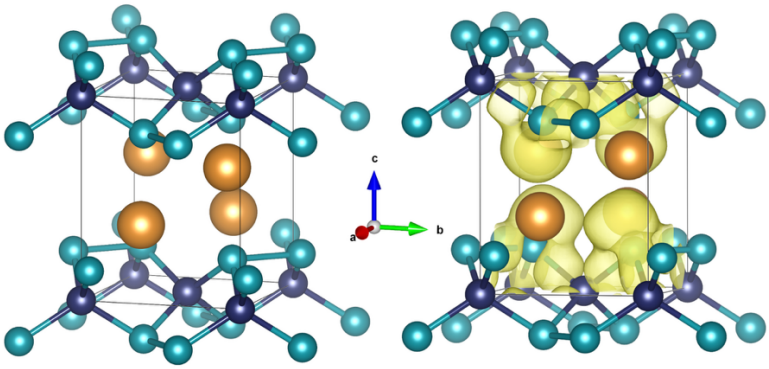

Figure 1. Crystal structure of tetragonal Na_2Si_3 at 5 GPa. The Na atoms are in orange, the four-coordinated Si1 atoms are in blue and the three-coordinated Si2 atoms are in cyan. The electron localization function (ELF) is shown in yellow with an isosurface value of 0.7.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T9.3-O2 Theoretical and Computational approaches

Introducing high-pressure physics into physics education through digital simulations

Ilia SHOLIN (Independent researcher, Bahrain)

Abstract

The current educational landscape of high-pressure physics remains relatively limited and fragmented. To the author's knowledge, high-pressure physics educational activities are largely confined to formats such as summer schools and workshops and primarily target postgraduate students. At the same time, this field of physics offers significant educational potential.

As a part of condensed matter physics, high-pressure physics explores the relationship between phenomena at the microscopic level and the macroscopic properties of matter. In this context, it provides a framework for connecting classical areas of physics in education, such as atomic physics, thermodynamics, and mechanics. Industrial applications of high-pressure physics, such as the synthesis of diamond, provide a relevant context for modernising physics education.

The ongoing digitalisation of education creates new opportunities to integrate high-pressure physics into education. This work presents digital educational simulations based on high-pressure physics (work-in-progress).

Digital Simulation of Sapphire and Diamond Anvil Cells (SAC and DAC)

The simulation enables users to explore the design and operating principles of SAC and DAC. Users can select one of the predefined samples for the SAC or the DAC and simulate an increase in pressure. A section of the screen shows what can be observed through a microscope as pressure increases. Visual observation is currently the only method used in the simulation.

The visual content used in the simulation is based on materials from multiple sources, including:

- photographs and video recordings obtained during our experiments in the SAC at pressures up to 9.5 GPa;
- images from key works in high-pressure physics, as well as video recordings from lecture courses by high-pressure researchers, for example the lecture series "The Diamond Anvil Cell" by Prof. William Bassett.

Pressure Scale

There is a wide range of simulations designed to develop an understanding of distance scales. To the author's knowledge, there are no comparable simulations for pressure. One possible reason is that distance is a much more intuitive physical quantity than pressure. The work presents an approach to understanding pressure scales in nature and technology by 'Pressure Scale' simulation.

The 'Pressure Scale' consists of several independent simulations. Each simulation is focused on a specific theme.

One simulation explores pressure scales in the context of pressures found in the cores of various astronomical bodies. The simulation includes the planets of the Solar System and their moons as reference points.

Another focuses on techniques for generating high pressures. It shows the range of pressures achieved in different high-pressure devices, such as piston–cylinder apparatus, SAC, and DAC. In addition to understanding pressure scales, this simulation also reflects the historical development of high-pressure physics.

Each simulation covers only the range of pressures relevant to the objects it represents.

To reinforce knowledge after engaging with the "Pressure Scale" simulation a mini-game titled "Which Option Has the Higher Pressure?" is used. In this mini-game, users choose between two options and select the one with the higher pressure. The options are drawn from various "Pressure Scale" simulations and allow users to integrate this knowledge into a unified framework. Additionally, the mini-game can be used as a standalone activity, independent of the "Pressure Scale" simulation. This can be done in a mode where the pressure values are either given directly or can be estimated by users with basic school-level physics knowledge, without requiring specialised knowledge in high-pressure physics.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T9.3-O3 Theoretical and Computational approaches

The anomalous melting of antimony hides a liquid-state transformation

Shir BEN SHALOM (Ben-Gurion University of the Negev, Israel)
Roee FRIEDMAN (Ben-Gurion University of the Negev, Israel)
Laura HENRY (Synchrotron SOLEIL, France)
Moran EMUNA (Nuclear Research Center Negev, Israel)
Eyal YAHEL (Nuclear Research Center Negev, Israel)
Guy MAKOV (Ben-Gurion University of the Negev, Israel)

Abstract

The relationship between liquid structure and anomalous melting behavior remains poorly understood, particularly in systems where no solid-phase transition accompanies changes in the slope of the melting curve. In this study, we investigate liquid antimony (Sb) under high-pressure and high-temperature conditions using synchrotron X-ray diffraction, density measurements, and *ab initio* molecular dynamics simulations. The melting curve of Sb initially displays a slightly negative slope, which becomes more pronounced above 3 GPa, reaching the triple point at 5.7 GPa and 840 K, in which three phases are in equilibrium: Sb-I (rhombohedral A7), Sb-II (tetragonal incommensurate host-guest structure), and the liquid phase. We observe a pronounced evolution of the short-range order with increasing pressure, marked by the gradual collapse of the characteristic shoulder in the structure factor *S(Q)* and pair distribution function *g(r)*. Around ~4 GPa, this structural evolution exhibits a distinct change in trend, coinciding with the pressure at which the slope of the melting curve changes. Analysis using the quasi-crystalline model reveals a reorganization of coordination environments consistent with a transformation in the liquid structure. At the same time, angular distribution functions indicate a concurrent modification of local bonding geometry. These results provide direct evidence that the anomalous melting behavior of Sb is governed by a transformation in the liquid state rather than by changes in the solid phase. More broadly, our findings highlight the role of liquid-state transformations in controlling melting behavior in elemental systems.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T9.4-O1 Theoretical and Computational approaches

A Continuous-Path Approach to Crystal Structure Prediction

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Abstract

The prediction of stable and metastable crystal structures at high pressures and finite temperatures remains among the central challenges in condensed matter physics. While existing heuristic algorithms, such as evolutionary structure searching or random sampling, have been widely and successfully used and have driven significant discoveries, they intrinsically lack the physical continuity required to accurately map complex free-energy landscapes. In this talk, we introduce a novel approach to phase space exploration: the cyclic strain-kinetic method. Rather than relying on discrete structural recombination or purely stochastic sampling, this method employs continuous pathways to efficiently traverse multidimensional potential energy surfaces at arbitrary pressure and temperature conditions. The algorithm deterministically escapes local topological traps and maps the true thermodynamic funnels of the system. We will demonstrate the applications of this method through a series of cases under extreme pressure, ranging from the phase transitions of simple elements to the high-pressure behavior of complex compounds. Finally, we will discuss the implications of this continuous-path approach for accelerating the discovery of novel high-pressure phases.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T9.4-O2 Theoretical and Computational approaches

Unconventional multicenter bonds in gold halide perovskites at room and high pressure

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Hussien Helmy Hassan OSMAN (Universidad de Oviedo, Spain)
Vinod PANCHAL (Royal College Mumbai, India)
Oscar GOMIS (Universitat Politècnica de València, Spain)
Alfonso MUÑOZ (Universidad de La Laguna, Spain)
Subrata MONDAL (Presidency University Bengaluru, India)
Ganapathy VAITHEESWARAN (University of Hyderabad, India)
Francisco Javier MANJÓN (Universitat Politècnica de València, Spain)

Abstract

Cesium gold halides are prominent lead-free distorted double perovskites with potential as photovoltaic, photocatalytic, and photosensitive materials. They exhibit $Cs_2Au_2X_6$ (X= Cl, Br, I) stoichiometry and crystallize in a tetragonal structure at room pressure due to the presence of mixed-valence gold states (Au^{I} and Au^{III}). At moderate pressures, they tend to undergo a phase transition to the cubic perovskite with $CsAuX_3$ stoichiometry, characterized by single-valence Au^{II} [1]. Despite the great effort in understanding the phase transitions and properties of these compounds, the chemical bonding present in the different phases of the cesium gold halides — and its relation to their properties— is far from being understood [2,3]. A systematic theoretical bonding analysis of $Cs_2Au_2Cl_6$ reveals that the pressure-induced tetragonal-to-cubic phase transition in the whole $Cs_2Au_2X_6$ family is governed by a fundamental change in the chemical bonding. In $Cs_2Au_2X_6$, bonding is dominated by 1D and 2D X–Au–X electron-rich multicenter bonds (ERMBs). In contrast, $CsAuX_3$ features 3D electron-deficient multicenter bonds (EDMBs) occurring as infinite linear –X–Au–X–Au–X– chains in the three directions (Figure 1). This transformation reflects the gradual pressure-induced polymerization of the $[Au^{I}Cl_2]^-$ and $[Au^{III}Cl_4]^-$ anions into a three dimensional network. The bonding change follows the stages recently proposed by the unified theory of multicenter bonding (UTMB), which explains the origin and mechanism of formation of ERMBs and EDMBs in compounds involving electron-rich elements with valence s- and p-type electrons [4-6]. Importantly, this study reveals that low-symmetry perovskites can feature ERMBs and that cubic perovskites, even those including elements with valence d-type electrons, such as gold, can exhibit EDMBs. These findings provide a bonding-based framework for understanding the unconventional properties of distorted and ideal perovskites that cannot be adequately described within the traditional classification of ionic, covalent, and metallic bonds.

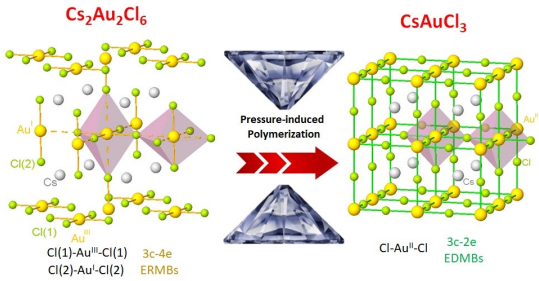

Figure 1. Tetragonal-to-cubic pressure-induced phase transition in the distorted tetragonal perovskite $Cs_2Au_2Cl_6$ leads to a pressure-induced polymerization of $Au^{I}Cl_2$ and $Au^{III}Cl_4$ units (with 1D and 2D ERMBs, respectively) that result in $Au^{II}Cl_6$ units in cubic perovskite $CsAuCl_3$ (with 3D EDMBs).

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[4] H. H. Osman et al., Electron-deficient multicenter bonding in pnictogens and chalcogens: Mechanism of formation. J. Mater. Chem. C 12, 10447 (2024).

[5] H. H. Osman et al., A Unified Theory of Electron-Rich and Electron-Deficient Multicenter Bonds in Molecules and Solids: A Change of Paradigms, J. Mater. Chem. C 13, 3774 (2025).

[6] F. J. Manjón et al., Introduction and Extension of the Unified Theory of Multicenter Bonding: The Role of the Charge-Shift Bonding, Molecules 31, 82 (2026).

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T9.4-O3 Theoretical and Computational approaches

Exploring Structural and non-trivial electronic properties of Ta_2NiSe_5 under pressure

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P. Modak(Bhabha Atomic Research Centre, Homi Bhabha National Institute, Mumbai, India)

Abstract

Ta_2NiSe_5 is a layered material that exhibits two ambient pressure crystallographic phases, orthorhombic Cmcm and monoclinic C2/c. The system undergoes structural transition from the high temperature orthorhombic phase to low temperature monoclinic phase C2/c below 300K [1]. In this work, both phases were optimized using semi-empirical DFT-D3 corrections in conjunction with the optB86b van der Waals functional to properly describe interlayer interactions. The monoclinic phase is a slight distortion of the orthorhombic structure, with $\beta \neq 90°$, while other lattice parameters remain nearly unchanged. Mechanical stability was confirmed by the Born stability criteria, and dynamical stability was verified through phonon dispersion calculations. Enthalpy pressure and volume pressure analyses indicate a pressure induced structural transition from the ambient pressure Cmcm phase to a Pmnm phase at 15 kbar within the same Bravair lattice, accompanied by a volume collapse of ~3%.

As Ta_2NiSe_5 is narrow band gap semi conductor (~100eV-300eV) [2], the calculated electronic band structure exhibits semi metallic behavior, which can be attributed to the well known underestimation of band gaps in density functional theory. The valence band is mainly composed of Ni-d orbitals and Se-p orbitals, while the conduction band is dominated by Ta-d orbitals, and multiple band inversions are observed near the Fermi level. Although the calculated band structure does not show a direct band crossing or touching, the Kane-Mele parity analysis reveals that both ambient pressure phases are topologically non-trivial, with a Z_2 index of (1;000), identifying them as strong topological insulators even in the absence of spin orbit coupling. With increasing pressure, the bands near the Fermi level move closer together, and the orthorhombic phase remains a strong topological insulator up to 15 kbar. Above this pressure, the closing of the bands drives a transition to a topological semimetal. Topological surface states were also calculated for all topologically non-trivial phases. Overall, this study provides a detailed understanding of the pressure driven structural and electronic evolution of Ta_2NiSe_5, highlighting its significance as a pressure tunable topological material.

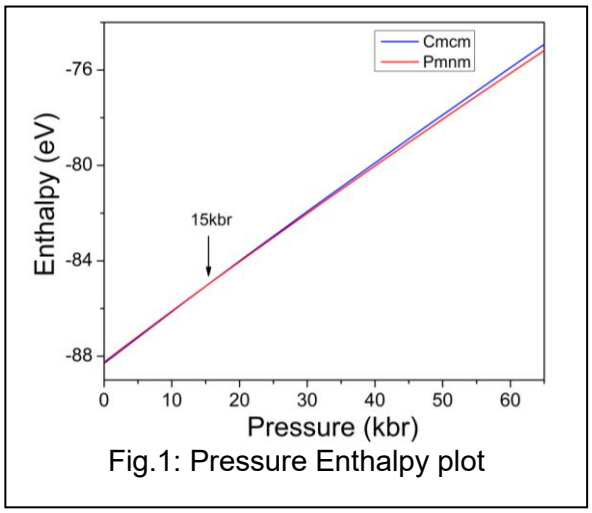

Fig.1: Pressure Enthalpy plot

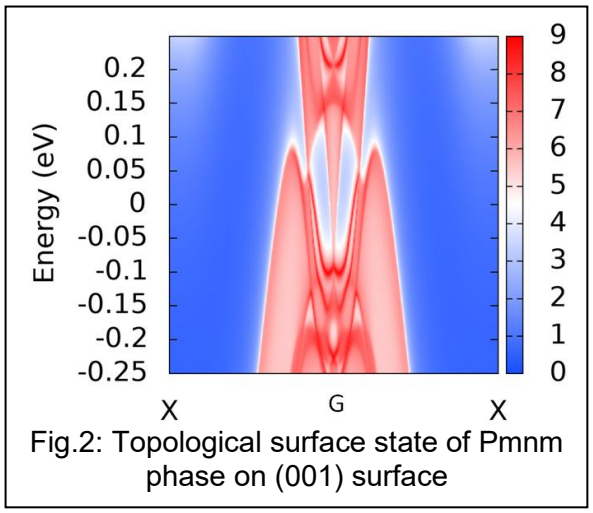

Fig.2: Topological surface state of Pmnm phase on (001) surface

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T9.4-O4 Theoretical and Computational approaches

Efficient Approach to Nuclear Quantum and Anharmonic Thermal Effects in Pressure-Constrained Relaxations

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Abstract

Accurately determining crystal structures under finite temperature and pressure remains one of the central challenges in computational solid-state physics. Standard methods such as the quasi-harmonic approximation (QHA) often lose reliability in systems dominated by strong anharmonic effects — hydrides and other light-element compounds being prime examples.

Molecular dynamics (MD) simulations naturally incorporate full P, T dependencies, but their computational cost grows rapidly with system size and simulation length, and they typically provide access only to time-averaged structural information.

The Temperature-Dependent Effective Potential (TDEP) method offers an appealing alternative by capturing anharmonic behavior through force-constant fitting to thermally sampled configurations. This approach enables the construction of temperature-dependent phonon spectra and free energies while remaining significantly more efficient than MD. I will present a new extension of the TDEP framework designed specifically for performing finite-temperature structural relaxations at high pressure. The method provides a direct route to equilibrium crystal geometries in regimes where anharmonicity is essential and traditional tools fail, thereby improving predictive accuracy for materials under extreme conditions.

I will explain the method and show benchmarks against experimental and previous simulation data for a range of systems.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T9.4-O5 Theoretical and Computational approaches

CrysViz: A Lightweight Browser-Based Platform for On-Device Crystal Structure Visualization and Simulation

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Abstract

Recent advances in machine learning (ML) have fundamentally transformed the discovery of new materials and molecules. Machine-learned interatomic potentials (MLIPs) have accelerated structure search calculations by orders of magnitude, while generative artificial intelligence (GenAI) is beginning to enable the direct prediction of materials with targeted properties. These developments are particularly impactful for high-pressure (HP) research, where the exploration of complex energy landscapes and direct comparison between simulation and experiment is crucial for discovering new chemistry and novel materials with advanced functionalities. However, the ability to generate millions or even billions [1] of candidate materials as well as the synthesis of increasingly complex materials [2], introduce new challenges: efficient methods are required to identify, evaluate, interpret, compare and communicate the underlying crystal structures and motifs, often containing new chemistry.

Bridging this gap requires intuitive, efficient, and customizable visualization tools. We present `CrysViz`, a light-weight browser-based crystal structure visualization and simulation platform that requires no software installation and can be run on any device with a browser, including laptops, tablets, smartphones, and more, while no user provided information is leaving the device. `CrysViz` is fully open source, supports easy user customization, and can be extended through a module system, specifically designed to address the diverse tasks in HP research. The platform allows (1) visualization, (2) MLIP simulations, and (3) data sharing:

(1) `CrysViz` supports a wide range of commonly used input formats (*e.g.,* CIF, POSCAR, OUTCAR, PWscf input, XYZ, …) as well as output formats (*e.g.,* OUTCAR, PWscf output, .res, extended XYZ, ...) with options for bulk upload of hundreds of structures in, *e.g.*, XYZ or .res format, to screen quickly through the results of structure search campaigns. If information about forces or spin states is present, these quantities are automatically read and can be visualized without additional user intervention. Three-dimensional fields, such as charge densities and electron localization functions (ELFs), can be imported from CHARGECAR or .cube files and visualized via isosurfaces and planar cuts. A structure comparison module allows the detailed comparison between, *e.g.*, synthesised and calculated crystal structures or structures under different pressure conditions, including calculation of relative lattice and volume difference. In addition, `CrysViz` provides tools for symmetry analysis and crystal structure symmetrization.

(2) Despite the increasing availability of machine-learning-based simulation methods, advanced MLIPs often require expertise in terminal-based workflows and access to HPC infrastructure, which limits their accessibility for non-computational scientists. `CrysViz` addresses this limitation by enabling lightweight, on-the-fly simulations directly in the browser, with all computations performed locally on the user's device. Users can run and monitor simulations in real time, including molecular dynamics and equation-of-state calculations relevant for high-pressure studies, as well as Birch Murnaghan EOS fitting, along with convergence analysis and visualization. This allows quick screening of results before further expensive calculations are started. Higher level potentials can be accessed via an ASE interface using the optional `CrysVizBackend` package that can be run by the user.

(3) Effective communication of results is equally crucial. CrysViz allows sharing results through link-based embedding, where the complete state of a visualization, including structure, orientation, coloring, and even inter-atomic distance or angle measurements, is encoded within the URL itself. This allows to highlight structural features and enables more efficient sharing of information with collaborators and in publications. By creating links on one device and rendering the visualization on another device only from the link, information is transferred securely with no data storage required and no reliance on server-side infrastructure.

I will present the full functionalities of `CrysViz` and demonstrate a range of different use cases.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T1-P01 Bio/Life Sciences, Food Science and Technology

High hydrostatic pressure as a modulator of microplastic–microbiome interactions: a deep-sea analogue approach

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Abstract

Microplastics (MPs) are now ubiquitous in the deep ocean, yet their fate and their interactions with deep-sea microbial communities remain poorly understood. Under the high hydrostatic pressures prevailing below 1000 m, both microbial physiology and polymer surface properties may be profoundly altered, with potential consequences for MP colonization, biodegradation, and additive release. The PLASTIS project addresses these questions through a multi-scale experimental approach combining high-pressure milli- and microfluidic devices with molecular and physicochemical analyses.

Polystyrene microbeads (PS, 6 µm) were incubated with natural marine microbial communities at atmospheric pressure (AP, 0.1 MPa) and high pressure (HP, 10 MPa) conditions in sapphire millifluidic tubes and all-sapphire microreactors (devices that withstand pressures up to 300 bar while remaining optically transparent), enabling *in situ* monitoring by Raman spectroscopy and optical microscopy. Artificial weathering of PS beads prior to incubation induced surface cracking, as confirmed by TEM and AFM, potentially promoting microbial colonization.

16S rRNA metabarcoding revealed that hydrostatic pressure significantly restructures microbial communities associated with MPs: *Pseudomonadota* were enriched under HP conditions, while *Bacteroidota* were proportionally more abundant at AP. These trends were confirmed across two independent datasets , the latter including a range of polymer types (LDPE, polypropylene, expanded PS, bioplastic). Bioplastics incubated under HP showed distinct taxonomic profiles compared to conventional plastics, suggesting a combined effect of polymer nature and pressure on microbial community assembly.

Raman and FTIR analyses of incubated polymers further revealed surface chemical modifications under both AP and HP conditions, consistent with biotic and/or abiotic alteration processes. These physicochemical signatures complement the microbiological data and support the establishment of correlations between community structure and polymer surface state.

Together, these results demonstrate that high hydrostatic pressure is a key modulator of MP–microbiome interactions in the deep ocean, and that high-pressure sapphire microfluidic devices offer a powerful platform for their controlled investigation.

Acknowledgments: This work was supported by the CNRS Mission pour les Initiatives Transverses et Interdisciplinaires (PLASTIS, PIB2024).

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T1-P02 Bio/Life Sciences, Food Science and Technology

The HHP-NMR unfolding study of the yeast Frataxin Yfh1 at variable temperature gives essential clues on the heat- and cold-induced denaturation of the protein.

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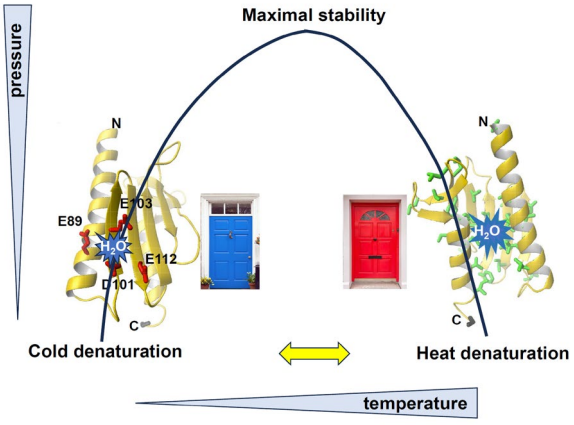
Abstract

Proteins unfold under different environmental insults, among which are heat, cold, high pressure and chaotropic agents. Understanding the mechanisms that determine unfolding under each of these conditions is an important problem that directly relates to the physical forces that determine the three-dimensional structure of a protein. Here, we studied the unfolding transitions of the marginally stable (in the absence of salt) yeast Frataxin Yfh1 using high-hydrostatic pressure nuclear magnetic resonance (HHP-NMR) at variable temperature: this technique is uniquely suited for protein unfolding studies at a residue-level resolution [1-3] , providing local information on the behaviour of different regions of a protein. We compared the cold, heat and pressure unfolded states. We show that the pressure-induced unfolding pathways at low and high temperatures differ [4], suggesting a synergic mechanism between pressure- and temperature-induced denaturation. Our observations help us to reconstruct the structural events determining unfolding and distinguish the mechanisms that rule the different processes of unfolding.



Cartoon showing the forces determining thermal unfolding at low and high temperature under mild pressures. The structure of Yfh1 is plotted to visualize where water starts entering in the two conditions symbolized as two different virtual doors (indicated in blue and red for cold and heat unfolding): at low temperature, where hydrophobic forces are weaker, the electrostatic repulsion between side chains near the N-terminus of the protein will determine opening of the structure, whereas at high temperature the partial exposure of the hydrophobic core due to the shorter C-terminus allows the structure to unfold starting from the C-terminus. The process becomes completely cooperative at high pressure and it is not longer possible to distinguish the two pathways..

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T1-P03 Bio/Life Sciences, Food Science and Technology

Influence of high hydrostatic pressure on Mexican jackfruit seed proteins

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Abstract

High hydrostatic pressure (HHP) modified the native structure of jackfruit seed proteins, with the greatest effect observed at 600 MPa for 30 min after pressure release. DLS revealed protein aggregation, while thermal analysis indicated changes in the energy required for denaturation, suggesting partial unfolding and the formation of aggregates stabilized by weak noncovalent interactions. These structural changes may improve techno-functional properties, although further optimization of HHP conditions and Native-PAGE analysis are required to characterize the aggregates and support their application as alternative food protein ingredients.

Continuous Flow Synthesis of Spin Crossover Materials for Solid-State Green Refrigeration

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The increasing global demand for cooling technologies represents a major environmental challenge. Recent reports indicate that refrigeration systems account for up to 20% of global electricity consumption and approximately 7.5% of total CO_2 emissions, arising from both energy use and refrigerant leakage [1]. In this context, the development of alternative solid-state cooling technologies is crucial to reduce the environmental impact of current vapor-compression systems. Among emerging solutions, barocaloric cooling based on mechanocaloric effects [2] has attracted significant attention. Spin-crossover (SCO) materials [3], in particular, exhibit large and reversible entropy changes associated with electronic transitions under external stimuli such as temperature or pressure. Their strong coupling between structural, electronic, and thermodynamic properties, combined with sensitivity to relatively low pressures, makes them promising candidates for next-generation cooling devices [4].

However, a major limitation for their technological implementation lies in their synthesis, processing and scaling up. SCO materials are typically obtained as poorly controlled polycrystalline powders through batch precipitation, leading to limited reproducibility, broad particle size distributions, and strong sensitivity to synthesis conditions. Since their functional properties are directly linked to microstructure, morphology, and phase identity, controlling nucleation and growth mechanisms is essential [5].

In this work, continuous flow chemistry is explored as a powerful strategy to overcome these limitations. Flow processes enable precise control over reaction parameters such as mixing, residence time, concentration, and temperature, allowing the decoupling of nucleation and growth steps [6]. This control directly impacts particle size and crystallinity, highlighting the importance of mixing regimes and concentration in determining final material properties. In particular, the implementation of quench strategies enables the limitation of particle growth by rapidly modifying reaction conditions, leading to smaller and more controlled particles [7].

In parallel, the integration of supercritical CO_2 ($scCO_2$) processing is investigated as a unique transport and extraction properties, enabling efficient solvent removal without capillary stresses and preserving particle morphology and microstructure [8]. The combination of continuous flow synthesis with $scCO_2$ drying (with or without co-solvents) provides a promising route toward controlled, reproducible, and scalable production of SCO molecular materials [7]. However, the implementation of such an approach for molecular coordination materials is far from trivial, as it involves fast precipitation reactions, strong sensitivity to mixing conditions, and complex nucleation–growth mechanisms that critically influence phase formation and final properties. The ultimate objective of this work is to develop an integrated and sustainable process enabling the large-scale production of spin-crossover materials for their integration into barocaloric heat exchangers, contributing to the emergence of alternative refrigeration technologies.

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HP/HT synthesis and in situ investigation of K doped Pb_2FeMoO_6 perovskite: tuning properties via A-site substitution

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The coexistence of magnetism and ferroelectricity requires very strict and specific symmetry conditions, which can be achieved in Pb-based double perovskites ($Pb_2BB'O_6$) due to the great tolerance of these systems to cationic substitutions and structural distortions. This study starts from the $Pb_2Fe^{3+}Mo^{5+}O_6$ (PFMO) system, a material that shows a semi-metallic to half-metallic transition at the FiM state (270 K) and an asymmetric magneto-resistivity below T_N. [1-2] In order to decrease the conductive character of the material, a strategy was devised to lower the electric charge on the A site and reduce the number of free electrons (by enhancing the Mo oxidation state) through the partial substitution of the Pb^{2+} ion with the alkali ion K^+.

The synthesis of $KPbFeMoO_6$ compounds was carried out using High Pressure/High Temperature (HP/HT) techniques with a multianvil press, which allows solid-state reactions in extreme regimes (up to 22 GPa and 2200°C). To find the best pressure-temperature stability conditions, the structural reactions were monitored in-situ in real-time via Energy-dispersive X-ray diffraction at the P61B Large-Volume press beamline at DESY.

The analysis of compounds ($K_xPb_{2-x}FeMoO_6$ with x=0.35-0.4) demonstrated the achievement of a phase isostructural to PFMO, with a perovskite purity of more than 92% considering some impurities and surface degradation products. Physical results reveal that the introduction of K^+ significantly modifies the material's behavior: the resistivity increases compared to PFMO, good dielectric constant values are recorded, and the magnetism shifts to a broad antiferromagnetic (AFM) transition with a T_N of ~50 K.

In conclusion, the combination of HP/HT synthesis and synchrotron investigations proves to be an indispensable approach to metastabilize unusual oxidation states, discover critical structural transformations that are completely inaccessible via standard ex-situ analysis, and fine-tune the properties of multifunctional materials. Further investigations, specifically at ESRF on ID14, will allow us to investigate iron and its surroundings.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T2–P06 Chemistry, Synthesis, Novel materials

Keep Cool with Crystals: Crystals under Pressure for the Refrigeration of the Future.

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Michaël JOSSE (Univ. Bordeaux, CNRS, Bordeaux INP, ICMCB, UMR 5026, FR),
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Abstract

Refrigeration devices we use in everyday life (air conditioners, refrigerators, etc.) are responsible for 8% of global greenhouse gas emissions. An alternative to refrigerant gases would be the use of a technology based on a solid, easily handled and recyclable, and its mechanical response to a pressure/depression cycle [1]. Among these materials, known as barocaloric materials, molecular spin-crossover (SCO) compounds have been identified as having promising barocaloric potential [2,3]. Although obtaining these materials in single-crystal form is complex, large quantities of polycrystalline powder can be produced from non-critical, inexpensive, abundant, and non-toxic elements. However, using powder in a technological application is challenging. Being able to process it into a more compact form, in order to facilitate the handling of the material of interest, is therefore a prerequisite for technological development.

While Cool-SPS (Spark Plasma Sintering) pelletizing has been demonstrated on various model systems to produce compact, centimeter-sized monoliths of brittle compounds [4], only one study has been reported for a molecular spin-crossover (SCO) material [5] leading to resulting densities comprising between 80 and 90% of the density of the corresponding crystal structure. The densification via Cool-SPS of new molecular SCO compounds has been investigated within the framework of FROSTBIT project (First Regenerative Solid-State Barocaloric Refrigerator) and will be presented. The FROSTBIT project relies on these molecular pellets to develop a regenerative cooling device with the aim of producing a fully functional refrigeration prototype.

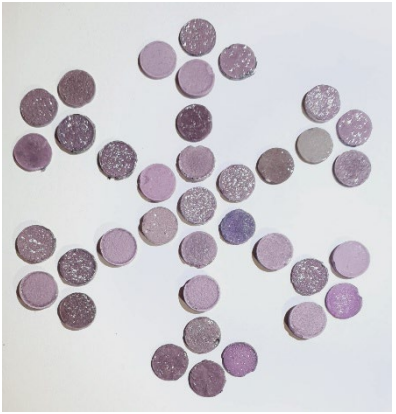

Figure: Pellets of molecular compounds for barocaloric refrigeration.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T2-P07 Chemistry, Synthesis, Novel materials

Caffeine enabling high-pressure research on new light element compounds

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Abstract

The combination of the elements H-C-N-O at extreme conditions serves as both a challenging and fundamental chemical system. Understanding it could be relevant for the chemistry inside the mantles of ice giants, the discovery of new materials, or even the origin of life itself.

High pressure has already revealed a remarkable richness of chemistry in light-element systems. Examples include polymeric nitrogen phases with exceptionally high energy density (Eremets et al., 2004), superionic water ice with simultaneous crystalline and liquid-like behavior (Prakapenka et al., 2021), and hydrogen-rich compounds exhibiting superconductivity at record-high temperatures (Drozdov et al., 2015). These discoveries highlight how compression can fundamentally alter chemical bonding and lead to entirely new classes of materials and physical properties.

While the binary, and to a lesser extent, ternary hydrogen-rich light-element systems (H_2, CH_4, H_2O, NH_3, etc.) have received extensive attention in the literature, there have been fewer efforts to explore the ternary and quaternary hydrogen-poor (H)-C-N-O phase diagram at extreme pressures. In order to shed light on this darker shade of chemical space, we utilize laser-heated Diamond Anvil Cells (LH-DACs) to synthesize new compounds and employ a range of spectroscopic and X-ray diffraction techniques to analyze their structure and properties.

The chemical reactions are facilitated by the high temperatures generated by the laser at the locally heated spot. While these temperatures usually enable the crystallization of thermodynamically stable phases, the steep thermal gradients can also result in the formation of kinetically stable phases. This makes the subsequent compositional and structural analysis particularly challenging. We employ primarily multi-grain X-ray diffraction to carefully analyze the composition of the resulting experiments at micron precision.

One of the main challenges in designing experiments for the synthesis of new phases is the choice of suitable precursors. Both multi-source and single-source precursors can be used, but single-source precursors offer the advantage that the chemical space within the laser-heated spot is homogeneous. This confinement is crucial for systematically exploring the complex chemical space of a multidimensional phase diagram. To investigate this light-element system, simple organic molecules may be used as single-source precursors with a fixed stoichiometry. Examples of such hydrogen-poor systems include cyanuric acid ($(HCNO)_3$), urazole ($H_3C_2N_3O_2$), and even caffeine ($C_8H_{10}N_4O_2$).

In this contribution, I will present the first results of my research dedicated to exploring this largely uncharted region of the H-C-N-O phase diagram at extreme pressures.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T2-PO8 Chemistry, Synthesis, Novel materials

Synthesis and characterisation of high-T_c metal hydride thin-films at megabar pressure

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Abstract

The discovery of the hydride superconductor H_3S in 2015 with a T_c record of 203 K at 155 GPa ignited the search for high-T_c superconductivity in compressed hydride compounds [1]. Since, several other hydride compounds have been synthesised such as LaH_{10} [2, 3], YH_6 [4, 5] and YH_9 [5], exhibiting superconductivity close to room temperature under megabar pressures. At present, hydride synthesis is typically carried out via *in-situ* laser heating of bulk precursors together with a hydrogen donor material at high-pressures inside a diamond anvil cell (DAC). One common challenge is the synthesis of single-phase hydrides, in-part due to partial or inhomogeneous hydrogenation during laser heating, yet it is important for careful interpretation of the intrinsic superconducting properties. Toward this objective, our group in Bristol has developed a novel approach to synthesise hydrides from an elemental thin film evaporated directly onto the diamond anvil, with ammonia borane (NH_3BH_3) as a hydrogen donor [6, 7]. Thin film deposition techniques are also used to fabricate robust electrodes, with low electrical resistance, capable of withstanding pressures of up to 250 GPa. This approach facilitates the formation of superhydrides by ensuring a high hydrogen to metal ratio during synthesis and permits accurate control over initial sample dimension and placement relative to the use of bulk precursors. Moreover, the thin films adhere very well to the culet surface, make excellent electrical contact to the underlying electrodes, and remove the requirement for the manipulation of very small (~ 10 µm) air sensitive bulk samples on the culet. Within our team, development of such techniques has greatly increased the success rate for hydride synthesis.

In this poster, we present a detailed overview of the methods used for the preparation of thin-film hydrides, including electrode preparation, film evaporation, and the laser-heating techniques. Experimental developments will be illustrated with examples such as the discovery of high-T_c superconductivity in the novel clathrate hydride La_4H_{23} [7], as well as our recent synthesis of the record superconductor LaH_{10}. We will present high-resolution structural and electrical characterisation of our high-T_c films and demonstrate that their properties are consistent with those reported in bulk samples. We believe thin-film hydride synthesis could pave the way for future detailed and controlled studies of promising ternary and quaternary hydrides.

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Funding Acknowledgement

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T2-P09 Chemistry, Synthesis, Novel materials

High pressure synthesis of manganese superhydride MnH_7

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Abstract

Through high-temperature, high-pressure diamond anvil cell studies combined with in situ synchrotron powder X-ray diffraction, we investigate the reactivity between manganese and hydrogen up to 182 GPa. Laser heating manganese in an H2 medium at 118 GPa yields body-centered tetragonal MnH_7, which has the highest hydrogen content ever observed in the binary hydrides of group IV-X11 transition metals. In addition, we also observe two other new hydrides as minor phases, MnH_2 with a tetragonal crystal structure and cubic $MnH_{3.67}$, formed at the pressures of 105 and 118 GPa, respectively. Upon decompression, $MnH_{3.67}$ and MnH_7 remain stable down to ~30 GPa before decomposing into the monohydride. Our ab initio quantum chemistry computations employing density-functional theory reveal that the key stabilization factor of $MnH_{3.67}$ and MnH_7 is zero-point energy, however, no isotope effect is observed on the crystal structures of the deuterated samples.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T3-P10 Electronic, Magnetic, Caloric and Transport properties

Pressure and Field Tuned Magnetism in the Honeycomb Antiferromagnet $Na_3Ni_2BiO_6$

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Abstract
Hydrostatic pressure offers a contolled and effective means to modifying the crystal structure and exchange interactions without chemical substitution. In this context, the layered nickelate compound $Na_3Ni_2BiO_6$ is a promising structure to test the influence of pressure on its magnetic properties. It crystallizes in the monoclinic α-$NaFeO_2$-type structure, where Ni^{2+} ions (S = 1) form two-dimensional honeycomb layers and develop long-range antiferromagnetic order with ($T_N \approx 10.4$ K) and a positive Curie–Weiss temperature, (θ_{CW} = 13.3 K) [1]. Here, we present a systematic study of the magnetic response of polycrystalline $Na_3Ni_2BiO_6$ as a combined function of applied magnetic field (H) and hydrostatic pressure (p).

At $\mu_0 H$ = 0.1 T and no applied pressure, we observe the antiferromagnetic transition at 10.5 K. The Curie-Weiss fit of the high-temperature susceptibility gives an effective moment μ_{eff} = 3.25 μ_B/Ni^{2+} and θ_{CW} = 13.7 K, consistent with earlier reports [1]. T_N decreases with increasing magnetic field, from 10.5 K at 0.1 T to 8.30 K at 7 T, in agreement with previous work [2]. Moreover, we find that hydrostatic pressure, in combination with the applied magnetic field, suppresses the antiferromagnetic transition temperature as shown in Fig. 1, $\Delta T_N/\Delta p$ increasing in magnitude from −0.2 to −0.58 K/GPa with increasing pressure and field. We tentatively attribute this shift to an anisotropic compression of the layered structure, as observed in the structurally similar compound $Na_3Co_2SbO_6$ [3]. These results show that the magnetic ground state of $Na_3Ni_2BiO_6$ is tuneable by the combined action of magnetic field and pressure. Future work will aim to extend these measurements to single crystals and to higher pressures accessible with diamond anvil cells.

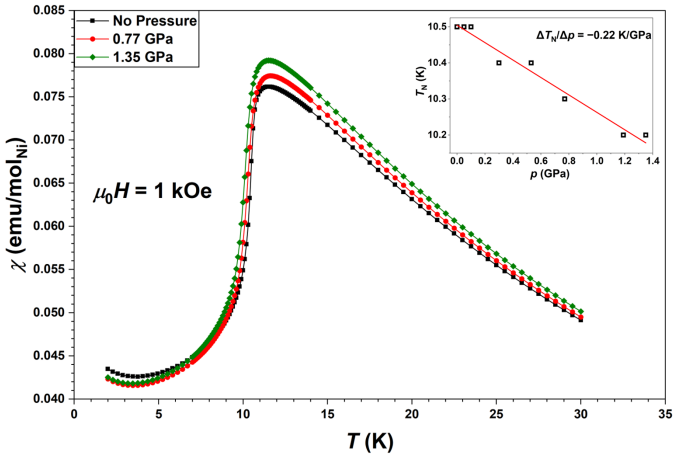

Fig. 1. Temperature dependent susceptibility of $Na_3Ni_2BiO_6$ at $\mu_0 H$ = 1 kOe under pressures of 0, 0.77, and 1.35 Gpa, respectively show a progressive suppression of the T_N. Decrease in T_N as a function of pressure (Inset).

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T3-P11 Electronic, Magnetic, Caloric and Transport properties

Quantitative and qualitative high pressure calorimetry for in situ studies

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Abstract

High pressure, high temperature calorimetry is a vast field that can include numerous measurements, most of which include implicit or explicit temperature measurements while heating, compressions or both. Historically, experimental calorimetry gave solid background not only in applied metallurgy, but also to numerous idea in fundamental physics, such as quantum theory of solids, superfluidity and superconductivity ; and in petrology, where calorimetry on silicates has provided useful inputs for modelling magmatic processes.

At present time, qualitative and quantitative high-pressure calorimetry remains a big challenge to petrology and fundamental physics aiming room-temperature superconductivity. Probing the chemical interactions and phase transformations would also be a big deal, since even qualitative calorimetric data would be an in house alternative to highly costly synchrotron in situ probing.

High pressure, high temperature conditions are typically attained in high pressure cells with cylindrical space [1] to be filled with sample, thermocouples, oven, etc. Adapted AC method [2] can be employed along with DTA variations [3, 4]. A number of successful applications related to Si materials will be presented and discussed [4, 5].

In the proposed poster we will highlight a number of examples of accomplished or preliminary calorimetric studies of light element compounds (Si, Na-Si) using various temperature and power regimes.

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Pressure-Enhanced Charge Density Wave Order and Anisotropic Lattice Strain in $BaFe_2Al_9$

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Abstract

The hexagonal intermetallic compound $BaFe_2Al_9$ provides an interesting platform to study the coupling between electronic ordering and lattice response under external pressure. In this work, we focus on the pressure evolution of its electrical transport and crystal structure using high-pressure resistivity and synchrotron powder X-ray diffraction measurements. At ambient pressure, $BaFe_2Al_9$ shows a clear resistivity anomaly near 112 K, associated with the onset of charge density wave order. With increasing pressure, this transition shifts systematically to higher temperatures and approaches room temperature at around 3.2 GPa. This behavior is unusual because pressure commonly suppresses charge density wave order, whereas in $BaFe_2Al_9$ it strongly enhances the transition temperature. The low-temperature resistivity follows a Fermi-liquid form, $\rho(T)= \rho_0+AT_2$. The pressure dependence of the residual resistivity and Fermi-liquid coefficient indicates a significant modification of the electronic scattering and suggests a pressure-induced reconstruction of the electronic structure.

High-pressure synchrotron X-ray diffraction measurements performed up to ~7 GPa show that the hexagonal crystal symmetry is preserved over the measured pressure range, with no evidence for a pressure-induced structural phase transition. However, the lattice parameters exhibit anisotropic compression, with a stronger response along the c-axis compared with the basal plane. In addition, the pressure-dependent microstrain parameters show a pronounced change at ~ 3.6 GPa, close to the pressure region where the charge density wave transition reaches room temperature. These results indicate that anisotropic lattice strain plays an important role in stabilizing the high-temperature charge density wave state in $BaFe_2Al_9$. Overall, the combined high-pressure transport and X-ray diffraction results reveal a strong coupling between lattice compression, microstrain, and electronic ordering in $BaFe_2Al_9$, making it a rare example of a three-dimensional intermetallic compound in which pressure promotes charge density wave order.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T5-P13 Instrumentation, Metrology and Techniques

Almax easyLab Solutions for Extreme Pressure Science

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Keywords: Diamond anvil cell, Megabar pressure, UV laser drilling

Abstract

Experiments above the megabar regime are increasingly important in modern high-pressure research but remain technically demanding. We present recent developments from Almax easyLab designed to facilitate routine experiments above 100 GPa.

The newly developed MegabarDAC (diamond anvil cell) improves diamond stability at ultra-high pressures by minimizing shear motion during compression [1,2], while providing a large optical aperture and compatibility with standard gas-loading systems (Figure Left).

In addition, the PulseCube UV laser drilling system enables precise gasket preparation with hole diameter down to 5 µm, producing higher quality results than conventional IR laser or EDM drilling methods (Figure Right).

Together, these developments contribute toward making routine multi-megabar experiments more accessible to the high-pressure community by improving experimental reliability, precision and ease of use.

Figure: (Left) The MegabarDAC cell, (Right) The PulseCube UV laser drilling system.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T5-P14 Instrumentation, Metrology and Techniques

Periodic dynamic oscillations of iron in diamond anvil cells

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Abstract

Dynamic diamond anvil cells (dDACs) are devices that can generate time-controlled stress. We used them to create periodic stress oscillations in order to study the viscoelastic behavior of hexagonal close-packed (hcp) iron. Iron with an hcp structure is considered to be a main component of the Earth's inner core[1]. Consequently, viscoelastic effects in iron are related to seismic attenuation deep within the Earth[2]. However, hcp iron only exists at pressures above ~15 GPa. For this reason, we had to perform experiments in a DAC.

Here, we compress iron foils in different pressure-transmitting media (PTMs) and apply different stress amplitudes at varying frequencies to observe the viscoelastic response of the system. The periodic stress oscillations are generated by a remotely controlled piezo element that pressed the DAC at pressures between 25 and 110 GPa. We derive the magnitude of the stress/strain oscillations in the pressure chamber by analyzing the variation in interplanar distances and peak widths by in-situ X-ray diffraction. Although our results require further investigation, we clearly observed a time shift in strain and stress between the iron and the different PTMs. This proves the fundamental possibility of studying viscoelasticity by dynamic oscillations in a DAC.

Periodic time dependencies of interplanar distances and peak widths show the time shift in these parameters between PTMs and iron sample. This time shift in periodic effects between PTM and iron points out to the occurrence of viscoelastic relaxation in the sample assembly. Based on the frequency of oscillation, we can recalculate the time shift to the phase lag and thus derive a version of quality factor Q. The experiments raise many questions regarding the origin of the observed quality factor Q. Therefore, our experimental work is being complemented with elasto-viscoplastic self-consistent (EVPSC) modeling of the deformation of iron and its response, as measured using X-ray diffraction. Ultimately, we expect to gain an understanding of the processes involved in periodic dynamic oscillations in a DAC. This should pave the way for the use of dDAC for viscoelasticity measurements under high-pressure conditions.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T6-P15 Crystallography at High Pressure

Pressure-Induced Helium Trapping in Sr_2FeIrO_6 Double Perovskite

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Abstract

Double perovskites containing transition-metal ions with strong electronic correlations and spin–orbit coupling provide an excellent platform to explore the coupling between crystal structure, lattice compressibility, and local electronic environments under extreme conditions. In this work, we report pressure-induced helium trapping in the double perovskite Sr_2FeIrO_6,[1] investigated using high-pressure synchrotron X-ray diffraction with helium as pressure-transmitting medium.

Our results show that, upon compression, helium atoms are incorporated into the Sr_2FeIrO_6 structure, producing a clear modification of its pressure–volume response. The trapped helium reduces the effective compressibility of the material and alters the equation of state with respect to the behaviour expected for a purely compressed framework. This demonstrates that helium, often considered an inert hydrostatic medium, can actively interact with host structures under pressure. The combined experimental and theoretical results therefore provide a consistent picture of pressure-induced helium uptake and its direct influence on the mechanical response of the material.

This study highlights the importance of considering pressure-transmitting media as active chemical agents in high-pressure experiments. The observation of helium trapping in Sr_2FeIrO_6 opens new perspectives for tuning the structural and electronic properties of complex oxides through the controlled incorporation of noble gases under compression.

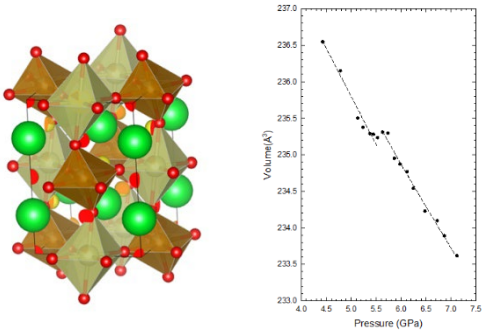

Figure1. (left) Scheme of the Sr_2FeIrO_6 with helium inclusions. (right) P-V Equation of state of SFIO with helium.

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Low-temperature High-pressure Sample Environment for Single Crystal and Powder X-ray Diffraction -for I15 beamline of Diamond Light Source

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Abstract

A low-temperature cryostat for high-pressure single-crystal and powder X-ray diffraction is currently in an advanced stage of commissioning in parallel at the Extreme Conditions beamline I15 at Diamond Light Source (DLS, UK) and at the ADDAMS beamline at the Paul Scherrer Institute (PSI, Switzerland). The I15 beamline operates in the high-energy range of 20–80 keV and ADDAMS beamline offers 5-40 keV. Both provide focussed and collimated X-ray beam well suited for high-pressure diffraction studies.

The cryostat for diamond anvil cells (DACs) is a custom-built cryogen flow system from DAC Tools (www.DACTools.com), using a controlled flow of liquid nitrogen or liquid helium to access cryogenic temperatures. Temperature control is achieved via heaters and sensors located near the sample and cold finger. A double-membrane DAC arrangement enables fine in-situ pressure control. The system provides optical access for pressure determination via ruby fluorescence. Sample temperatures as low as 11 K and 80 K can be achieved using liquid helium and liquid nitrogen, respectively. Cu-Be made mSSDAC-80-BeCu diamond anvil cells from DAC Tools (www.DACTools.com) are being used for efficient cooling and better thermal stability.

This capability will provide a powerful platform for structural investigations of pressure and temperature-tuned phenomena such as superconductivity [1], charge density waves [2], and structural phase transitions, as well as materials relevant to extreme planetary environments, including icy moon hydrospheres [3–4]. High-pressure, low-temperature phase boundaries can also be accurately mapped. The ability to perform experiments under cryogenic conditions further suppresses unwanted chemical reactions and diffusion processes, which is particularly important for reactive systems such as alkali metals and hydrogen-rich compounds.

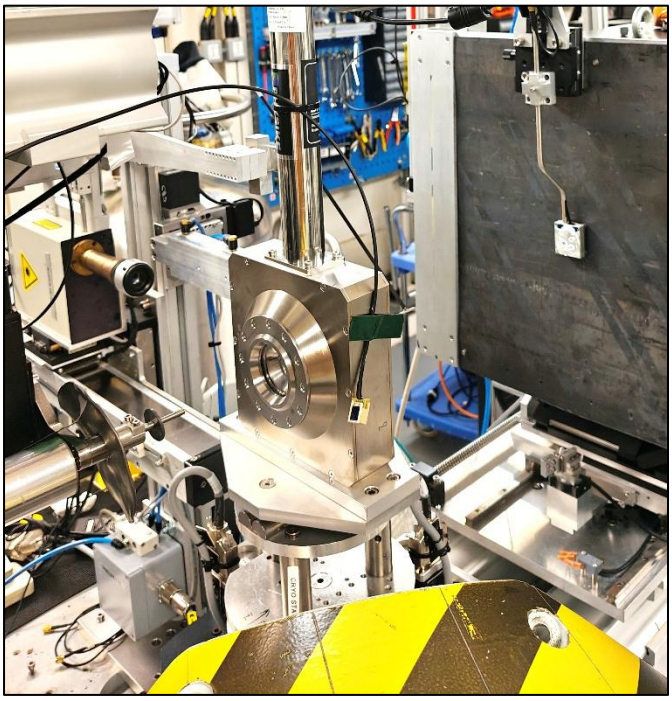

Figure 1: Cryostat on the diffractometer of I15 beamline

The cryostat is being optimized for reliable, user-friendly operation and seamless integration with beamline instrumentation. This poster presents the current configuration and highlights recent results from commissioning activities, with a focus on developments at DLS, demonstrating the current performance and potential of the system for advanced high-pressure, low-temperature diffraction studies.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T6-P17 Crystallography at High Pressure

Structural characterization of amorphized quartz resulting from diamond anvil cell and shock experiments

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Abstract

Amorphous silica is among the most extensively studied disordered materials owing to its fundamental importance in a wide range of technical applications and scientific research fields. While vitreous silica is the archetypical glass produced by rapid quenching of an SiO_2 melt to ambient temperature, amorphous silica can also form through amorphization of quartz in the solid state at high pressures [1, 2, 3]. A particularly intriguing modification of amorphous silica is formed through the extreme conditions of meteorite impacts and shock experiments in the laboratory. For peak shock pressures ranging between approximately 10 to 35 GPa, planar deformation features are formed in quartz, which are sets of amorphous lamellae oriented parallel to low-index crystallographic planes [4, 5, 6]. For even higher peak shock pressures, quartz transforms completely into a so-called diaplectic glass.

Diaplectic glasses possess intriguing properties that are distinct from those of vitreous silica. For example, diaplectic glasses exhibit enhanced densities and refractive indices [4] and display a different annealing behavior [7]. Despite few investigations on the structures of diaplectic glasses [8], the structural characteristics leading to the distinct behavior of diaplectic glasses remain unclear to date.

Here, we investigated and compared the short-range order in the structures of amorphized quartz resulting from different experiments under extreme conditions – namely shock experiments on single crystals of quartz [5] and rapid compression experiments on powder samples of quartz at room temperature using the membrane-driven diamond anvil cell (mDAC). From the collected diffuse scattering of the amorphous silica, we calculated and analyzed structure factors and pair distribution functions. These indicate several differences in the short-range order of the amorphous silica samples. The structures of amorphized quartz are denser than the structure of vitreous silica. In agreement with previous results of shock-recovery experiments [4, 5], this compaction apparently decreases with increasing peak shock pressure, because the residual temperatures increase as a function of pressure. This is corroborated by DAC experiments at room temperature, which indicate that the density of amorphized quartz is increased. We can explain the differences also with the residual increased coordination of the silicon atoms in amorphized quartz after pressure decay. Detailed structural characteristics are provided by means of pair distribution functions, that may explain the distinct behavior of diaplectic glasses.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T6-P18 Crystallography at High Pressure

The stishovite to post-stishovite phase boundary studied by stress cycling experiments in a dDAC

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Abstract

Stishovite and post-stishovite, the stable forms of SiO_2 at mantle conditions, are important mineral phases in the lower mantle, in particular in subduction zone environments, where Mid-Ocean Ridge Basalt (MORB), the crustal component of the subducting slabs, contains up to 20 Vol.% of SiO_2. Deeper, where MORB might delaminate from the rest of the subducting slab, it might stagnate at around 600-1000 km depth. Ultimately, MORB will sink toward the base of the mantle, potentially feeding the LLSVPs or other heterogeneities near the CMB. Other scenarii also propose that SiO_2 can exsolve into the mantle from the crystallising core, or that SiO_2-rich regions can exist as remnants of the magma ocean.

Stishovite and post-stishovite are thus important components of the dynamic mantle, in the regions that are the most crucial to image by seismology and advance our understanding of the dynamics of the Earth's interior.

The stishovite to post-stishovite transition is characterised by elastic anomalies, but its impact on mantle physical properties and seismic wave propagation has not yet been completely understood. For instance previous studies have reported softening of the shear modulus of stishovite near the phase boundary, with strong differences depending on the stress condition of the sample (isostress vs isostrain). Another study has highlighted a strong sensitivity of the phase transition to stress. Hence the real-world physical behaviour of polycrystalline SiO_2 across the stishovite to post-stishovite boundary under a cyclic loading, as imposed by a seismic wave in the mantle, could be different to what is expected based on hydrostatic equation of states or classic compression experiments. In addition, non-elastic responses to cyclic stresses, including attenuation, are poorly explored by experiments.

To directly investigate the response of stishovite and post-stishovite to a passing seismic wave, we performed cyclic loading experiments using the dynamic diamond anvil cell (dDAC). We used the dDAC setup available at the synchrotron beamline P02.2, at PETRA III, DESY, to simulate seismic waves in stishovite/post-stishovite samples, and followed the evolution of their unit cell and lattice strain using time-resolved X-ray diffraction.

Our preliminary results show that at pressure of about 50 GPa, volume strain response to stress in our samples arrives ~15 s later than lattice strain response, when the oscillation frequency is 0.01 s^{-1}. This lag of the volume strain response, however, decreases when increasing the cycling frequency from 0.01 to 0.1 s^{-1}. We will discuss the possible causes of this observation and, in particular, try to discriminate between an elastic or attenuation origin.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T6-P19 Crystallography at High Pressure

Crystal structure of $EuZn_2X_2$ Zintl phases in elevated pressure

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Abstract

$EuZn_2P_2$ and $EuZn_2As_2$ belong to the family of the Zintl-like phases being recently is in the focus of interest with respect to magnetic and transport properties [1,2]. Materials belonging to this group of Zintl phases (ionic entities covalently bonded) have been studied since several decades for their chemical properties. Their (ambient-pressure) structure was characterized, but the point of view of electronic properties became subject of interest rather later. Incorporating magnetic ions in these compounds represents the opportunity to study the interplay of magnetic degrees of freedom and electronic structure. Upon the pressure application the systems can undergo either increase of magnetic ordering, change of the type of transition, change of the crystal structure or insulator-metal transition.

Our recent interest in magnetic and transport properties of the Zintl phases has a special focus in the development of their behavior upon application of pressure [1,3] with variations of the lattice properties, namely the magnetic-entities distance variations. The transport and magnetic properties of $EuZn_2P_2$ have shown that hydrostatic pressure strongly affects both magnetic (increase of the Néel temperature) and electronic (suppression of the band gap and semimetallic behavior) properties, indicating a strong interplay of structure with magnetic and electronic degrees of freedom. In this paper we deal mainly with the lattice evolution as a lattice background of the observed pressure-induced changes in the magnetic behavior for $EuZn_2P_2$ and its $EuZn_2As_2$ analogue.

The recent measured pressure dependence of the structural properties (lattice parameters) signify anisotropic evolution of the particular lattice constants signifying *a*-*a* plane to be less compressible than the *c*-parameter. Compared to another Zintl phase UCu_2P_2 it represents rather opposite trend. This experimentally confirmed fact stays behind the anisotropy in magnetic interactions and major type of magnetic order of the particular compound.

$EuZn_2As_2$ represents As-based counterpart of $EuZn_2P_2$ with larger unit-cell volume. By the pressure application, we are thus able to cover the whole range to continuously follow physical properties of the Eu-based Zintl systems within the volume-dependence from the “ambient-$EuZn_2As_2$” down to “high-pressure $EuZn_2P_2$” structural relations. Aspects of the crystal structure including the anisotropy of $EuZn_2P_2$ and $EuZn_2As_2$ upon application of pressure are to be main subject of the presentation.

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Keywords: Zintl phase, EuZn2P2, EuZn2As2, anisotropy, structure.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T6-P20 Crystallography at High Pressure

Extreme conditions X-ray diffraction and imaging beamline ID15B on the ESRF extremely brilliant source

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Abstract
In recent decades, high-pressure research has experienced a remarkable expansion, deepening our understanding of how materials behave under extreme compression. At the ESRF and other third-generation synchrotron facilities, X-ray studies under extreme conditions have become a major research focus. A broad range of techniques is now routinely applied: X-ray diffraction, inelastic and nuclear inelastic scattering, X-ray absorption and emission spectroscopy, magnetic circular dichroism, Compton and magnetic scattering, and more. These tools have enabled breakthroughs across many fields: from fundamental physics and Earth sciences to materials chemistry and even biophysics, shedding light on how life and biological systems might function under extreme conditions. With the launch of the ESRF-EBS (Extremely Brilliant Source) in August 2020, a new generation of synchrotron science has begun. Beamlines ID15B and ID27, dedicated to high-pressure crystallography, now benefit from dramatically improved beam coherence and focusing capabilities. Their recent upgrades, together with enhanced support from the High-Pressure Laboratory, make it possible to explore the structure of materials at pressures up to 3 Mbar and temperatures from 3 K to 6000 K—pushing the frontiers of extreme condition science.
We present in this overview, the main features of the ID15B beamline on the new ESRF Extremely Bright Source (EBS). The ID15B beamline was fully reconstructed in 2015, considering the new capabilities of the future EBS machine. We will introduce the ID15 project, the ID15B undulator X-ray source, the optical scheme and the experimental hutch. The beamline ID15B is mostly dedicated to the determination of structural properties of solids at high pressure using angle-dispersive diffraction with diamond anvil cells. We will present different selected research examples illustrating the capabilities of this instrument.

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https://doi.org/10.1080/08957959.2024.2379294

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T7-P21 Simple Systems and Experiments at extreme conditions

Determining High-Pressure Binary Phase Diagram Evolution through Thermodynamics and Electrical Measurements

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Abstract

Understanding phase diagrams under high pressure is essential for predicting phase stability and transformations in materials. In this work, pressure-dependent phase diagrams of the Ga-based (Ga-Sn, Ga-In) and Bi-Pb binary systems were investigated using thermodynamic modeling and experimentally validated with electrical measurements in the Paris-Edinburgh press.

The phase diagrams were calculated using a pressure-dependent sub-regular solution model that incorporates the effect of pressure on Gibbs free energy and interaction parameters. The model also includes the effects of solid-phase transitions in the elements. The results demonstrate that pressure significantly modifies phase equilibria, shifting invariance temperatures and compositions, and altering liquidus curvature. A key finding is that pressure-induced solid-state phase transitions in the elemental constituents (Ga, Sn, Bi) strongly influence the topology of the phase diagrams. These transitions lead to the appearance or disappearance of phase regions, liquidus branching, and changes in phase stability fields. Across all systems, good agreement between calculated and experimental data confirms the reliability of the combined thermodynamic-experimental approach.

This study highlights the critical role of elemental phase transitions in shaping high-pressure phase diagrams and demonstrates the effectiveness of coupling thermodynamic modeling with high P-T electrical measurements to investigate phase behavior under extreme conditions.

23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T7-P22 Simple Systems and Experiments at extreme conditions

Periodic table of phase diagrams of the elements

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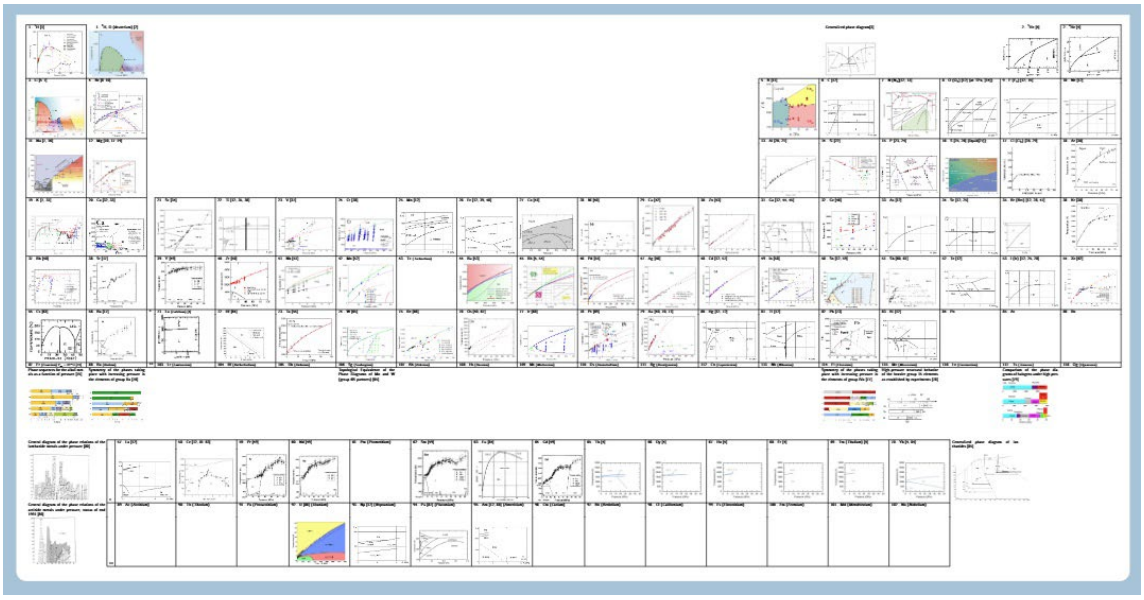
Abstract

This poster proposes an up-to-date overview of all the thermodynamical phase diagrams of the pure elements. This work is inspired by the seminal books of D. A. Young [1] and E. Yu. Tonkov & E. G. Ponyatovsky [4]. Some phase diagrams of isotopes of light elements were added. The phase diagrams are arranged in the shape of the periodic table to highlight the trends in groups (columns) and in periods (rows). In addition, a few illustrative charts from the literature are proposed, such as “generalized phase diagrams” [3], or colored crystalline phases sequences with increasing pressure. A similar approach, illustrating the structural diversity of the elements, was done by W. B. Holzapfel [4, 5]. This type of methodology could help determine the unknown parts of phase diagrams.



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Raman study of $[Ru(bpy)(CN)_4Mg(H_2O)_5]\cdot H_2O$ crystal at high pressure

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Abstract

$[Ru(bpy)(CN)_4]^{2-}$, where bpy denotes 2,2′-bipyridine, is a luminescent anionic Ru(II) complex with pronounced solvatochromic behavior, enabling substantial tuning of its absorption and emission spectra in different solvent environments [1]. Luminescent coordination polymers, where metal ions or clusters are connected by bridging ligands into extended networks, can be prepared by combining this complex anion with various mono- and divalent metal cations, including alkali and alkaline-earth cations such as K^+, Na^+, Li^+, Cs^+, Ca^{2+}, Sr^{2+}, and Ba^{2+}[1,2,3].

In this work, we report on a high pressure Raman study of crystalline $[Ru(bpy)(CN)_4Mg(H_2O)_5]\cdot H_2O$. Yellowish crystals were obtained when reacting the appropriate salts, following previously reported preparation routes [1]. Single crystal X-ray diffraction (sc-XRD) data can be indexed using a disordered P2/c structural model, where the expected polymeric connectivity is disrupted, due to partial occupancy of $Mg(H_2O)_5$ units bonded to cyanido groups on both trans positions to the bipyridine nitrogen atoms with equal occupation factors. Raman spectra were excited at 785 nm, to minimize any absorption or luminescence contributions, and recorded using a LabRAM HR spectrometer. Pressure was applied using a membrane diamond-anvil cell. Daphne 7676 oil, solidifying at ~5 GPa at room temperature, was used as the pressure transmitting medium (PTM) and pressure was determined using the ruby fluorescence method.

The ambient pressure Raman spectrum is rich in features. External lattice modes and low-frequency internal modes of the molecular complex dominate the spectral region below 300 cm^{-1}. The intermediate-frequency region, extending up to 1700 cm^{-1}, contains peaks associated mainly with internal vibrational modes of the complex, while bands observed in the 2000-2200 cm^{-1} range are assigned to C≡N stretching modes [3,4,5]. Ar or N_2 atmosphere or vacuum, lead to a rapid and clearly visible change in crystal colour, often accompanied by a change in sample texture. The Raman spectra are strongly modified, in a similar manner in all cases, particularly in the low-frequency and C≡N stretching regions. These changes are attributed to desorption of water molecules, as previously reported for related materials [3].

Upon compression, most Raman bands shift to higher frequencies, consistent with bond stiffening under volume contraction. Abrupt spectral changes are observed already at ~0.2 GPa, indicating a pressure-induced structural modification. They are most pronounced in the cyanido-stretching region, where relatively broad bands are replaced by stronger and narrower features, and in the low-frequency lattice-mode region, where the spectral profile changes substantially. The high-pressure phase persists up to the maximum attained pressure of 1 GPa in this experiment and reverts to the ambient-pressure phase upon decompression. In a subsequent experiment up to ~5 GPa, additional spectral changes were observed between 3.3 and 4.1 GPa. The affected spectral regions are again the cyanido-stretching and low-frequency lattice-mode. The C≡N stretching Raman peaks become broader and asymmetric, suggesting a phase with a larger number of crystallographically or chemically inequivalent cyanido groups. Upon decompression, this second high-pressure phase persists down to ambient pressure inside the cell.

Both pressure-induced transformations are expected to be distinct from those observed at ambient pressure associated with the water desorption. However, the detailed structure determination of the studied system by XRD under different environments and high pressure is essential for clarifying the nature of the observed structural modifications.

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T8-P24 Spectroscopic and Structural studies

Metallization of Solid Oxygen: Optical Gap Closure and Structural Evolution up to 100 GPa

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Abstract
Solid oxygen occupies a unique place among molecular solids because of the interplay between van der Waals interactions and the spin S=1 magnetic moment carried by the O2 molecule. This competition gives rise to a remarkably rich pressure–temperature phase diagram. Above 10 GPa, oxygen transforms into the ε-phase [1], a monoclinic C2/m structure composed of layered (O2)4 molecular clusters [2,3]. Compression progressively suppresses the magnetic degrees of freedom [4,5] and eventually drives an insulator-to-metal transition near 96 GPa [6,7]. Although metallic oxygen was discovered more than three decades ago, the microscopic mechanism of metallization and the structural nature of the metallic ζ-phase remain unclear.

To investigate this transition, we performed infrared absorption spectroscopy at 20 K and 300 K, up to metallization, complemented by Raman spectroscopy and high-pressure single-crystal x-ray diffraction. Raman measurements show no evidence of a structural phase transition between 20 K and 300 K throughout the stability domain of the ε-phase. Infrared absorption measurements reveal a continuous reduction of the optical gap with pressure. Analysis of the absorption edge indicates that an indirect gap closes near 85 GPa, while a finite direct gap persists up to the metallization pressure. The metallic state emerges through the collapse of this direct gap at 96 GPa.

The use of highly hydrostatic conditions and high-quality single crystals allowed us to determine the evolution of the atomic positions up to 101 GPa, extending previous structural studies into the megabar regime. We find that the layered arrangement of (O2)4 clusters remains essentially preserved up to metallization. The indirect gap closure produces no detectable structural signature, whereas the collapse of the direct gap is accompanied by a lattice instability leading to the ε-to-ζ transition. Structural refinements indicate that the metallic state retains a strongly layered character, suggesting that charge delocalization develops primarily within the molecular planes and that ζ-oxygen may constitute a highly anisotropic, quasi-two-dimensional molecular metal.

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T8-P25 Spectroscopic and Structural studies

$Zn_{1-x}Mn_xTe$ & $Zn_{1-x}Be_xSe$ High-pressure lattice structure/dynamics

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Abstract

Due to their simplicity (two chemical bonds arranged at random on a high-symmetry lattice), the pseudo-binary cubic (zincblende-type) $A_{1-x}B_xC$ disordered semiconductor alloys set a benchmark to explore how the lattice is distorted by mixing crystals, as needed to accommodate locally the difference in A-C and B-C bond lengths. The lattice dynamics offers the possibility to address the raised issue at all length scales since the wavelength (λ) of lattice vibrations ranges from quasi infinite, "averaging" over the alloy disorder, for the phonon-photon coupled modes called phonon-polaritons that propagate near the Brillouin zone center (BZC), all the way down to ultimately small wavelengths nearly matching the lattice constant a, "zooming" into the alloy disorder, achieved by phonons near the Brillouin zone boundary (BZB). Further, the optical (O) modes, reflecting an effective bond-stretching, potentially offer a more local (bond-related) insight into the lattice distortion induced by alloying than the acoustic (A) modes, the genuine collective modes of the crystal conveying all bond species into the same dynamics, *i.e.*, at the same frequency, hence providing a macroscopic (bond-collective) insight into the alloy disorder. Experimentally, the phonon-polariton dispersion near the BZC ($\lambda \to 10^4 \times a$) and the phonon dispersion across the Brillouin zone ($10^2 \times a > \lambda > a$) can be measured by forward inelastic light (Raman) scattering (RS, schematically operated in "transmission") and by inelastic neutron (INS, nuclear reactor) or x-ray (IXS, synchrotron) scattering using national facilities, as specified in brackets.

Two "extreme" II-VI alloys are considered, *i.e.*, the well-matched $Zn_{1-x}Mn_xTe$ ($\Delta a/a \sim 3.8\%$) and highly-mismatched $Zn_{1-x}Be_xSe$ ($\Delta a/a \sim 9.4\%$) ones, subject to minimum and maximum lattice distortions, respectively.

$Zn_{1-x}Mn_xTe$: Two compositions (x= 0.12, 0.37) situated on each side of the Mn-Te bond percolation threshold[1] ($x_c \sim 0.19$, corresponding to the first self-connection of the minor Mn-Te bonds into a pseudo-infinite treelike chain across the crystal, a purely statistical effect of the random Zn↔Mn substitution) are studied at large length scale by combining high-pressure X-ray diffraction (HP-XRD, PSICHÉ beamline – synchrotron SOLEIL) and near-forward-RS. The bulk modulus B_0 obtained by fitting the pressure dependence of the unit-cell volume (a^3) via a Birch–Murnaghan equation of state suffers a major drop below linearity on crossing x_c, below both parent values. This suggests a dramatic lattice fragilization from this limit onwards (to be further documented/studied). Besides, the dramatic dispersion of the phonon-polariton regime probed by forward-RS ($\lambda \to \infty$) unveils a dual fine structure behind the ZnTe-like O-mode at both studied x values, distinguishing *homo* (Zn-like) from *hetero* (Mn-like) local environments, as explained by the percolation model.[2] The O-duo is hardly visible in the phonon regime, whether probed near the BZC in backward-RS or near the BZB at ultimately small λ "zooming" into the alloy disorder by INS (IN22 beamline – ILL). Hence, even though $Zn_{1-x}Mn_xTe$ is well-matched, it suffers an effective lattice distortion, evidenced both at large (HP-XRD) and short (*homo* vs. *hetero* local bond environments) length scales.

$Zn_{1-x}Be_xSe$: The large lattice distortion gives rise to a distinct percolation-type Be-Se O-duo (split by ~40 cm^{-1}) already visible in the phonon regime probed by conventional backward-RS near the BZC at large λ "averaging" over the alloy disorder ($\lambda \sim 10^2 \times a$). Under pressure, the Raman O-duo converges, until crossing at the critical pressure $P_c \sim 14\ GPa$.[3] Beyond P_c, only the upper (*hetero*) O-submode survives, the lower (*homo*) O-submode is quenched, independently verified by *ab initio* phonon calculations using the SIESTA code. The trend is reversible in the downstroke. The quenching was explained and modeled within a concept of a phonon exceptional point being achieved at the resonance/crossing.[4] Not surprisingly, the Be-Se O-duo clarifies (further splits) at ultimately small λ "zooming" into the alloy disorder near the BZB, as observed by INS (IN8 beamline, ILL).[5] The BZB is thus most suitable to investigate whether the percolation model worked out for the *bond-specific* O-modes of semiconductor alloys is echoed, or not, in the, *a priori* less discriminating, *bond-collective* A-modes. High-pressure IXS has recently been done in this line on $Zn_{1-x}Be_xSe$ (ID28 beamline, ESRF) at maximum alloying ($x \sim 0.5$) across the BZ. The studied A-mode consists of a unique well-defined feature near the BZC, but dramatically broadens halfway the dispersion and eventually splits into a distinct A-duo near the BZB. Further, the upper A-submode is quenched above P_c. The trend is reversible in the downstroke. Altogether, the A-duo strongly reminds of the O-duo.

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T8-P26 Spectroscopic and Structural studies

High Pressure as a Potential Route to Correlation Physics in Mott Insulator Nb_3Cl_8

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Abstract
A central question in high-T_c superconductivity is how doping transforms a Mott insulator parent state dominated by strong Coulomb repulsion ($U \gg W$) into a correlated metal and, ultimately, a superconductor (Figure 1). Theoretical efforts to explain these phenomena have been hampered by (1) the lack of an exact solution for the 2D single-band Mott-Hubbard model, (2) obfuscating material specifics (parasitic bands, interlayer coupling, defects, etc.), and (3) an inability to tune key parameters. Experimental systems that offer controlled access to different regions of the U/W–doping phase diagram without these drawbacks are highly sought after.

The Kagome cluster Mott insulators Nb_3X_8 (X = Cl, Br, I) are uniquely suited to this problem. A breathing mode distortion of the lattice (Figure 1) creates isolated, narrow electronic bands near the Fermi level, producing an effectively single-band Mott insulating ground state. The crystals are easily exfoliable, chemically stable and largely free from substitutional disorder. Theoretical models predict that Nb_3Cl_8 and Nb_3I_8 lie in a regime where modest carrier doping may generate correlated electronic states at the Fermi level [1]. High pressure experiments have indeed already demonstrated that bulk Nb_3Cl_8 undergoes a pressure-driven insulator-to-metal transition above ~70 GPa accompanied by bandgap closure, a reversal in dominant carrier type and an as-yet unidentified structural reconstruction [2].

In this poster, I will show our progress toward spectroscopic and transport measurements of bulk Nb_3Cl_8 at even higher pressures, using diamond anvil cells. I will also introduce our multi-parameter approach of combining chemical doping, extreme pressures and electrostatic doping to tune Nb_3X_8 away from Mottness and into regimes of strong electronic correlations, where superconductivity and strange metallicity may emerge.

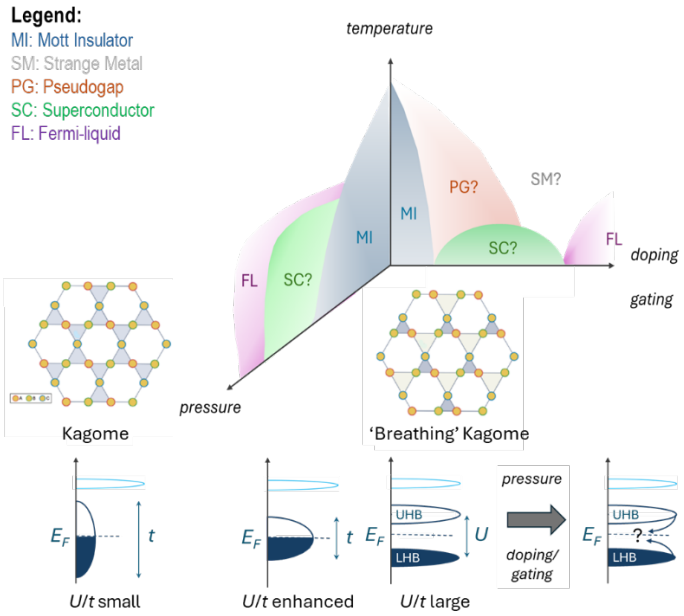

Figure 1: Generalised phase diagram showing the evolution of a Mott insulating parent state into a superconducting ground state via chemical doping, electrostatic doping or physical pressure. The ratio of U (Coulomb energy) and t (bandwidth) sets the energy scale, which can be adjusted using a combination of these tuning knobs.

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T8-P27 Spectroscopic and Structural studies

Pressure-induced hydrogen formation and phase transitions in H_2S-THF clathrate hydrate

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Abstract

Hydrogen-bearing compounds are attracting increasing attention because they provide valuable model systems to investigate the behaviour of hydrogen under extreme conditions, while also offering potential routes for hydrogen storage and release [1]. Among hydrogen-containing molecules, hydrogen sulfide (H_2S) is particularly appealing as it exhibits a remarkably rich high-pressure chemistry, such as molecular dissociation and the formation of hydrogen-rich hydrides, including phases exhibiting near-record superconducting critical temperatures [2].

In this framework, H_2S hydrates offer an unexplored platform to investigate how a hydrogen-bearing guest molecule interacts with a hydrogen-bonded host lattice under compression. Indeed, H_2S is known to form clathrate hydrates which are believed to play an important role in planetary environments by promoting the trapping of volatile species and thus influencing out-gassing processes [3]. However, despite their significance for the interiors of icy moons and satellites, the behaviour of H_2S hydrates has been studied exclusively at low pressure [4, 5, 6], while at pressures in the GPa range, typical of subduction processes and of the interiors of icy bodies, its chemistry remains unexplored.

We investigated the room temperature compression (0.1 -10 GPa) of the H_2S-THF clathrate hydrate (THF acts as a clathrate stabiliser) in membrane Diamond Anvil Cells (mDACs) using Raman spectroscopy and synchrotron x-ray diffraction, finding multiple phase transitions below 3 GPa. Beyond establishing the clathrate high-pressure stability field, we observed a pressure-induced decomposition associated with sulfur segregation and the direct formation of molecular hydrogen, which remains trapped within a hydrate phase. These remarkable findings provide new insights into the mechanisms of hydrogen generation and release from hydrogen-bearing compounds under extreme conditions, firmly establishing H_2S hydrates as a model system for studying pressure-driven hydrogen synthesis in molecular systems.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T8-P28 Spectroscopic and Structural studies

Anomalous pressure modulation of the lowest B_{1g} lattice vibration in semimetal zirconium diphosphide, ZrP_2

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Abstract

Lattice dynamics of ZrP_2, a semimetal compound with non-trivial topology of electronic bands, has been studied through measurements of inelastic light scattering and extensive ab initio calculations at riange of static pressures up to 20 GPa. We found that lattice vibrations of the lowest energy exhibited anomalous properties.

An abnormal change in the energy of the lowest B_{1g} phonon mode revealing alternate softening (energy decrease) and hardening (energy increase) regimes has been observed within 16 GPa pressure range. This finding substantially complements the very recent observation of the softening of the lowest A_g lattice mode in $ZrPAs_2$ [1] and ZrP_2 [2] under compression. Our study demonstrates a complex behavior of optically active lattice vibrations, the reason for which is yet to be understood.

In a broader context, detecting lattice instability manifested through the soft phonon modes in the low energy region might be of high relevance to the mechanism of driving superconductive state observed recently in several semimetal compounds under compression urging for further scrupulous investigation.

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23-28 August 2026, Palavas-les-Flots/Montpellier, France: 63rd meeting of the European High Pressure Research Group
T2-P30 Chemistry, Synthesis, Novel materials

Halogen Chains with One-Dimensional Semi-Metallic Electronic Structure and Peierls Physics in Polymorphs of Na_4X_5 (X = I, Br, Cl) Compounds

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Abstract

Since the pioneering works of Peierls, one-dimensional materials have attracted great attention due to the possibility to study spin-charge separation, charge and spin-density waves, and topological spin excitations. Discoveries of quasi-one-dimensional materials made it possible to investigate at least some aspects of hypothetical theoretical models experimentally. Still, the synthesis of truly monoatomic chains remains elusive. In this study, we explore a novel path of experimental synthesis of monoatomic one-dimensional chains by their chemical stabilization in ionic compounds. We demonstrate that in synthesized at high pressure sodium halides Na_4X_5 (X = I, Br, Cl) with *hP*18 Ga_4Ti_5-type structures, transfer of valence electrons from cations to anions leads to the formation of halogen chains connected with other atoms only by ionic interaction and having one-dimensional electronic structure. The Peierls physics in the systems is confirmed by newly synthesized incommensurately modulated *i-hP*18-Na_4X_5 (X = I, Br, Cl) compounds, as well as by the discovered *hP*36 phases of Na_4Cl_5 and Na_4Br_5. Our theoretical calculations demonstrate that at zero temperature, in agreement with what is expected for Peierls materials, the electron-phonon interactions destabilize the linear monoatomic metallic chains of halogen anions, leading to opening band gaps in the electronic structure. However, at finite temperature, anharmonic effects of lattice vibrations lead to stabilization of regular monoatomic chains of equidistant halogen anions, as experimentally observed in the *hP*18-Na_4X_5 polymorphs, closing the band gaps, and making the one-dimensional chains semi-metallic.

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T6-P31 High-Pressure Crystallography

High-pressure studies of hydrogen bonding in gypsum via Quantum Crystallography methods

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Abstract

Gypsum, $CaSO_4 \cdot 2H_2O$, is a model hydrous mineral in which pressure-induced structural transformations are governed not only by the compression of the crystal lattice, but also by the response of molecular water and hydrogen bonding. The ambient-pressure hydrogen geometry was established by neutron diffraction, showing two significantly different O–H distances of 0.942(3) and 0.959(3) Å and two non-equivalent hydrogen bonds to sulfate oxygen atoms, with H···O distances of 1.856(2) and 1.941(2) Å (Pedersen and Semmingsen, 1981). High-pressure single-crystal X-ray diffraction later showed that gypsum-I preserves its C2/c structure up to ca. 4.0 GPa, where the compression curve displays a discontinuity accompanied by a 2.5% volume contraction (Comodi et al., 2008). In that pressure range, the [CaO_8–SO_4] polyhedral layer remains comparatively incompressible, whereas the water-bearing interlayer is much more compressible, highlighting the central role of hydrogen bonding in the compression mechanism (Comodi et al., 2008). The structure of gypsum-II was subsequently solved from synchrotron single-crystal XRD with monoclinic $P2_1/n$ symmetry, with enhanced SO_4 tetrahedral distortion and a strong change in the bonding style of water molecules (Nazzareni et al., 2010). Spectroscopic studies also suggested that the transition is reversible and related primarily to the hydrogen-bonding network and water-molecule symmetry rather than to sulfate distortion (Knittle et al., 2001; Nazzareni et al., 2010).

Here we present a high-pressure quantum-crystallographic study of synthetic gypsum single crystals compressed in a diamond anvil cell. Synchrotron single-crystal X-ray diffraction data were collected over a dense pressure series from ambient pressure to 14.1 GPa, covering gypsum-I, the transition region, gypsum-II, and further structural transformations above 9 GPa with triclinic crystal symmetry. Despite the low monoclinic symmetry and the severe reciprocal-space restrictions imposed by the diamond anvil cell, high-pressure datasets reached up to ca. 90% completeness by merging measurements from several crystals collected at the same pressure point. This multi-crystal strategy is crucial for quantum crystallography, because multipole refinement, Hirshfeld Atom Refinement, and experimental electron-density analysis require not only accurate intensities, but also high completeness and reliable weak high-resolution reflections.

As an ambient-pressure reference, an in-house Mo Kα dataset was collected and refined using Hirshfeld Atom Refinement with anisotropic hydrogen atoms. The HAR-refined O–H distances, 0.965(10) and 0.929(11) Å, agree within uncertainty with the neutron-derived values of Pedersen and Semmingsen and confirm the intrinsic asymmetry of the water molecule in gypsum. Structures were solved and refined within the independent atom model for each observed phase, and compressibilities and bulk moduli were determined separately for the corresponding stability fields. Selected datasets were further treated using Hirshfeld Atom Refinement, multipole-model refinement, and topological analysis of the electron density within Bader's Quantum Theory of Atoms in Molecules and Crystals.

This combined structural and topological approach allows us to follow the evolution of O–H bonds, O–H···O hydrogen bonds, water-layer compression, and electron-density descriptors at bond critical points across the pressure-induced phase transformation. In contrast to previous studies, which established the ambient neutron reference structure, the pre-transition equation of state, or the structural model of gypsum-II, the present work provides a pressure-resolved experimental description of hydrogen-bond evolution at the level of electron density. The results show how hydrogen bonding accommodates compression, contributes to symmetry lowering, and evolves towards structural degradation, demonstrating the potential of high-pressure quantum crystallography for studying hydrated minerals and weak interactions under extreme conditions.

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T9-P29 Theoretical and Computational approaches

Pressure-dependent structural, elastic, electronic and vibrational studies of Sr_2InSbO_6 from first principles simulations.

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Abstract

Perovskite materials have interesting and unusual physical properties that have been studied a lot for both real-world applications and theoretical modelling. The science of perovskites and how they can be used, has been a large area of research that has led to many new device ideas based on revolutionary discoveries. Double perovskite compounds, first identified in the 1950s, are remarkable for their characteristics and the wide range of uses they find in industry. A2BB0O6 double perovskite oxides have gained considerable attention over the past two decades due to their extensive structural diversity, as well as potential technological applications in microwave dielectric ceramics, optoelectronic device materials The ideal double perovskite structure of the general formula A2BB0O6 is derived from the perovskite structure ABO3 when the octahedrally coordinated two B-cations are occupied by a B cation and a B0-cation in an ordered 1:1 way, where B and B0 cations are largely different in charge or size.

First-principles calculations have been performed to study the structural, elastic, electronic, and lattice dynamical properties of Sr_2InSbO_6. Our first-principles density functional theory, DFT, calculations were performed with the pseudo-potential plane-wave method as implemented in the Vienna ab initio Simulations Package, VASP.In this work, we present a study of the evolution of the structural, vibrational, elastic, and electronic properties under hydrostatic pressure.

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