The role of homonuclear bonds in the stability of the high-pressure polymorphs of III-V compounds

Andrés MUJICA (Universidad de La Laguna, Spain),
Enrique ZANARDI (Universidad de La Laguna, Spain),
Silvana RADESCU (Universidad de La Laguna, Spain)
Barbara LAVINA (University of Chicago, USA)

Abstract

In this contribution we give an account of the recently discovered high-pressure *mS16* phase of GaP [1] and the theoretical possibility of similar phases in other members of the III-V family of technologically relevant binary compounds. Two decades after the high-pressure polymorphism of the binary III-V compounds was considered a substantially settled matter [2], recent findings in GaP have revealed the occurrence of new structure types that challenge previous views concerning the effect of homonuclear bonds on the energetics of their high-pressure phases and emphasize the role of structures based on the stacking of NaCl-type layers, including partial interlayer dimerization, as a relevant type of ordering in these compounds [1,3]. The new data for GaP have unraveled a marked complexity in the high-pressure metallic phases, arising from strong bonding differentiation and finely tuned pressure dependence of the degree of phosphorus dimerization allowed by the different stackings of NaCl-type layers. Distinct ordering sequences of such layers, and therefore new structures, are likely to occur in other octect compounds as well, an aspect relevant to material design, as phases and properties might be finely tunable with pressure.

[1] B. Lavina, E. Zanardi, A. Mujica, H. Cynn, Y. Meng, W.V. Prakapenka, J.S. Smith, Mater. Today Phys. **53** (2025) 101686.

[2] A. Mujica, A. Rubio, A. Muñoz, R.J. Needs, Rev. Mod. Phys. **75** (2003) 863.

[3] B. Lavina, E. Kim, H. Cynn, P.F. Weck, K. Seaborg, E. Siska, Y. Meng, W. Evans, Inorg. Chem. **57** (2018) 2432.