High Pressure as a Potential Route to Correlation Physics in Mott Insulator Nb_3Cl_8

Rebecca Nicholls (University of Bristol, UK)
Jonathan Buhot (University of Bristol, UK)
Sam Cross (University of Bristol, UK)
Nigel Hussey (University of Bristol, UK)

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.

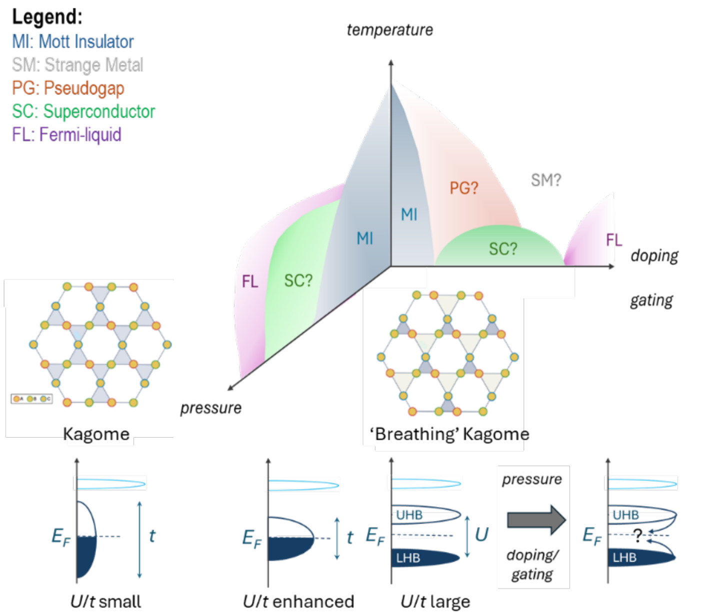

Figure 1: Generalised phase diagram showing the evolution of a Mott insulating parent state into a superconducting ground state via chemical doping, electrostatic doping or physical pressure. The ratio of U (Coulomb energy) and t (bandwidth) sets the energy scale, which can be adjusted using a combination of these tuning knobs.

[1] Aretz et al., Phys. Rev. X 15, 041042 (2025).
[2] Shan el al., Materials Today Physics, 38 101267 (2023).