Abstract for IAS Quantum Forum on Altermagnetism and Beyond (August 10-13, 2026)

Layered Mott Insulator Nb_3Cl_8

Hongming WENG

Institute of Physics, Chinese Academy of Sciences, P.R. China

Email: hmweng@iphy.ac.cn

Mott insulators are prototypical strongly correlated systems that can give rise to many exotic quantum states, such as antiferromagnetic order, high-temperature superconductivity, quantum spin liquids, and more. The Hubbard model is an important theoretical framework for understanding their physical mechanisms. However, in real material systems, strong correlation effects typically involve multiple orbitals such as *d* and *f* orbitals, making Mott insulators that perfectly realize the single-band, single-occupancy Hubbard model exceedingly rare — a circumstance that introduces considerable complexity into the understanding and control of Mott insulators. Through a combination of theory and experiment, we have discovered that the layered compound Nb_3Cl_8 is an ideal Hubbard–Mott insulator. Its high-temperature phase (α-phase) exhibits weak interlayer coupling, with each single layer behaving as an ideal two-dimensional Mott insulator displaying characteristic Curie–Weiss paramagnetism. At low temperatures (β-phase), a structural phase transition involving interlayer dimerization occurs: the interlayer pairing is enhanced, leading to the formation of spin singlets and typical nonmagnetic insulating behavior. Calculations reveal that although the internal energy of the α-phase is higher than that of the β-phase, the α-phase possesses substantially larger spin entropy and lattice vibrational (phonon) entropy at elevated temperatures, because the enhanced interlayer coupling in the β-phase suppresses both spin and phonon entropy. These factors jointly drive the changes in electronic structure and crystal structure that occur with decreasing temperature. Further calculations indicate that applying pressure can suppress this phase transition and stabilize the α-phase, thereby offering a tuning strategy for realizing a quantum spin liquid state.