Unconventional Phase Transitions in Layered 2D Crystals

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In this talk, we will introduce our recent studies on anomalous phase transitions in physical properties of layered materials. First, we will show a metal-to-Mott insulating phase transition (MIT) as a function of a number of layers in 1T-$TaSe_2$ [1]. Using our newly developed first-principles calculation method for the extended Hubbard functionals [2], we reveal that the intricate competition between the strong screened Coulomb interaction and kinetic energy gain across the layers is a key to the MIT here. We show that our simulations of spectroscopic signals near the MIT agree with experiments from our collaborators very well. Second, we will present a new theory on anomalous charge density wave (CDW) transition in kagome metals of AV_3Sb_5 (A = K, Rb, Cs) [3]. Using our newly developed molecular dynamics simulation tools, we uncover asynchronous condensation processes to the charge density wave states in kagome metals. We demonstrate that the CDW forms first within each layer but their phases fluctuate across the kagome layers owing to unavoidable degeneracy in energetic costs for stacking CDWs. We will discuss several consequences and experimental implications for kagome metal physics and layered crystals based on our discoveries of condensation of preformed CDW orders. If time allowed, we also present strain-induced magnetic transitions in a new carbon 2D crystal of Biphenylene Network (BPN) [4,5].

References

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[2] S.-H. Lee and Y.-W. Son, arXiv:1911.05967.
[3] C. Park and Y.-W. Son, arXiv:2303.08598.
[4] Y.-W. Son, H. Jin and S. Kim, arXiv:2201.09456.
[5] S. Kim, H. Jin and Y.-W. Son, *in preparation*.