Quantum Materials by Design: First-Principles Pathways

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April 28th, 2025

at Ajou University

Technological revolutions throughout history have been driven by advances in materials—from stone and steel to silicon. As we enter the Quantum Age, the search for novel quantum materials becomes more urgent, especially in light of the growing demand for computing power and the limitations of conventional semiconductors. In this talk, I will discuss a computational strategy for quantum materials design based on a synergy of density functional theory (DFT) and dynamical mean-field theory (DMFT), which enables a realistic treatment of strong correlation effects beyond single-particle approximations. Focusing on Hund's coupling and spin-orbit coupling—two energy scales that have historically received less attention—I will highlight how their interplay gives rise to emergent phenomena such as metal-insulator transitions, Hund's metallicity, and spin-orbital entangled states. These effects are particularly rich in systems such as ruthenates and cuprates, where orbital degrees of freedom play a central role. I will also present recent results about correlated topological phases that emerge when spin-orbit coupling is embedded within strongly interacting electronic systems.