“Theoretical investigation of superconducting infinite-layer nickelates”

The recent discovery of superconductivity in oxygen-reduced monovalent nickelates $R\mathrm{NiO_2}$ offers a new platform for the study of unconventional superconductivity, with similarities and differences with cuprates. In this talk, I discuss our recent theoretical investigations of the electronic structure[1][2], superconductivity, and competing orders[3] of infinite-layer nickelates. Unlike cuprates where the underlying low-energy physics is dominated by the strongly correlated single-band physics, the electronic structure of infinite-layer nickelates essentially features multi-orbital physics. Our density functional theory studies show the low energy physics of $R\mathrm{NiO_2}$ is dominated by a three-dimensional 5*d* metallic state at the rare-earth *R* spacer layer hybridizing with a quasi-two-dimensional, strongly correlated state with primarily Ni $3d_{x2\text{-}y2}$ orbital character in the NiO_2 layer. Density matrix renormalization group calculations for the ground state of such a two-orbital Hubbard model show a metallic state at half-filling and a superconducting state upon doping. This two-band Hubbard model also gives rise to charge density modulations in both rare earth and Ni layers. The consistency between our theoretical results and experiments suggests the two-band Hubbard model provides fundamental insights to infinite-layer nickelates.

References:

[1] Hepting et al, Nature Materials 19 (4), 381-385 (2020)

[2] Been et al, Physical Review X 11, 011050 (2021)

[3] Peng et al, arXiv:2110.07593 (2021)