Understanding correlated d- and f-electron systems using DFT and eDMFT methods

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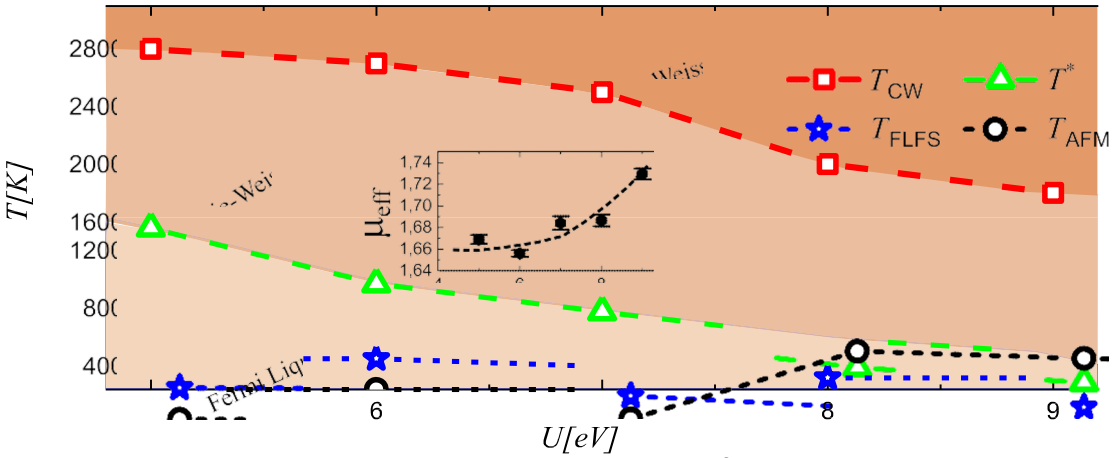
Novel materials whose properties are influenced by the presence of d- and/or f-electrons have been of sustained interest to the condensed matter community. Innovative material syntheses, together with thermodynamic, transport and cutting-edge spectroscopy experiments have been revealing an intriguing array of properties. These have also brought to fore theoretical challenges posed by the presence of strong electronic correlations. Large-scale first-principle computational approaches have been valuable in deciphering experimental findings and predicting new results. Recently, we proposed* a correlation-temperature (U-T) phase diagram for the undoped nickelates, showing low-T Fermi liquid phases (partially screened and fully screened nickel d-electron moments), a high-T Curie-Weiss phase of fluctuating nickel d-electron moment, and an antiferromagnetic phase at large U. I will briefly discuss basic ideas underlying self-consistent DFT + embedded dynamical mean field (eDMFT) method. Then I will present our current work on doped nickelate superconductors, exploring possible changes in the phase diagram. At the end, I will discuss our first-principles work on a class of transition metal (A)-Beryllium(Be) compounds with distorted Kagome lattice features**.

Correlation-temperature phase diagram of prototypical infinite layer rare earth nickelates, G. L. Pascut, L. Cosovanu, K. Haule, K. F. Quader, Communications Physics **6, Article number: 45 (2023)*
***First-principles study of transition metal-Beryllium (ABe_2) Laves phases with distorted Kagome layers, L. Bleys, G. L. Pascut, M. Widom, K. Quader, draft (2024).*



Correlation-temperature phase diagram of undoped nickelate