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Structural Predictions and Dynamic Stability of Correlated Electron Materials using Embedded Dynamical Mean Field Theory Functional Approach

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Materials with strong electronic correlations have long resisted abinitio modeling due to their complexity arising from non-perturbative strength of the interaction. The Dynamical Mean Field Theory in combination with the Density Functional Theory has recently allowed accurate modeling of the electronic structure of many complex materials, such as the heavy fermions, transition metal oxides, iron superconductors, etc. The stationary implementation of the Dynamical Mean Field Theory functional [1] and its derivative [2] has been recently achieved, which allows one to predict forces for structural relaxation at finite temperature across the metal-insulator transition, and *ab-initio* prediction of the coupling between magnetism and phonons at finite temperature. We will show how the electronic correlations enhance the electron-phonon coupling strength in FeSe[3], how the coupling of magnetism and crystal structure in rare earth nickelates leads to the metal insulator transition[4], and why is the BCC structures of elemental iron stable at high temperature[5].

1. Haule, K. and Birol, T., "Free Energy from Stationary Implementation of the DFT + DMFT Functional". Phys. Rev. Lett. **115**, 256402 (2015).
2. Haule, K and Pascut G.L., "Forces for structural optimizations in correlated materials within a DFT+embedded DMFT functional approach". Phys. Rev. B **94**, 195146 (2016).
3. Mandal, S. and Cohen, R.E. and Haule, K. "Strong pressure-dependent electron-phonon coupling in FeSe". Phys. Rev. B **89**, 220502(R) (2014).
4. Haule, K. and L. G. Pascut, "Mott Transition and Magnetism in Rare Earth Nickelates and its Fingerprint on the X-ray Scattering", arXiv:1703.08196.
5. Han, Q. and Birol, T. and Haule K. "The phonon softening due to melting of the ferromagnetic order in elemental iron", arXiv:1705.06877.