Electronic Structure and Lattice Stability of Correlated Electron Materials

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The computational studies of the electronic structure and magnetism of strongly correlated electron materials is one of the most challenging theoretical problems. In this talk, I will discuss an application of the novel computational scheme DFT+DMFT to explore the electronic and structural properties of correlated materials [1]. In particular, I will present our recent results for the pressure-induced magnetic collapse and Mott insulator-metal transition in paramagnetic monoxides MnO, FeO, CoO, and NiO. Our calculations reveal that under pressure these materials exhibit a Mott insulator-metal transition (IMT) which is accompanied by a simultaneous collapse of local magnetic moments and lattice volume, implying a complex interplay between chemical bonding and electronic correlations. In addition, I report the electronic properties and phase stability of Fe_2O_3 near a pressure-induced Mott metal-insulator transition. Our results reveal that upon compression Fe_2O_3 undergoes a Mott insulator (MI) to site-selective MI phase transition, which is characterized by a collapse of local moments and emergence of metallic state only on half of the Fe sites. In agreement with experiment, it was found that the IMT is accompanied by a structural transformation from corundum to a double perovskite lattice structure. Our results for the electronic state, equilibrium crystal structure, and structural phase stability are in quantitative agreement with experimental data. We find that electronic correlations are important to explain the lattice stability of correlated materials, e.g., in the vicinity of a Mott insulator-metal transition.

[1] I. Leonov et al., Phys. Rev. Lett. 106, 106405 (2011); I. Leonov et al., Phys. Rev. Lett. 115, 106402 (2015); I. Leonov et al., Phys. Rev. B 91, 195115 (2015); I. Leonov et al., Phys. Rev. B 94, 155135 (2016).