Title: Head-to-head comparison of spectral properties of binary transition-metal oxides using DFT and beyond-DFT methods

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The development of computational tools for the accurate prediction of the electronic structure of strongly correlated materials has been an active field of research for several decades. As a result, a variety of methods, including density functional theory (DFT), DFT+U, hybrid functionals, meta-GGAs, GW quasiparticle approaches, and DFT-embedded dynamical mean field theory (EDMFT), are now available. Among these, the beyond-DFT methods have been instrumental for understanding the electronic structure of strongly correlated systems, but it is unclear how reliable are those methods when applied to typical strongly correlated solids. It is thus of pressing interest to compare the quality of these methods as they apply to different categories of materials. Here we systematically test these methods on transition-metal oxides (TMOs) such as FeO, CoO, MnO, and NiO, which provide a suitable platform since conventional DFT methods are known to fail to predict their electronic structure accurately. We present a head-to-head comparison of spectral properties as obtained using the listed methods in the antiferromagnetic (AFM) phase. Comparing with experimental photoemission data, we find both B3LYP and EDMFT can reproduce the experiments reasonably well. The comparisons with EDMFT are however much superior. Using EDMFT, we further investigate the paramagnetic phase, where the spectral function becomes incoherent compared to AFM phase, and the first valence band predominately change near the Gamma-point. Overall the spectral function and the insulating gap remain unchanged during this phase transition. Comparing optical properties with available experiments, we find the excitonic effects arising from the vertex correction are not important for TMOs.