

Reformulation of DFT+ U as a pseudo-hybrid Hubbard density functional

Luis A. Agapito,^{1,2,*} Stefano Curtarolo,^{2,3} and Marco Buongiorno Nardelli^{1,2,†}

¹*Department of Physics, University of North Texas, Denton, TX 76203, USA*

²*Center for Materials Genomics, Duke University, Durham, NC 27708, USA*

³*Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC 27708, USA*

We introduce the Agapito-Curtarolo-Buongiorno Nardelli (ACBN0) pseudo-hybrid Hubbard density functional as a fast, accurate and parameter-free alternative to traditional DFT+ U and hybrid exact exchange methods. In ACBN0 the Hubbard energy of DFT+ U is calculated via the direct evaluation of the local Coulomb (\bar{U}) and exchange (\bar{J}) integrals in which the screening of the bare Coulomb potential is accounted for by a renormalization of the density matrix. Through this procedure, the values of \bar{U} and \bar{J} are thus functionals of the electron density and depend not only on the atomic species, but also on the chemical environment and crystalline field, introducing an effective way of giving the proper description of Mott insulators and other strongly correlated systems. As a first application, we discuss the electronic properties of a series of transition metal oxides calculated with ACBN0 that show excellent agreement with hybrid functionals, the GW approximation and experimental results at a fraction of the computational cost.