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ACBN0-tool for accelerated materials discovery. PRIYA GOPAL, Central Michigan University, LAALITHA LIYANAGE, LUIS AGAPITO, University of North Texas, SEUNGHUN LEE, ICHIRO TAKEUCHI, University of Maryland, GUS HART, Brigham Young University, STEFANO CURTAROLO, Duke University, MARCO FORNARI, Central Michigan University, MARCO BUONGIORNO NARDELLI, University of North Texas — High-Throughput QM computation of material properties by abinitio methods has become the foundation of an effective approach to materials design. One of the major challenges in mapping the materials genome is in developing efficient computational tools that are cost-effective and accurate at the same time. In this talk, we discuss the newly developed ACBN0 pseudo-hybrid Hubbard density functional where the Hubbard energy within the DFT + U formulation is calculated self consistently. The U depends on the electron density and depends both on the geometry and chemical environment of the system. We show that ACBN0 improves the description of both the structural and electronic properties in a range of complex materials from Zn/Cd based chalcogenides to the TMOs. The magnetic properties are better described compared to the LDA/GGA functionals. We will also discuss the application of the ACBN0 approach to surfaces, doped and multi-valent systems where it is possible to evaluate U for different sites and chemical bonding. For all the complex materials studied here, we find that the electronic properties are significantly improved over the DFT values and the accuracy is at par with the HSE values at a fraction of the computational cost.

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