High-throughput determination of Hubbard U for cubic per-ovskites using the ACBN0 functional. LAALITHA LIYANAGE, University of North Texas, ANDREW SUPKA, PRIYA GOPAL, Central Michigan University, LUIS AGAPITO, University of North Texas, GUS HART, Brigham Young University , MARCO FORNARI, Central Michigan University, STEFANO CURTAROLO, Duke University, MARCO BUONGIORNO NARDELLI, University of North Texas — High-throughput (HT) density functional theory (DFT) computations are the method of choice for rapid screening of materials properties and materials development. However, traditional DFT is not adequate for the investigation of all systems. For materials containing transition metal elements, methods such as DFT+U or hybrid functionals are needed for an accurate prediction of the electronic structure. As an efficient and accurate alternative we have recently introduced the ACBN0 functional for DFT as a new pseudo-hybrid Hubbard density functional that is a parameter-free extension of traditional DFT+U that has been proved to correct both the band gap and the relative position of the different bands in transition metal compounds. We implemented ACBN0 in a Medium-Throughput Framework (MTFrame) designed to automate DFT calculations for systems that share a single reference crystal structure. Using the MTFrame, we have determined the effective U values for 3969 cubic perovskites (ABO3) built by permutating 63 different elements in the A and B sites. Analysis of resulting data reveals the effects of Hubbard U on the electronic properties and crystal structure. Finally, machine learning algorithms are used to find correlations in the extracted data and the U values.

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