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Improved predictions of the electronic and structural properties of Zn- and Cd- based compounds. An ACBN0 study PRIYA GOPAL, MARCO FORNARI, Central Michigan University, STEFANO CURTAROLO, Duke University, LUIS AGAPITO, LAALITHA LIYANAGE, MARCO BUONGIORNO NARDELLI, University of North Texas — In this talk, we will present our results of the performance of the recently developed ACBN0 pseudo-hybrid Hubbard density functional in predicting the electronic and structural properties of the Zn- and Cd- based semiconductors. ACBN0 is a fast, accurate and parameter-free extension of traditional DFT+U proved to correct the band gap in transition metal compounds. Within ACBN0, the values of U and J are functionals of the electron density and depend directly on the chemical environment and crystalline field.[1]) We will compare the structural and electronic properties of ZnX and CdX (X=0,S,Se,Te) semiconductors calculated in *rs*,*wz* and *zb* phases using ACBN0 with the results obtained by semi-local PBE, hybrid HSE06 functionals and experiments whenever available. Our results demonstrate that the lattice constants, bulk modulii and band-gaps are more accurately described by ACBN0 compared to the PBE functionals. Overall, we show that ACBN0 is a powerful tool which preserves the accuracy of the HSE calculations with higher computational efficiency.

[1]L. Agapito, S. Curtarolo and M. Buongiorno Nardelli, arXiv:1406.3259

Priya Gopal
Central Michigan University

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