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Effect of uniaxial and biaxial strain on the electronic and dynamical properties of CdO: ACBN0 functional study JACOB GALLAWAY, University of North Texas, PRIYA GOPAL, MARCO FORNARI, Central Michigan University, STEFANO CURTAROLO, Duke University, MARCO BUONGIORNO NARDELLI, University of North Texas — We have investigated the influence of uniaxial and biaxial strain on the electronic and vibrational properties of CdO in the rocksalt structure using Density functional theory calculations with our newly developed ACBN0 pseudo–hybrid Hubbard density functional.[1] ACBN0 is a fast, accurate and parameter-free extension of traditional DFT+U proved to correct both the band gap and the relative position of the different bands in transition metal compounds. CdO is a technologically important materials with a direct band-gap of 2.2 eV, which makes it a potential candidate for applications as transparent conductor (TCO) in optoelectronic devices. In such devices, CdO is often grown as a thin film on a substrate and this substrate induces strain that alters the electronic properties. It is clearly very important to understand this phenomenon to properly predict the performance of these devices. All earlier first principles making the system semimetallic. In this talk, we show that the newly developed ACBN0 functional opens up the gap in closer agreement with the experiments, thus making possible to study band-gap modulation. We will discuss in detail the variation of the electronic and vibrational properties under epitaxial strain.

[1]Agapito, L *et.al.*, arXiv:1406.3259

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