Abstract Submitted
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A LSDA+U Study on Bulk CuO: Electronic Structures and Native Defects[1] DANGXIN WU, QIMING ZHANG, Department of Physics, the University of Texas at Arlington, LONGCHENG WANG, MENG TAO, Department of Electrical Engineering, the University of Texas at Arlington — We have performed a first-principles study on the electronic structure and the formation of native defects in the monoclinic CuO by using the LSDA+U method with the PAW potentials. The optimized structural parameters of the crystal are in good agreement with the experimental data. The band structure of the crystal is calculated. An indirect band-gap of 1.0 eV is obtained, which agree with the experimental semiconducting property of the material. This is qualitatively different from a LDA or LSDA calculation, which predicts a metal with the Fermi level below the top of valence band. The formation energies of various native defects as well as their charged states in CuO are carefully studied. The influence of Fermi level and the stoichiometry to the defects formation will be discussed.

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