

Abstract Submitted
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Corrected Band Gap Of Zinc Oxide ZnO using DFT + U KESHAB BAYSHAL, ALEXEY ZAYAK, Bowling Green State University — ZnO is a wide band gap semiconductor with potential for many electronic applications. The major challenge of ZnO is the problem of controlling defects. Unfortunately, DFT has limitations that lead to underestimated values of the energy band gap, which is critical for the energetics of defects. In this work, we employ DFT+U and HSE functional calculations to study native point defects and formation energy for ZnO Wurtzite structure. The incorrect DFT band gap was calculated to be 1.1 eV. The extremely costly HSE calculations led to an improved band gap value of 2.5 eV, which is still significantly smaller than the experimentally observed 3.4 eV. In order to make a major improvement we use the Hubbard correction (DFT+U), which introduces on-site corrections for Zn 3d and O 2p electrons. We performed a large set of calculations covering a broad range of all possible combinations of U-parameters for Zn and O, and found that the right band gap of 3.4 eV can be obtained by using numerous combinations. Such ambiguity leads to a poorly defined methodology and probably unreliable results. In order to resolve this ambiguity, we use the concept of relating the U - corrections to the electronegativities of the atoms, which gives a physically meaningful criteria for choosing U-parameters.

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