DFT study of structural, electronic, optical, and electrical properties of CuO based on GGA+U and TB-mBJ approximations

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Abstract

The structural, electronic, optical, and electrical properties of CuO were studied using the density functional theory (DFT) based on the Full Potential Linearized Augmented Plane Wave (FP-LAPW) method as implemented in the Wien2k code. The structural parameters are optimized by using the 4D-optimize option and the PBE-sol functional. The electronic and optical properties were analysed adopting Generalized Gradient approximation plus the screened Coulomb interaction (GGA+U) and the modified Becke-Johnson (GGA-TB-mBJ) potential for comparison. The calculated band energies have been used with the Boltzmann transport equation to calculate the thermoelectric properties. It is shown that the gap energy obtained by the (TB-mBJ) approximation potential is 2.02 eV more close to the experimental values comparing to that given by the GGA+U (E_g=1.57 eV). The optical properties reveal a high absorption coefficient in the UV region with an average transmittance of around 65% in the visible range, which covers a high range of light using TB-mBJ exchange potential and an average reflectivity of approximately 18% in visible light. The CuO conductivity is limited by the carrier mobility at low temperature and primarily defined by the carrier concentration at high temperature. These properties make CuO a promising material for solar cell applications as an absorbent layer and antireflection coating.

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