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Electronic Properties of ZnO: Band Structure and Directional Compton Profiles

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The electronic band structure and directional Compton profiles (DCPs) of ZnO are studied in this work. Calculations are performed considering a set of three schemes based on density functional theory (DFT), the Hartree–Fock (HF) method, and a hybrid scheme. All band structures predict direct bandgaps. The best agreement with experiment is, however, shown by the hybrid scheme. The three schemes are also applied to compute DCPs along [100], [110], and [001] directions. These are compared with measurements made on single crystals of ZnO employing a 59.54 keV gamma-ray Compton spectrometer. Calculations overestimate the momentum density in the low-momentum region while underestimate the anisotropies. Positions of extremes in anisotropies deduced from calculations are well reproduced by the measured anisotropies in some cases. Within the experimental limits, the DCPs from the HF method are in better agreement with the measurements compared with DFT.

Key words: Oxides, semiconductors, ZnO, *ab initio* calculations, electronic structure, Compton profile

INTRODUCTION

There is a resurgence of interest in the study of ZnO, a wide-bandgap semiconductor, due to its applications in electronics, optoelectronics, spintronics, and nanodevices.[1] It crystallizes in wurtzite, zincblende, CsCl-type, and rocksalt structures. However, under ambient conditions, wurtzite is the stable phase of ZnO.[2,3]

A number of theoretical and experimental studies exploring the electronic, structural, and optical properties of doped and undoped ZnO have been reported in the literature.[4–18] Earlier band structure calculations were aimed at locating the energy of the *d* bands and computing the bandgap. Moreover, the effect of *pd* repulsion on the formation of bands in wurtzite and other polymorphs of ZnO and CdO has been examined.[14–19] It has been observed that the role of 3*d* or *4*d electrons in the band structure of these two compounds is qualitatively similar, but the computed bandgaps diverge. It is claimed that a correct bandgap estimate is obtained by computing quasiparticle (QP) shift and *GW* calculations.[14–19] It is suggested that the correction term resulting from the QP is negligibly small when 25% Hartree–Fock (HF) exchange is mixed with the 75% exchange derived from density functionals.[15,17,19] Therefore, it would be interesting to compute the band structure for this compound considering the hybrid functional, i.e., hybrid-25 (HY-25).[20] Further, band energies calculated by the density functional theory (DFT) and HF methods would enable logical comparison with the HY-25 scheme.

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