Bonding Formation and Orbitals Nature of Zno Structure

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Abstract:

The structural and electronic properties of wurtzite ZnO structure have been theoretically investigated within the framework of the density functional theory and plane wave pseudopotential method. In contrast to recent studies, our calculations reveal that the Zn-O bonds have a pure ionic nature and no appreciable degree of covalency has been observed. The highest occupied and lowest unoccupied states have been found to originate from the p orbitals of the Zn atoms, suggesting different approach of charge transfer between the O and Zn atoms. Detailed calculations on the fundamental structural and electronic properties of the ZnO structure have been determined and compared with the available studies.