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Calculation of Electronic and Structural Properties of the Semi-Conductor MgS_xSe_{1-x} by Using the FP-LAPW Method

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The structural, electronic properties of three chalcogenide compounds MgS, MgSe in rockslat phase have been investigated by using the full-potential linearized augmented plane-wave method (FP-LAPW) within density functional theory(DFT). We employed the local density approximation (LDA) and generalized gradient approximation (GGA) for the exchange-correlation (XC) potential.The equilibrium lattice constants are in agreement with the values reported in the literature.From the study of the electronic properties, we find that these binary compounds MgS and MgSe have indirect band gaps.

For ternary alloy MgS_xSe_{1-x} the study of these various properties are calculated, particularly the variation of structural and electronic parameters with concentration x. We focused our attention on the origins of bowing parameters corresponding to these physical properties.

In this study, we compare these predictions to the results already obtained experimentally as well as theoretical work in this regard.

Keywords: DFT, FP-LAPW, magnesium chalcogenides, ternary alloys, bowing parameter.