In Press, Corrected Proof (?)

Electronic and optical properties of Quasi-1D barium zinc chalcogenides Ba_2ZnX_3 (X = S, Se, Te): A DFT approach

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Highlights

- Ba_2ZnS_3, Ba_2ZnSe_3 and Ba_2ZnTe_3 were investigated using density functional theory with PBE and HSE06 functionals.
- All materials exhibit quasi-one-dimensional structure with infinite chains of corner sharing ZnX_4 distorted tetrahedra.
- Electronic structure calculations show that all materials are wide band gap semiconductors with direct band gap.
- All materials exhibit high optical anisotropy and large birefringence.

Abstract

We investigated structural, electronic and optical properties of quasi-one-dimensional barium zinc chalcogenides Ba_2ZnS_3, Ba_2ZnSe_3 and Ba_2ZnTe_3 using density functional theory as implemented in VASP. The structures crystallise in the orthorhombic space group D_{2h}^{16} – Pnma and were studied using PBE and HSE06 functionals incorporating van der Waals corrections using DFT-D3 method. It was found that the calculated structures agree well with experimental