Abstract Submitted
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Effect of pressure on band structure properties of Zinc Chalcogenides[1] DHARMBIR SINGH, PIET, Samalkha, Panipat, India — The first principal calculations have been carried out to study the effect of pressure on band structure of Zinc Chalcogenides. The tight-binding linear muffin-tin orbital method (TB-LMTO) within local density approximation (LDA) has been used to study the band structure properties at abmbient and high pressure. The phase stability is determined from the total energy calculations within the atomic-sphere approximation (ASA). The purely theoretical calculations show that in these materials (i) at ambient pressure, zinc blende type (B3) phase is more stable than rock salt type (B1) phase; and (ii) it exhibits a phase transition from zinc blende (B3) type to NaCl type (B1) type structure at high pressure. At further ultrahigh pressure there is phase transition from NaCl type (B1) phase to CsCl type ($B2$) phase. Although the calculated lattice parameter, transition pressure, volume of collapse is found to be little less than the experimentally observed value, but this has been explained from the fact that the calculation has been carried out at 0 K while the experiments have been performed at room temperature. Ambient & high pressure band structural results are compared with earlier obtained similar results and explained in details.

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