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Structural Properties of CuCl, CuBr, and CuI Compounds under Hydrostatic Pressure

Authors : S. Louhibi-Fasla, H. Rekab Djabri, H. Achour

Abstract : The aim of this work is to investigate the structural phase-transitions and electronic properties of copper halides. Our calculations were performed within the PLW extension to the first principle FPLMTO method, which enables an accurate treatment of all kinds of structures including the open ones. Results are given for lattice parameters, bulk modulus and its first derivatives in five different surface phases, and are compared with the available theoretical and experimental data. In the zinc-blende (B3) and PbO (B10) phases, the fundamental gap remains direct with both the top of VB and the bottom of CB located at Γ.

Keywords : FPLMTO, structural properties, Copper halides, phase transitions, ground state phase
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