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DFT calculation of the electronic and optical properties of Ag_2PdO_2 from X-ray and neutron crystallographic data

Abstract

Electronic and optical properties of ternary silver palladium oxide (Ag2PdO2) are investigated using density functional theory. Two different possible approximations for the exchange correlation potentials were employed. The X-ray and neutron crystallographic data were optimized by minimization of the forces (1 mRy/a.u.) acting on the atoms. The electronic structure, electron space charge density, chemical bonding and optical dielectric were determined from the relaxed geometry seeking deep insight understanding of this material. Our calculated energy band gap (0.15 eV) shows a good agreement with the experimental value (0.18 eV).

Keywords

Ag2PdO2; Electronic structure; Optical properties; Semiconductors