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Structural, Mechanical, Electronic, Elastic and Chemical Bonding Properties of the Complex K2PtCl6-Structure Hydrides Sr2RuH6 First-Principles Study

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Abstract : We report a systematic study of the structural, electronic and elastic properties of the ternary ruthenium-based hydrides Sr2RuH6 within two complementary first-principles approaches. We describe the properties of the Sr2RuH6 systems looking for trends on different properties. Our results are in agreement with experimental ones when the latter are available. In particular, our theoretical lattice parameters obtained using the GGA-PBEsol to include the exchange-correlation functional are in good agreement with experiment. Analysis of the calculated electronic band structure diagrams suggests that these hydrides are wide nearly direct band semiconductors, with a very slight deviation from the ideal direct-band gap behaviour and they are expected to have a poor hole-type electrical conductivity. The TB-mBJ potential has been used to correct the deficiency of the standard GGA for predicting the optoelectronic properties. The calculated TB-mBJ fundamental band gap is about 2.99eV. Calculated density of states spectra demonstrate that the topmost valence bands consist of d orbitals of the Ru atoms, classifying these materials as d-type hydrides. Analysis of charge density maps tells that these systems can be classified as mixed ionic-covalent bonding materials. The single-crystal and polycrystalline elastic moduli and their related properties have been numerically estimated and analysed for the first time.

Keywords : Ruthenium-based hydrides; first-principles calculations; elastic constants; electronic structure