

Structural, electronic, optical and elastic properties of the complex K₂PtCl₆-structure hydrides ARuH₆ (A = Mg, Ca, Sr and Ba): first-principles study

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Abstract: We report a systematic study of the structural, electronic, optical and elastic properties of the ternary ruthenium-based hydrides A₂RuH₆ (A = Mg, Ca, Sr and Ba) within two complementary first-principles approaches. We describe the properties of the A₂RuH₆ systems looking for trends on different properties as a function of the A sublattice. 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 gaps are about 3.53, 3.11, 2.99 and 2.68 eV for Mg₂RuH₆, Ca₂RuH₆, Sr₂RuH₆ and Ba₂RuH₆, respectively. Calculated density of states spectra demonstrates 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. Optical spectra in a wide energy range from 0 to 30 eV have been provided and the origin of the observed peaks and structures has been assigned. Optical spectra in the visible range of solar spectrum suggest these hydrides for use as antireflection coatings. 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; optical properties; electronic