Structural, electronic, optical and elastic properties, vibrational 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 deviationfrom 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. Analysisof 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, vibrational properties, electronic structure.