7th African Conference on Non Destructive Testing ACNDT 2016 & the 5th International Conference on NDT and Materials Industry and Alloys (IC-WNDT-MI)

2016

Structural, Mechanical, Electronic, Elastic andChemical Bonding Properties of the Complex K_2PtCl_6-Structure Hydrides Sr_2RuH_6: First Principles Study

BOUDRIFA OUASSILA, ABDELMADJID BOUHEADOU

Abstract : We report a systematic study of the structural, electronic and elastic properties of the ternary ruthenium-based hydrides Sr_2RuH_6 within two complementary first-principles approaches. We describe the properties of the Sr_2RuH_6 systems looking for trends on different properties. Our results are in agreement with experimental ones when the latter areavailable. 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 topmostvalence 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