Structural, mechanical and optical properties of the complex K2PtCl6-structure hydrides Ba2OsH6: ab initio study

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Abstract: Several applications of hydrides have been found so far, e.g. switchable mirrors [1–2], energy storage [3,4], rechargeable batteries [4], etc. Using first-principals density functional calculations, we report a systematic investigations of the structural and optical properties of the ternary ruthenium-based hydrides Ba2OsH6 within two complementary first-principles approaches. We describe the properties of the Ba2RuH6 systems looking for trends on different properties as a function of the A sublattice. Our results are in agreement with experimental ones when the later are available. In particular, our theoretical lattice parameters obtained using the GGA-PBE to include the exchange-correlation functional are in excellent agreement with experiment. The mechanical stability of the considered materials has been examined on the light of the pressure dependence of the elastic constants. Optical spectra in a wide energy range from 0 to 40 eV have been provided. Optical spectra in the visible range of solar spectrum suggest these hydrides for use as antireflection coatings.

Keywords: structural, Ab initio calculations, Ternary Hydrides, mechanical properties, optical properties