Structural, elastic, electronic and chemical bonding properties of the semi-conductor matérials Ba2OsH6: An ab initio study

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Abstract : Several applications of hydrides have been found so far. During the last decade, applications such as hydrogen storage/economy [1,2], rechargeable batteries [2], etc., have been the subject of intensive research efforts. After the discovery of the switchable optical properties of yttrium and lanthanum hydride films [3], hydrides have found another application as smart windows [3–4]. For the above listed specific applications of hydrides fast kinetics of hydrogenation/dehydrogenation processes, low temperature at which the hydrogenation/dehydrogenation occurs, large hydrogen content, low total weight and powder form of hydrides are extremely important. However, hydrides with large total weight, low concentration of hydrogen atoms and high temperature for activation of hydrogenation/dehydrogenation processes have received little or no attention. Recently, this class of hydrides has been suggested as a source of important applications in semiconductor electronics, such as transparent conducting materials [5] and semiconductor p–n junctions [6].

Keywords : structural, elastic, electronic, chemical bonding ab initio calculations, Electronic band, densities of states, Charge density.