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Pressure induced phase transition and superconducting properties of PtH and IrH: a first principles study

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Abstract. The electronic, structural, mechanical and superconducting properties of PtH and IrH are investigated using first principles calculation based on density functional theory with generalized gradient approximation. The calculated lattice constants at normal pressure are in good agreement with experimental and other theoretical results. Among the five crystallographic proposed structures investigated, the cubic phase is found to be more stable than the hexagonal ones. A new high pressure CsCl phase is predicted for Iridium hydride. The maximum superconducting transition temperature achieved in Platinum hydride and Iridium hydride are 23.8K and 10K respectively. The calculated elastic constants indicate that both the hydrides are mechanically stable at ambient pressure.

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Key words: structural phase transition, electronic structure, elastic properties, superconducting transition temperature

1 Introduction

Density functional theory (DFT) calculations of metal- hydrogen systems represent a growing field of research [1]. Hydrogen is known to form compounds with many elements in the periodic table [2]. Among those, the metal hydrides are of particular interest due to their application in hydrogen storage for fuel cells [3, 4] or heat storage for the solar-energy industry [5]. Platinum (Pt) and Iridium (Ir) are frequently used to form electrodes (which allow measurements of electrical resistance, the concentration of electrical

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carriers and the Hall mobility) and as heat coupler. Pt and Ir play a very important role in high pressure studies [6-8]. Although a number of transition metal hydrides have been synthesized under high pressure conditions [9], the investigation of platinum hydride (PtH) and iridium hydride (IrH) is rare especially in its high pressure behavior. There are only a few works on high pressure study of platinum hydride [10-13] and there are no experimental and theoretical investigations on the structural phase transition of IrH. Experimentally Thomas Scheler et.al [14] found two hexagonal phases of PtH, one is stable at low pressure and another predicted P63/mmc structure appears as a single phase of PtH above 42 GPa. Theoretically Papaconstantopoulos et al. [15] has showed NaCl PtH is stable at ambient pressure. Duck Young Kim et al. [16] investigated the superconducting properties of some transition metal hydrides TMH (TM=Rh, Pd, Ag, Pt, Ir and Au) and observed high superconducting transition temperature in fcc phase of platinum hydride (T_c=24.5 K). Still there is a contradiction about the stable structure of Platinum hydride. This motivated us to analyze the structural stability of platinum hydride. Moreover, to the best of our knowledge the structural phase transition and pressure dependence of superconductivity in Iridium hydride have not been reported yet. In the present paper the electronic and elastic properties of PtH and IrH are analyzed under normal pressure. Also a pressure induced structural phase transition and superconducting properties of PtH and IrH are investigated.

2 Computational details

The DFT calculations are carried out using the Vienna ab initio simulation package (VASP) [17-19]. The generalized gradient approximation (GGA) is used for the correlation energy functional with the Perdew-Burke-Ernzehof functional (PBE) [20-21]. In the present computation, the hydrides are assumed to be defect free and the stoichiometric composition for all the hydrides is taken as 1:1 ratio of metal and hydrogen atom. The electronic wave functions are expanded in a plane wave basis set with an energy cut-off of 500 eV and 600 eV for PtH and IrH respectively. To predict the stable structure of PtH and IrH, five possible phases are considered. The space group and atomic positions are tabulated in Table 1.

The valence electron configuration for H, Pt and Ir atoms are $1s^1$, $6s^1$ $5d^9$ and $6s^2$ $5d^7$ respectively. For both PtH and IrH, relaxations are performed so that the convergence of Hellmann-Feynman forces is better than 1 meV/Å. The self-consistent total energy is converged with energy difference less than 0.01 meV. A dense grid of k points in the irreducible wedge of Brillouin zone is used with the sampling generated by the Monkhorst-pack procedure [22]. The Crystalline structure, k-point set, energy cut-off and smearing width of PtH and IrH are given in Table 2.The density of states (DOS) are obtained using the linear tetrahedron method with Blöchl corrections on the relaxed structures.

The tight binding linear muffin tin orbital method [23-27] is used for the estimation of electron-phonon coupling constant and electron-electron interaction parameter. This