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Research Article

Role of hydrogen and hydrogen storage in lithium hydride

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Abstract

Tight binding linear muffin-tin orbitals atomic sphere approximation have been used to examine the structural stability, electronic properties, charge density and magnetization of lithium hydride (LiH).In our study, the direct band gap (4.25 eV) detected between the valence bands (especially dominated by hydrogen) and conduction bands implies that LiH is insulating in nature with strong ionic bonds and weak orbitals-hybridization. Furthermore, we noticed that the hydrogen contributed more to the total density of states than the lithium in the complete system, based on the spin polarised partial density of states of H and Li. Because our calculated band gap accords with experiment, the results found in LiH suggest that it is a better choice for optoelectronic devices. The strength of hybridization of orbitals and band gap properties improve energy storage as well.

1. Introduction:

The utilization of hydrogen as a fuel depends on the development of energy storage materials with a high mass content of hydrogen [1].Due to the hydrogen capacities of lithium hydride, it is considered to be attractive metal hydrides. Many researches have been performed on the metals and perovskites hydrides to improve their performance [2-4]. Various theoretical and experimental groups [5-8] have found the energy separation for LiH to be in the range of (2.8 eV - 5.7 eV). The significant variance in band structure of the same material when measured using different methods, as well as the inconsistency in band gap measurements in earlier studies, motivated us to look into it more. The electronic band structure, density of states (DoS), orbitals contributions, and functions of hydrogen in LiH in terms of both electronic structure and magnetic properties of materials are all addressed in this paper.

2. Method:

Computer simulation is being greatly used in the field of research in scientific community. The standard local density approximation is used to address exchange correlation potential. We have only included the energetically higher-lying valence states in the self-consistent calculations of the effective crystal potential according to the norms of the TB-LMTO-ASA approach [9, 10] with the applications of approach to understand the properties of materials [11-14].The core states are treated fully relativistically while the semi-core and valence states as treated semi-relativistically. All the calculations were iterated to self-consistency along with accuracy of 10^{-6}Rydberg.

3. Result and Discussion:

Crystal Structure of LiH:

A crystal structure is formed by the addition of a basis to every lattice point: a lattice combined with a basis creates a crystal structure.

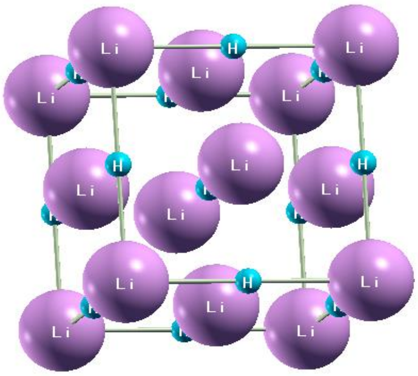

Figure 1: Crystal Structure of Li, each face centered atom is shared by two unit cells. There are six faces of a cube and six face centered atoms.

Electronic Band Structure of LiH:

Band structures represent energy difference between the lowest point of the conduction band (conduction band edge) and the highest point of the valence band (valence band edge).The band structure of Lithium hydride is as shown in the figure below. The energy bands above the Fermi level (E_F) are known as the conduction bands and energy band below the E_F are known as valence bands.

In the band structure of lithium hydride, we found the finite gap between the valence band and conduction band. This finite gap between conduction band and valence band conclude that lithium hydride is insulator in nature.

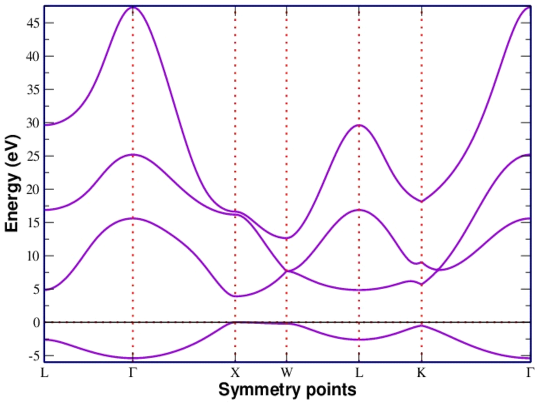

Figure 2: Electronic Band structure of Lithium Hydride (LiH)

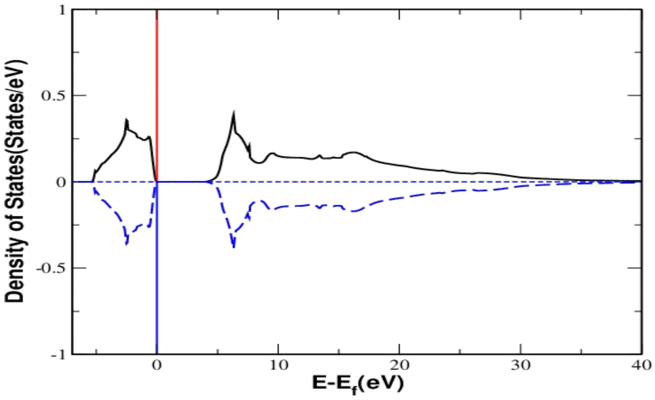

Figure 3: Up and down spin channels of LiH

There are altogether three bands in the conduction band region and only one band in the valence band region. The conduction band originates from transitions at L K and X, The minimum value of energy of conduction band at symmetry point-X was found to be 3.92 eV. The maximum value of energy of valence band was found to be -0.23 eV. The difference between minimum values of energy of conduction band and the maximum value of valence band is said to be direct band gap, which was found to be 4.2 eV. Our result agrees with previously reported experimental energy band gap of 4.9eV [8].

Density of States (DoS) of LiH:

The number of orbitals per unit energy range at each energy level that are accessible to be occupied is known as density of states. It's also known as the number of quantum states that can exist in a given energy range. The number of quantum states is vital in determining a material's optical properties, hence studying density of state is significantly more relevant.

Calculations based on DoS can be used to establish the pattern of states as a function of energy, as well as the spacing between energy bands. A high DoS at a specific energy level indicates that there are many states available for occupation. The bond between them is fully ionic in nature, as found from charge and density of states analysis. The density of states of Lithium hydride is as shown in figure 3.

As seen in figure 3, The Fermi energy, which is the reference between up and down spin of LiH, is taken as a zero line parallel to the X-axis. In the valence bands, we noticed two mounted peaks. The non-magnetic character of LiH is demonstrated by the symmetric nature of up and down spin channels.

Density of States of Lithium:

From the figure 4, contribution of Li is lesser in the valence band but contribution of Li is greater in the conduction band. Four principal peaks were observed at 0.032 States/eV, 0.030 States/eV, 0.023 States/eV and 0.008 States/eV. Low hybridization is seen among the orbitals.

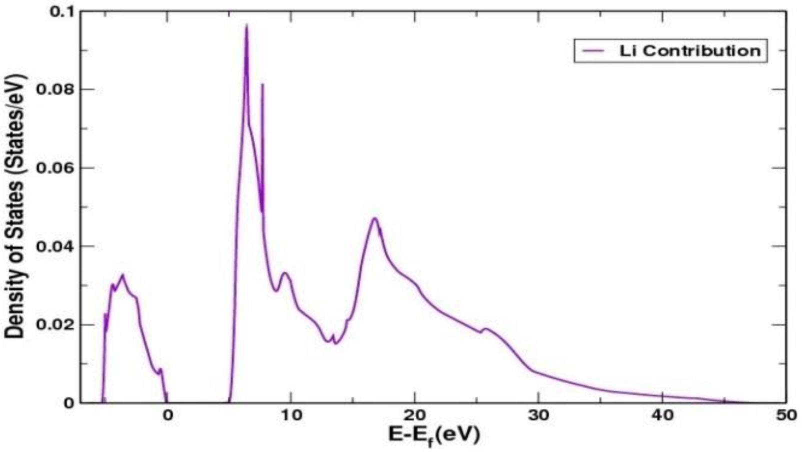

Figure 4: DoS of Lithium

Density of States of Hydrogen:

The electrons DoS of H is as shown in the figure below. From the figure the contribution of H is greater in valence band; however, contribution of H is lesser in conduction band. In the figure 5, we found two peaks appeared in the valence band. The values of two peaks were found to be 0.205 States/eV and 0.196 States/eV.

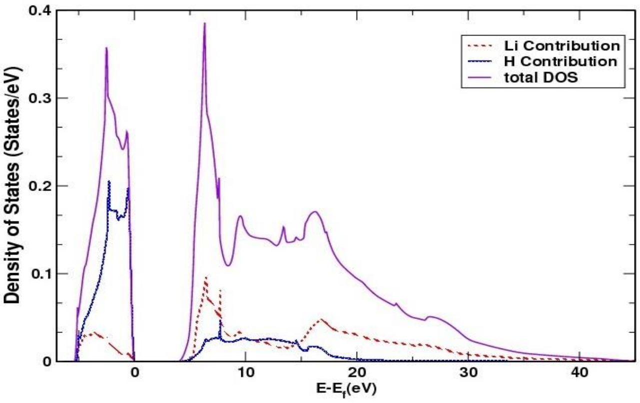

Figure 5: DoS of hydrogen

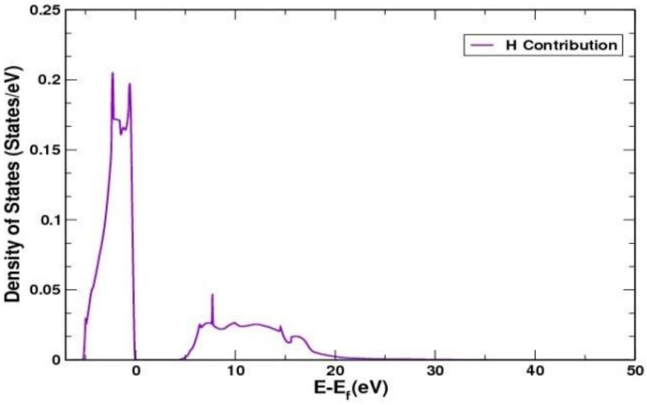

Figure 6: Partial DoS of Li and H of LiH

Partial Density of States of Li and H of LiH:

From the figure 6, we observed 2 and 4 peaks of hydrogen and Lithium respectively. Among them, 0.20 states/eV of hydrogen is the highest one. Hydrogen plays the significant role to increase the total states in LiH.

Li-s state hybridizes to H-s state nearby 15.23 eV and -4.10 eV. Difference in electronegativity along with electrostatic force are responsible to change the character of lithium after adding hydrogen.

Distribution of charge (Q=ne) takes place with ionic bonding. The outer most electrons from Li region are shifted to region of hydrogen as a result majority of charges are accumulated on site of hydrogen.

4. Conclusion and Concluding Remarks:

LiH can be employed as insulating devices due to the finite gap between the valence and conduction bands. Valence band is dominated by hydrogen. LiH's non-magnetic behavior is corroborated by its symmetric up and down states. The greatest peak positions are 0.20 and 0.19 states/eV, respectively, revealing that hydrogen plays a major role in increasing the total density of states, supportive to the fact that lithium (metal) hydrides are the leading hydrogen storage materials. This mechanism is related to hydrogen storage [15, 16] in terms of charge transfer from metals to metal sheet.

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Compliance with Ethical Standards:

The author declare that they have no conflict of interest.

Availability of data and material

The findings of this study are obtained from the corresponding author.

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