Eng. Sci., 2022, **18**, 98–104

Engineered Science
DOI: https://dx.doi.org/10.30919/es8d658

Computational Investigation on Lithium Fluoride for Efficient Hydrogen Storage System

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Abstract

Lithium fluoride (LiF) serving as a template for an efficient hydrogen storage system has been expressed in this article. The structure optimization, stability, and reactivity of the derived LiF systems have been studied with density functional theory (DFT) based reactivity descriptors. The binding energy/H_2 gives support to the quasi-molecular type adsorption process. According to natural bond orbital (NBO) data analysis, the charge on the Li atom decreases gradually with each successive H_2 adsorption, and a charge transfer interaction occurs from H_2 molecules to the Li of the LiF. From atoms-in-molecule (AIM) analysis, molecular hydrogen interacts with building blocks through electrovalent-type interaction. The astonishing gravimetric wt% result (43.48 upon ten hydrogen adsorption in a single LiF) justifies this template to be a potential hydrogen storage material. The Gibbs free energy changes suggest a spontaneous hydrogen adsorption process at or below 54 K.

Keywords: Lithium fluoride; Density functional theory; Binding energy; Quasi-molecular adsorption; Gravimetric wt%.
Received: 02 February 2022; Revised: 17 February 2022; Accepted: 19 February 2022.
Article type: Communication.

1. Introduction

Energy and climate change are the most imperative issues in the present time throughout the world. Energy consumption is increasing day by day. Within a few decades, the demand for carbon-based fossil fuels will likely outpace its rate of production. It is seen that three times of mass of gasoline is required to supply the same energy as compared to hydrogen. In addition, the emission of CO_2 during the combustion of fossil fuels also can't be overlooked. In a combustion reaction of hydrocarbons, the energy contribution of hydrogen per gram is more comparable to carbon. To reduce the dependency on carbon-based fossil fuels, the limelight comes to hydrogen, which might be a promising clean alternative energy carrier because of its higher energy density proficiency and sustainable environment-friendly combustible nature.[1-5] However, one of the major challenges in this context is the storage of hydrogen. On a large volumetric scale, hydrogen being gas at standard temperature and pressure is necessary to meet the same energy as provided by gasoline being liquid under the same condition.[6] To deal with this low volumetric density problem, the designing of solid-state hydrogen storage materials has drawn the keen interest of researchers.[7,8] The density of hydrogen storage becomes a key issue for its portable applications. The density of hydrogen at atmospheric pressure and temperature is very low (1/14 of the air density) and thus the hydrogen storage density of the system is a key factor for hydrogen energy applications.[9,10] Presently, for the mobile applications of hydrogen, two storage paths are established, *i.e.*, high-pressure gas storage and low-temperature liquid storage. The gas storage density, high-pressure tank, hydrogenation station, and safety, are the main challenges for a high-pressure hydrogen gas storage path.[11,12] Physisorption and chemisorption are the two storage routes for solid hydrogen storage materials and a series of materials have been theoretically predicted.[5] But high hydrogen storage capacity cannot be achieved by physisorption, although in this process, the desorption of hydrogen can occur under ambient conditions. Chemisorption is a simple way to store a large

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quantity of hydrogen. But since it's not a reversible process, chemisorption cannot satisfy the storage criteria.[13-17] It appears that for materials to possess promising storage capacity, the hydrogen adsorption process should be reversible and the concerned energy should lie in between that of physisorption and chemisorption (quasi-sorption).[18,19] Keeping in view all these things, we recently started to find out some suitable hydrogen storage materials, which can meet the target set up by the U.S. Department of Energy (DOE)[20] (6.0% in 2010, and 9.0% in 2015) with a high gravimetric wt%.[18,19] Due to the small size of lithium fluoride and greater charge density of Li, we choose this template LiF for storing hydrogen with satisfactory results. We communicate the results in this article.

2. Theory and Computational Details

The Gaussian 16w computer program has been used to optimize ground state geometries of all the studied systems by using numerous functionals, including B3LYP, CAM-B3LYP, *ω*B97X-D, and two distinct basis sets, LanL2DZ and 6-311+G(d,p) to get the ground state energy minima of the structures.[19,21-23] Here we have taken two basis sets to know whether there has been any significant change in reactivity parameter values. Frequency optimization is also performed in the same functional and basis set to ensure their location at the minimum of the potential energy surface. All the geometries have been optimized without any symmetry constraints and the default optimization criteria embedded in Gaussian16 software have been used.

The employment of CAM-B3LYP and *ω*B97X-D is largely to rectify the long-range interaction. All the optimized geometry along with their ground state energy and point groups are depicted in Fig. 1, Figs. S1, S2, S3, and S5. The cartesian coordinates of optimized geometries were listed in the data set. D1 of supporting information file. Hardness (η), electrophilicity (ω), the average adsorption energy per hydrogen molecule (E_{ads}/H_2), the donor-acceptor (bonding–antibonding) charge-transfer interaction, the gravimetric wt%,

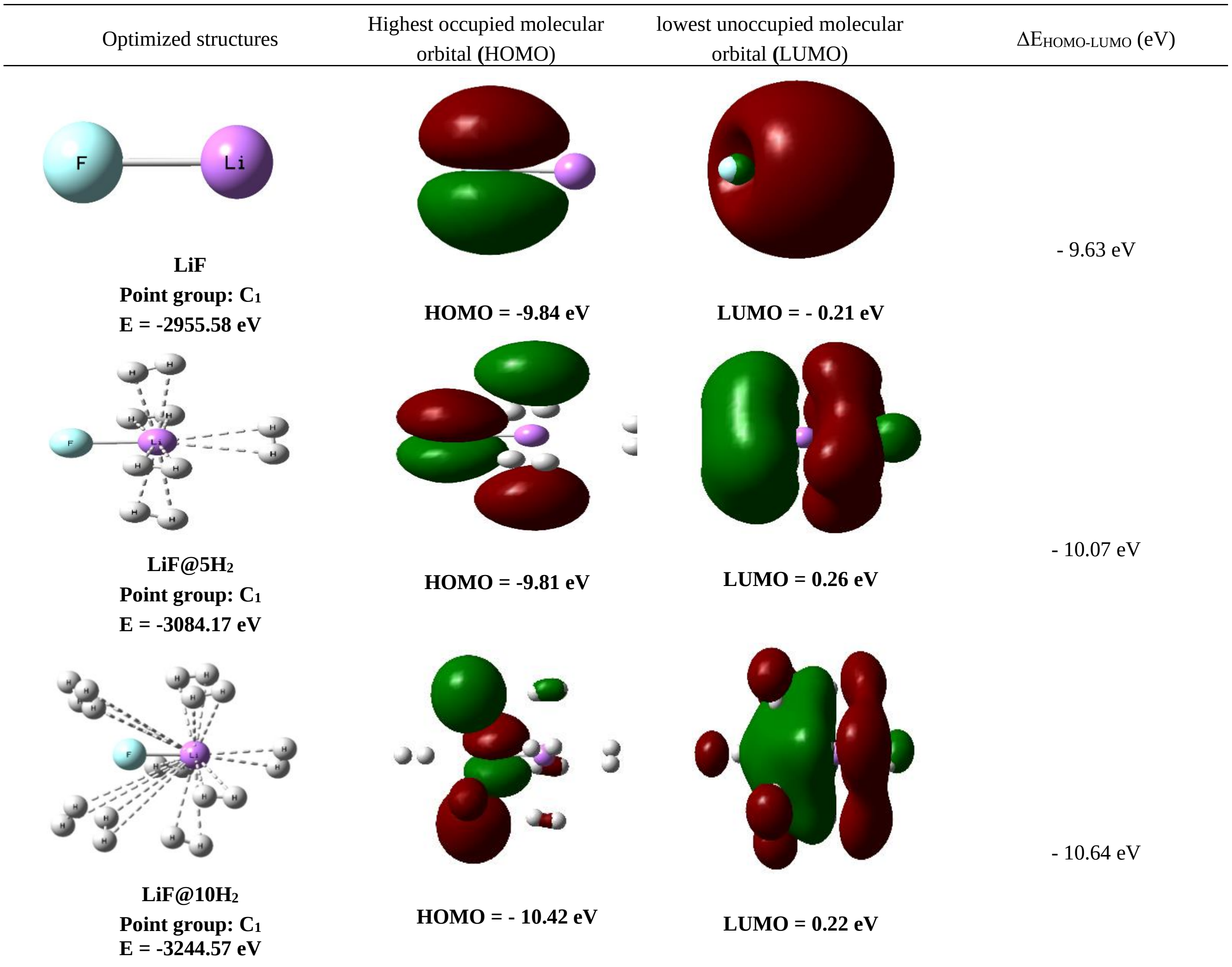

Fig. 1 Optimized geometries, energy, point group, HOMO, LUMO, and $\Delta E_{HOMO-LUMO}$ (eV) of LiF, $LiF@5H_2$, and $LiF@10H_2$ systems at the ωB97X-D/6-311+ G (d, p) level of theory.

and the Gibbs free energy change of the LiF@nH_2 systems, as well as the adsorption ability (Er) of LiF, have been calculated by using standard techniques.[18,19,24-35] To understand the binding nature of this trapping mechanism, the Multiwfn package[36] was used to perform the atoms-in-molecules (AIM) analysis.[37] The Multiwfn software is an extremely powerful program for realizing electronic wavefunction analysis, which is a key ingredient of quantum chemistry. The details have been given in supporting information.

3. Results and discussion

3.1 LiF@nH_2: Stability, reactivity, and average adsorption energy per H_2 (E_{ads}/H_2)

The dipolar LiF molecule can adsorb up to 10 H_2 molecules (up to five around the Li center and after that around the whole LiF molecule). The optimized structures, energy, point group, frontier molecular orbitals such as HOMO/LUMO of the systems, and corresponding bandgap ($\Delta E_{\text{HOMO-LUMO}}$) have been given in Fig. 1 and Figs. S1, S2, and S3 (supporting information file). From Tables S1 and S2, it is evident that the hardness (η, eV) has gradually increased and electrophilicity (ω, eV) has relatively decreased when molecular H_2 is adsorbed one after another on the LiF surface. This trend is found similar for all types of basis sets (B3LYP, CAM-B3LYP, and ωB97X-D) used during the calculation. This has been perfectly manifested in Fig. S4. This is the indication of increasing stability and decreasing reactivity trends and respectively upon gradual H_2 adsorption. Again, the higher the bandgap ($\Delta E_{\text{HOMO-LUMO}}$) higher is the stability and the lower the reactivity,[38] which is clearly observed in Fig. 1 and detail given in Figs. S1, S2, and S3.

The average adsorption energy per molecule of hydrogen (Eads/H_2) of LiF@nH_2 systems (Fig. 2 and Table S3) is decreased with the increase of the number of adsorbed H_2 molecules around the Li center and whole LiF. The reason behind that with the increase of the number of adsorbed H_2 molecules around the Li center and whole LiF, the natural bond orbital (NBO) charges on the Li are decreased (Table 1 and Fig. S5). As a result, the dipole-induced dipole interaction decreases, which directly influences the lowering of average adsorption energy per hydrogen molecule (Eads/H_2). But moving from eight H_2 to nine and ten, the NBO charges on the Li center remain unchanged, this may be attributed to the lowering of dipole-induced dipole interaction due to the movement of adsorbed molecular hydrogen towards the fluorine (F) center. Now, another important parameter, namely adsorption ability (E_r), is the indication of how many adsorbed H_2 molecules will be considered to be calculated (Table 1). The result reflects that up to ten adsorbed H_2, its values are decreased; after that, its value is negligible. Thus, we have considered LiF can adsorb a maximum of ten molecular hydrogens. Next, the gravimetric wt% of all H_2 adsorbed systems has been recorded (Table 1). This is an excellent result when we compare it with the reference value of the U.S. D.O.E. standard value[20] as well as other reported systems[18,19] reported in Table S7.

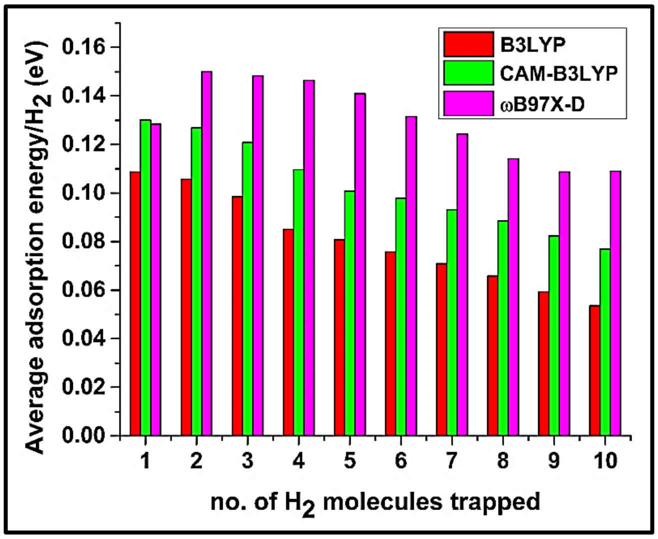

Fig. 2 Plot of average adsorption energy/H_2 [eV] *vs* no. of H_2 molecules trapped of LiF@nH_2 systems at the B3LYP, CAM-B3LYP, and ωB97X-D/6-311+ G(d,p) level of theory.

Table 1. NBO charges of LiF@nH_2 systems at CAM-B3LYP/6-311+G(d,p) level of theory, adsorption ability (E_r) of LiF@nH_2 systems at the B3LYP and CAM-B3LYP/6-311+G(d,p) level of theory and Gravimetric wt% of LiF@nH_2 systems.

System	NBO charges	Adsorption ability (E_r)		Gravimetric wt%
		B3LYP	CAM-B3LYP	
LiF@H_2	0.96	0.109	0.130	7.14
LiF@2H_2	0.95	0.103	0.124	13.33
LiF@3H_2	0.93	0.084	0.109	18.75
LiF@4H_2	0.91	0.045	0.076	23.53
LiF@5H_2	0.89	0.064	0.065	27.78
LiF@6H_2	0.88	0.051	0.083	31.58
LiF@7H_2	0.88	0.042	0.065	35.00
LiF@8H_2	0.88	0.029	0.056	38.10
LiF@9H_2	0.89	0.008	0.033	40.91
LiF@10H_2	0.89	0.001	0.028	43.48

3.1.1 Bonding nature

The delocalization correction energy (ΔE_{CT}) and it's average (ΔE_{CT}^{av}) values have been expressed through Fig. S6 (the detailed results in Table S4) indicating that a charge transfer interaction happened from the bonding orbital (BD) of the trapped H_2 molecules to the anti-bonding lone pair orbital (LP*) of Li^+ ions. One interesting observation here is that up to five adsorbed H_2, the (ΔE_{CT}^{av}) values increase; after that, upon adsorption of 6H_2 onwards, the trend decreases. This may be due to the load of the adsorbed hydrogen shift towards the F center of the LiF molecule. We used topological analysis at the bond critical point (BCP) to find the bonding nature controlling parameters like electron density [$\rho(r_c)$], Laplacian of electron density [$\nabla^2\rho(r_c)$], local electron energy density [$H(r_c)$], kinetic energy density [$G(r_c)$], and potential energy density [$v(r_c)$] of the LiF@H_2. Using the multi-win package,[36] we developed three figures (Fig. 3 and Figs. S7 and S8) to show the bonding behavior of LiF@H_2. The top and lower sections of Fig. 3 demonstrate the variations in the electron density. We can see that there is no electron density between the Li center and the adsorbed H_2 molecule. This supports the ionic bonding between the Li center and the adsorbed molecular hydrogen. In Fig. S7 the areas of charge depletion (green solid lines) and charge concentration (blue dotted lines) are depicted. The solid brown lines represent the bond paths, while the solid bold blue lines represent the zero-flux molecular plane surfaces.[39] The light blue spheres indicate the bond critical points (BCPs), where the bond path and zero-flux surfaces intersect. No electron density between Li and the molecular hydrogen suggests ionic bonding. Fig. S8 shows the electron localization function (ELF) of the systems. There are no localized electrons between Li and the adsorbed molecular hydrogen in this image. To determine the bonding type, $\nabla^2\rho(r_c)$, $H(r_c)$, and [$-G(r_c)/V(r_c)$] values have been calculated at the BCP [Table S5]. As the values of both $\nabla^2\rho(r_c)$ and $H(r_c)$ are positive (0.04 and 0.002) and the ratio of $-G(r_c)$ to $V(r_c)$ is larger than 1, we may assume that FLi$\cdots H_2$ interactions are non-covalent.[40-42]

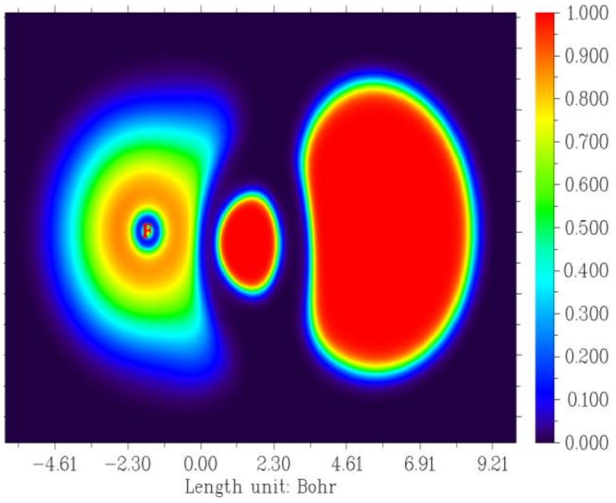

Fig. 3 The plot of the ELF of the LiF@H_2 systems generated at the ωB97X-D/6-311+G(d,p) level of theory.

3.1.2 Effect of temperature on hydrogen adsorption

The Gibbs free energy change analysis has been carried out (Fig. 4 and Table S6) to make an idea about the spontaneous H_2 adsorption temperature of LiF. Results reveal that at 54 K or below this temperature, this adsorption process will be spontaneous.

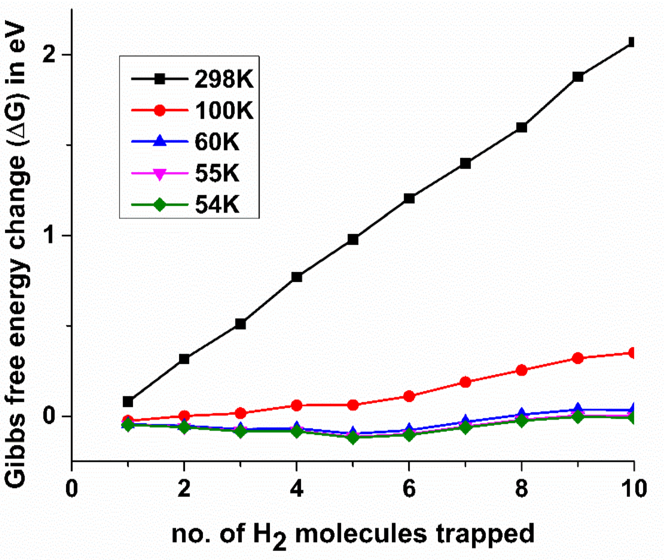

Fig. 4 Plot of Gibb's free energy change [eV] *vs* no. of H_2 molecules trapped of LiF@nH_2 systems at the ωB97X-D/6-311+G(d,p) level of theory.

4. Conclusion

The LiF molecule has been identified as a promising hydrogen storage material since the average adsorption energy per H_2 molecule supports a quasi-molecular adsorption process. According to the NBO analysis, the charge on the Li atom progressively drops with the gradual increase of H_2 adsorptions, indicating that a charge transfer interaction occurs between the bonding orbitals of H_2 molecules and the antibonding orbitals of Li. A single LiF molecule can adsorb up to 10 H_2 (LiF@10H_2) with a high gravimetric wt% value (43.48) which is found to be a much better system than our previously reported systems (Table S7). The amazing results demonstrate the LiF molecule as a promising hydrogen storage material w.r.t U.S.D.O.E. standards.[20] According to the atoms in molecule (AIM) analysis, molecular hydrogen interacts with the building units in electrovalent interactions. At or below 54 K, the changes in Gibbs free energy indicate that the hydrogen adsorption process is spontaneous. The findings are very encouraging and exciting for synthetic chemists and technologists in terms of the possibility of synthesizing this material as a potential hydrogen storage option in the pursuit of green fuel storage. Based on the findings reported in this article we are trying to develop a study on LiF clusters, a molecule-to-material approach that may help to design a new type of gas storage device by using the material which will help the real laboratory to land application.

Acknowledgment

All authors are thankful to the Haldia Institute of Technology for providing research infrastructure.

Conflict of interest

There are no conflicts to declare.

Supporting information

Applicable.

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