

Hydrogen storage in lithium-terminated boron chains

Hydrogen can be used as alternative energy source because of many advantages. Despite the high energy content by mass, hydrogen has low density, and it is necessary to develop an efficient storage medium to use this technology widely. The hydrogen-rich materials, such as metal-hydrides, have high desorption temperatures, slow desorption and often not reversible. This is because of the breaking of strong bonds, such as covalent and/or ionic bonds, during the release of hydrogen. Thus, hydrogen should be stored in molecular form. This requirement led to the adsorption-based storage of hydrogen on high-surface materials, such as carbon nanotubes and metal-organic frameworks. Despite having large storage capacity, the hydrogen molecules bind very weakly to these nanomaterials, which would release H₂ molecules at very low temperatures.

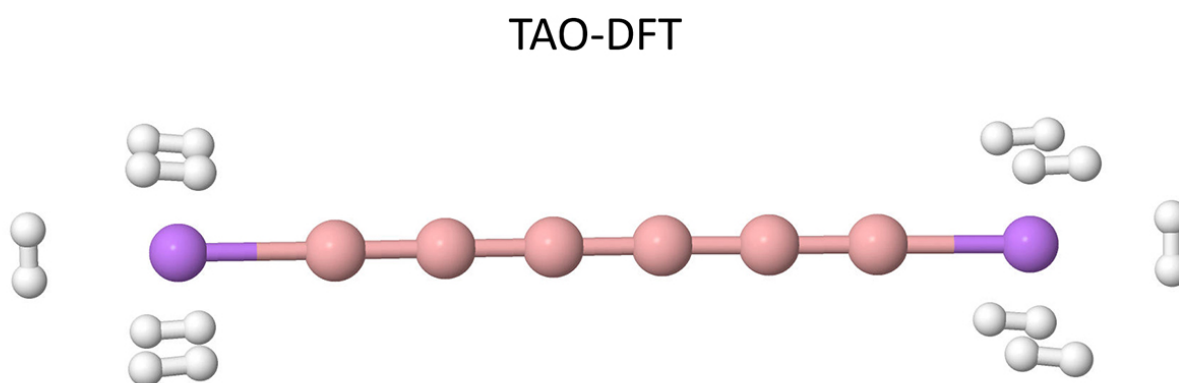


Fig. 1. Hydrogen storage in lithium-terminated boron chains.

In addition to large storage capacity, the hydrogen should be attracted to the host material with the suitable strength (about 20 to 40 kJ/mol per H₂) so that the hydrogen can be released at temperatures slightly higher than room temperature. In this research article, a novel hydrogen storage medium that promises high-capacity hydrogen storage at temperatures well-above the liquid nitrogen temperature has been reported. Boron, being light weight can increase the weight percentage. However, we found that the pure boron chains cannot store hydrogen at the desired range of strength. Thus, to increase the strength of the hydrogen interaction with the boron chains, we terminated the chains with lithium (Li) atoms. Generally, the terminating atoms used to enhance the interaction and storage capacity should be light weight, should not form clusters, and should bind hydrogen molecularly. In this research, lithium is used because it satisfies all these criteria.

We found that these Li-terminated boron chains have radical nature. Because of this, reliable

calculations on such materials are highly challenging using conventional theoretical methods. In this work, we adopt thermally-assisted-occupation density functional theory (TAO-DFT), a very efficient electronic structure method for systems with radical nature, to study the electronic and hydrogen storage properties of Li-terminated linear boron chains (Li_2B_n), with n boron atoms ($n = 6, 8, \dots$, and 16). From our TAO-DFT results, Li_2B_n , which have radical nature, can bind up to 4 H_2 molecules per Li, with the ideal binding energies. The hydrogen gravimetric storage capacities of Li_2B_n range from 7.9 to 17.0 wt%, achieving the ultimate goal of the United States Department of Energy. Therefore, Li_2B_n could be ideal media for storing and releasing H_2 at temperatures much higher than the boiling point of liquid nitrogen.

When used as fuel, the engines (hydrogen fuel cells) emit water vapor as the only effluent during the combustion of the engine giving balance to the environment. This research shows that Li-terminated boron chains are potential candidates for hydrogen storage application. The molecular adsorption of hydrogen guarantees favorable kinetics such as fast filling, and release when needed.

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