Joint CQSE and CASTS Seminar

Weekly Seminar
May 26, 2017 (Friday)

TIME May 26, 2017, 14:30 ~ 15:30
TITLE Electronic and Hydrogen Storage Properties of Strongly Correlated Materials: A TAO-DFT Study
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Abstract

Accurate prediction of the electronic and hydrogen storage properties of materials with strong static correlation has been very challenging for the traditional electronic structure methods. To meet the challenge, we use our newly developed thermally-assisted-occupation density functional theory (TAO-DFT) which is an efficient electronic structure method for the study of large systems with strong static correlation effects. Firstly, we show that Li-adsorbed n-acenes are strongly correlated materials and possess multireference character. Further, we show that the Li-adsorbed n-acenes are the potential candidates for hydrogen storage applications. The first and second set of H2 molecules adsorb on Li-adsorbed n-acene with the ideal binding energy range (20-40 kJ/mol per H2), promising the adsorption and desorption at near ambient condition. The hydrogen storage capacity of Li-adsorbed n-acene is 9.91–10.78 wt%. Then, we focus on linear carbon chains (Cn). Owing to the alteration of the reactivity of Cn and Li2Cn with n, odd-even oscillations in their electronic properties are found. In contrast to Cn, the binding energies of H2 molecules on Li2Cn are in (or close to) the ideal binding energy range. In addition, the H2 gravimetric storage capacities of Li2Cn are in the range of 10.7 to 17.9 wt%. On the basis of our TAO-DFT calculations, Li-adsorbed n-acene and Li2Cn can be high-capacity hydrogen storage materials that satisfy the USDOE's ultimate system target of 7.5 wt%.

References

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- Seenithurai, S., & Chai, J. D. Effect of Li Termination on the Electronic and Hydrogen Storage Properties of Linear Carbon Chains: A TAO-DFT Study. arXiv preprint, arXiv:1702.03055 (2017).