INVESTIGATION OF LITHIUM-CORANNULENE COMPLEX VIA AB INITIO CALCULATIONS AS MOLECULAR SYSTEM FOR HYDROGEN STORAGE

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In our prior work (1), molecular orbital (MO) calculations have been performed to investigate the influence of curved and planar carbon lattices on the nature of lithium bonding in lithium intercalated carbon anodes, in order to correlate molecular structure with that required for high-capacity lithium carbon anodes. It was found that molecular orbitals composed only of lithiums can be formed when the spin multiplicity is 2 and the carbon molecular system is fullerene C_{60} or corannulene $C_{20}H_{10}$. In this investigation, the lithium-corannulene molecular system was used to determine if hydrogen storage could be achieved through the interaction of a paramagnetic complex and hydrogen molecules. Figure 1 shows the optimized geometry for Li_5-$C_{20}H_{10}$-H_2 using density functional theory, B3LYP, and the 6-31G(d) basis set. The calculated hydrogen-hydrogen bond distance is 0.756 Å as compared with the calculated value of 0.743 Å in the neutral molecule. The lithium-hydrogen molecule separation is 2.08 Å. The binding energy of the hydrogen to the lithium is 1.95 Kcal mol^{-1}. Figure 2 shows the calculated structure for Li_5-$C_{20}H_{10}$-$3H_2$. In this case the hydrogen atom separation for the hydrogen directly over the lithium is 0.754 Å with a binding energy of 0.71 kcal mol^{-1}/H_2. As a comparison, figure 3 shows the calculated structure for Li_6-$C_{20}H_{10}$-$3H_2$. The hydrogen molecule directly over the lithium is separated by a distance of 2.18 Å from the lithium. The hydrogen atom separation is 0.750 Å. However, in this molecular system the binding energy/H_2 is 3.38 kcal mol^{-1}. In this paper, higher number of hydrogen molecules i.e., 5 to 9 molecules will be investigated.

References

1. G. Sandí, R. E. Gerald, L. G. Scanlon, C. Johnson, R. J. Klingler, and J. W. Rathke. *J. New Mater. Electrochem. Systs*. **3**, 13, 2000.

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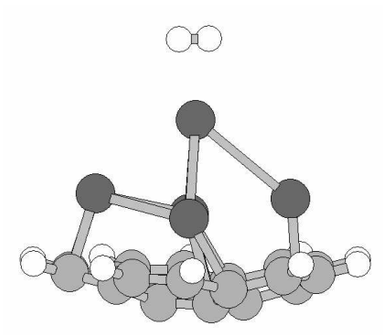

Figure 1: Calculated structure for Li_5-$C_{20}H_{10}$-H_2.

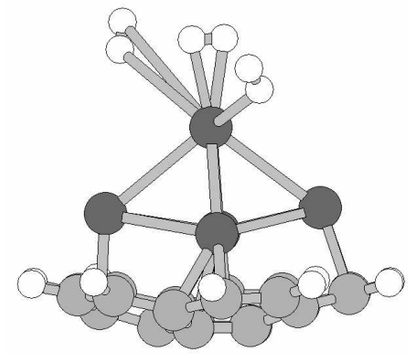

Figure 2: Calculated structure for Li_5-$C_{20}H_{10}$-$3H_2$.

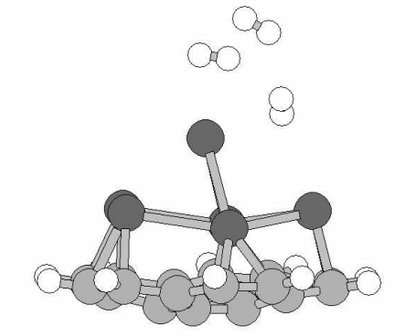

Figure 3: Calculated structure for Li_6-$C_{20}H_{10}$-$3H_2$.