

## **548b Investigation of Corannulene as Molecular System for Hydrogen Storage**

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Recent experiments have shown that a curved carbon lattice can adsorb 4 % by weight hydrogen at room temperature and at a pressure of 100 bars. In this system, hydrogen is fully released at 80°C. Carbon hydrogen bonds exist in the carbon lattice as confirmed by neutron experiments. Typically one expects 2 % by weight hydrogen storage at -80°C and 100 bars in carbon nanotubes. Physisorption of hydrogen is most likely the mechanism of storage in these cases where resonant fluctuations in charge distributions or van der Waals interactions are important. In order to gain an understanding of the increased hydrogen storage capability in the first case over that of carbon nanotubes, corannulene was chosen to model the curved carbon lattice with carbon-hydrogen bonds. Corannulene is an interesting molecule because it has a dipole moment that facilitates dipole-dipole interactions and it contains electropositive sites on the hydrogen atoms located along the periphery of the molecule. The importance of the positive charges on hydrogen atoms is evident from the crystal structure of corannulene in which corannulenes adopt a T shaped structure with one corannulene ring at ninety degrees to another. The positive hydrogen atoms are interacting with the negative electrostatic potential located in the center of the corannulene ring. Ab initio calculations using Moller-Plesset perturbation theory (MP2) are used to model hydrogen molecule interactions with either monomer or dimeric corannulene molecular systems since it has been previously shown that MP2 types of calculations can effectively model small cation-molecular hydrogen interactions. Besides neutral molecular systems consisting of corannulene, we are investigating the effect of doping corannulene with lithium. Lithium doping usually increases the dipole moment of the molecular system and provides extra electropositive sites for interaction with molecular hydrogen since there is electron transfer from the lithium to the corannulene ring. Molecular dynamics (MD) calculations demonstrate the reversibility of hydrogen storage in corannulene at room temperature and at pressures of approximately 100 bars. The MD results also suggest that spacing between rings is an important parameter to control for hydrogen storage.