440e Hydrogen Adsorption in Self-Assembled LI-Doped Corannulene

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Hydrogen is of great interest as future fuel because it is a clean and sustainable energy system. However, to use hydrogen as energy source, the key challenge is how to store and release hydrogen effectively under ambient conditions. Different lightweight carbon materials have been studied for H2 storage to meet the DOE target (6.5 wt%). However, pure carbon materials have low H2 storage capacity at ambient conditions. Alkali metal-doped corannulene is investigated as a candidate material for hydrogen storage at different temperatures and pressures, using molecular dynamics simulations. Three advantages might favor the H2 uptake in alkali metal-doped corannulene, (i) polar corannulene enhances the interaction between H2 and corannulene; (ii) charge-induced dipole moment by doped alkali metal further enhances the interaction; and (iii) doping provides more space for H2 to be adsorbed. We report molecular dynamics simulation results suggesting that about 4 wt% H2 adsorbed at room temperature can be obtained at a pressure of 250 bar.