A Theoretical Study of Platinum Decorated Carbon Nanocones on Hydrogen Storage Reactions: Effect of Spillover Mechanism

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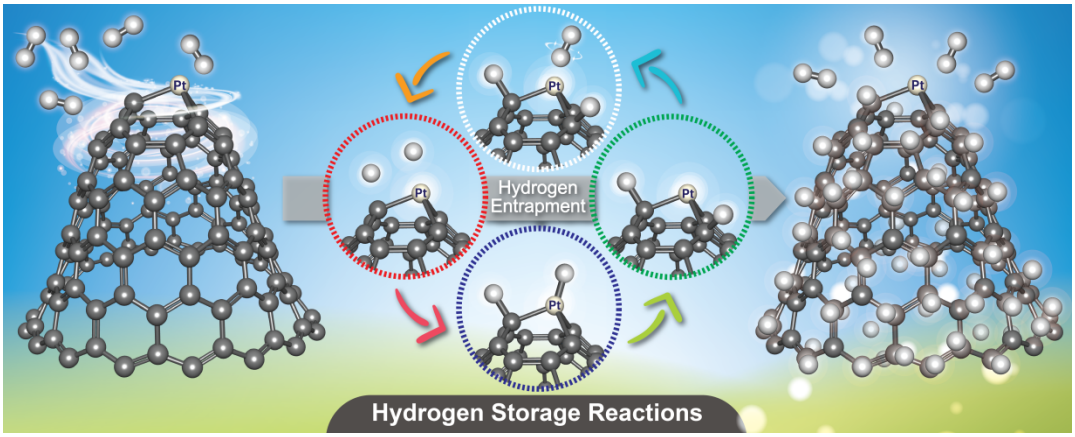
Abstract

Carbon nanocones (CNC) are an important material for hydrogen storage. We used density functional theory (DFT) to investigate hydrogen adsorption and storage on platinum (Pt)-decorated CNC (Pt-CNC). The acute curvature present in the conical section of CNC materials enhances metal and molecular hydrogen binding. Our calculations reveal that Pt atoms deposit at bridge sites between pentagons on pristine CNC. H_2 adsorption energies on Pt-CNC are more favorable than they are on pristine CNC; the Pt atom serves as an active site for H_2 adsorption. We investigated the effects of CNC shape on storage capacity by varying the number of pentagons from 1 to 6. With Pt as the active site for H_2 adsorption, a maximum of two hydrogen molecules can bind to 4-pentagon pristine carbon nanocone (4CNC), with average adsorption energy of 0.47 eV/H_2. This contrasts with 4-pentagon defective carbon nanocone (d4CNC), which can bind only one hydrogen molecule, with average adsorption energy of 0.56 eV/H_2. We investigated hydrogen spillover mechanisms on d4CNC using first principle calculations. We found that spillover process can enhance hydrogen uptake by up to 3 hydrogen molecules per Pt atom.



Keywords: hydrogen storage, carbon nanocone, DFT, spillover mechanism