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Metal clustering and catalytic spillover on the nanotubes and graphene for hydrogen storage FENG DING, PAVEL KRASNOV, YU LIN, BORIS I. YAKOBSON, Rice University — Energies and kinetic barriers associated with transition metal (Sc) clustering on a single-walled carbon nanotube (SWNT) and graphene were studied by all-electron density functional method. The analysis shows that the binding energy of Sc atom on SWNT is highly sensitive to the tube diameter and chirality. The metal atoms do cluster on common SWNT, with diameters ∼1-2 nm. Hydrogen binds to the metal cluster chemically and thus opens a way for hydrogen storage via catalytic spillover. However the hydrogen chemisorption on graphene receptor-substrate is difficult to reconcile with a single H atom binding to carbon being weaker than it is within initial molecular H_2. This paradox is resolved by presenting the process as phase nucleation. Atomistic calculations bridge remarkably with the macroscopic-continuum description, and show a feasible path to 7.7 wt% H-content at nearly ambient conditions. P. O. Krasnov, F. Ding, et.al., J. Phys. Chem. C, in press (2007).

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