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Hydrogenation of graphitic nanocarbons[1] SAVAS BERBER, DAVID TOMÁNEK, Michigan State University, EUNJA KIM, PHILIPPE F. WECK, University of Nevada Las Vegas, GLEN P. MILLER, University of New Hampshire —
We apply *ab initio* density functional calculations to study the hydrogenation of graphitic nanocarbons including fullerenes, onions and nanotubes using diethylenetriamine (DETA) as hydrogenation reagent. Our results indicate that transfer of atomic hydrogen from the amine end-group of chemisorbed DETA molecules to nanocarbons is an exothermic reaction. We explore the optimum pathway for the hydrogenation reaction and find the activation energy associated with sigmatropic rearrangement of chemisorbed hydrogen atoms to lie near 1 eV, thus facilitating formation of energetically favorable adsorbate structures by surface diffusion. Chemisorbed hydrogen assists in a local sp^2 to sp^3 bonding conversion of the graphitic nanocarbons, causing large-scale structural changes ranging from local relaxations in nanotubes to shell opening in multi-wall onions.

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Savas Berber
Michigan State University

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