Abstract Submitted
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First Principles Study of Metal Adatom Adsorption on Carbon Nanotubes[1] KEVIN T. CHAN, University of California, Berkeley, JEFFREY B. NEATON, The Molecular Foundry, Lawrence Berkeley National Laboratory, MARVIN L. COHEN, University of California, Berkeley and Lawrence Berkeley National Laboratory — Recent experiments observed bias-induced mass transport between indium nanoparticles on a carbon nanotube. Ab initio studies later suggested that electromigration in this case can be explained by charge transfer from indium adatoms to the nanotube and small diffusion barriers, and that defects can serve as nucleation sites for nanoparticle formation. Here we use ab initio calculations to explore adhesion, diffusion, and the possibility of mass transport on nanotube surfaces for other metallic species. We will present calculations examining binding energy, binding site, diffusion barriers, and charge transfer for a range of metal adsorbates on surfaces, defects, and vacancies of carbon nanotubes and sheets. Adatom coverage dependence and the role of curvature effects will also be discussed.

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