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Mechanism for bias-assisted mass transport of indium on carbon nanotube surfaces FILIPE J. RIBEIRO, North Carolina State University, J.B. NEATON, The Molecular Foundry, Lawrence Berkeley National Laboratory, STEVEN G. LOUIE, MARVIN L. COHEN, University of California Berkeley, Lawrence Berkeley National Laboratory — We have preformed *ab initio* pseudopotential density functional calculations to study the adsorption and diffusion of indium atoms on graphite-like and carbon nanotube surfaces. The adsorption energy was calculated as a function of In coverage, and it is shown that, for low surface densities, In becomes positively charged by donating one electron to the surface. This explains the experimental evidence that In deposited on carbon nanotubes migrates towards the cathode under an applied voltage. The effects of nanotube surface curvature on In adsorption are shown to be small. Based on the calculated energy barrier between two neighboring adsorption sites and the calculated vibrational frequencies of the adsorbate, the hopping rate for In adsorbed on graphene is estimated. Finally, In adsorption is shown to be stronger near a Stone-Wales defect, which could be linked to the nucleation of In nanocrystals. This work was supported by National Science Foundation Grant No. DMR04-39768 and by the Director, Office of Science, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, U.S.Department of Energy under Contract No. DE-AC03-76SF00098. Computational resources have been provided by NPACI and NERSC.

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