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Multiscale Modeling of Functionalized Single-Wall Carbon Nanotubes SOUMYA PATNAIK, Air Force Research Laboratory, Materials and Manufacturing Directorate, XIAOFENG DUAN, Aeronautical Systems Center Major Shared Resource Center for HPC, BRAHIM AKDIM, RUTH PACHTER, Air Force Research Laboratory, Materials and Manufacturing Directorate — Funtionalization of carbon nanotubes is significant for many reasons. Along with enhancing the processability of the nanotubes which can aid in applications such as nanotube reinforced composites, covalent chemical functionalization provides a means for better control over their electronic and mechanical properties. Functionalization of single-wall carbon nanotubes (SWCNTs) has been observed to exhibit diameter selectivity and proposed as a method for SWCNT purification [1]. In the present work, we report a multiscale modeling approach, combining atomistic molecular dynamics (MD) and first principles density functional theory (DFT) methods, to study the effects of SWCNTs carboxy functionalization. The MD simulations provide important information regarding intertube interactions upon functionalization. This was used in subsequent DFT calculations for a correct prediction of resonant Raman modes shifts in SWCNT bundles. The MD simulations, electronic structure calculations, and predicted Raman shifts in comparison with experiment [1] will be discussed in detail. [1] Kuzmany, H., Kukovecz, A., Simon, F., Holzweber, M., Kramberger, Ch., and Pichler, T., *Syn. Met.* 2004, 141, 113-122.

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