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Effects of hydrogen chemisorption on the structure of carbon nanotubes ANDRE MUNIZ, TEJINDER SINGH, DIMITRIOS MAROUDAS, University of Massachusetts at Amherst — We report results of a computational atomic-scale analysis of the effects of atomic hydrogen chemisorption on the structure of single-walled and multi-walled carbon nanotubes (SWCNTs and MWCNTs). The analysis combines classical molecular-dynamics simulations with first-principles density functional theory calculations. We find that H chemisorption induces structural changes in SWCNTs associated with sp^2-to-sp^3 bonding transitions; increasing the H coverage beyond a critical level leads to axial and radial expansion of the SWCNTs that increases monotonically with H coverage. We also investigated the possibility of H-induced inter-shell sp^3 C–C bond formation in MWCNTs. We find several pathways that lead to stable inter-shell bonded structures, which can act as seeds for nucleation of various crystalline carbon phases embedded into the MWCNTs. Finally, we show how the chiralities and relative alignments of adjacent graphene walls in MWCNTs determine the resulting crystalline structures.

Andre Muniz
University of Massachusetts at Amherst

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