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Atomic-Scale Theory and Modeling of Electronic and Molecular Transport through Carbon Nanotubes YONGQIANG XUE, SUNY-Albany — In this talk, we investigate the application of carbon nanotubes as novel transport channels for electrons and molecules using atomistic simulation. (1) Electronic transport: In this talk, we present a Green's function based self-consistent tight-binding study of electron transport through SWNT junction devices, which takes fully into account the 3D atomistic nature of the electronic processes. We discuss insights obtained from such atomistic study on the contact/diameter dependence of junction conductance and self-consistent study of current transport through metal-SWNT-metal junctions. (2) Molecular transport: Carbon nanotube could also be used to build assemblies for controlled transport of biomolecules for nanofluidic devices. Water confinement inside such nanoscale cylindrical core plays a significant role in determining the insertion and flow of biomolecules through the nanotube channel, which can be strongly affected by surface functionalization. Molecular dynamics simulations have been carried out to study the structure and thermodynamics of water in carbon nanotube and its effect on the spontaneous insertion of DNA molecules inside the nanotube channel. The simulations can provide valuable insights into the transport of molecules through nanoscale pore or channel structures.

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