

Computational Modeling and Applications of Nanostructured Materials

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Using a variety of computational methods, we have performed computational modeling and simulations to investigate various properties of nanostructured materials and to design potential applications. In this talk, I will present some of our results. First, thermal and thermal mechanical properties of carbon nanotubes will be presented. Using the equilibrium and non-equilibrium Green-Kubo formalism based on molecular dynamics simulations, we have shown that nanotubes exhibit very high thermal conductivity, even higher at room temperature than diamond, which has been known to be the highest thermal conductor. Unusual thermal contraction behaviors of carbon nanotubes and fullerenes will be presented. As a second topic, I will discuss a “holy grail” in nanoscience and technology fields: separation of semiconducting or metallic nanotubes from a mixture of different chiral tubes. I will show our device modeling describing a pathway toward 100% semiconducting nanotube devices from a network composed of a mixture of different chiral nanotubes. Finally I will present a couple of potential applications, such as memory devices, nano-velcroTM, and hydrogen storage. Especially, I will discuss some issues for the last application, which is one of most important problems in current research and development of sustainable energy, which would eventually replace current major energy source, fossil fuels.