Carbon nanomaterials: atomistic interfaces and the hunt for a payoff on the $\$10^{12}$ investment

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A quick search on the Internet for information about "carbon nanotubes" yields a long list of record-breaking properties for this particular arrangement of some of the most abundant atoms in the universe. Carbon nanotubes are the strongest, stiffest, most thermally conductive materials on earth. They demonstrate exotic physical properties like electronic conduction that is independent of length (no wasted power dissipated as heat as in copper with electrons scattering every ~40 nanometers—imagine perfectly efficient power transmission lines). They also possess a very low density, suggesting their utility in a broad range of applications for engineering materials in applications demanding lightweight strength, as in both aerospace and terrestrial transportation. Given their characteristics, the potential for carbon nanotubes to make an impact on our everyday lives seems obvious in terms of reduced energy consumption, energy delivery costs, and a more robust power grid as examples. However, after spending trillions of dollars on research over the course of 20 years, the long and impressive list describing the attributes of carbon nanotubes under the heading "Properties" is generally found adjacent to a disappointingly short list under the heading "Applications". Why? Carbon nanotubes should be critical building blocks for many lightweight, multifunctional structures and devices, but the mechanical, thermal, and electrical properties of macroscale assemblies of carbon nanotubes, where the tubes are making contact with each other or with more ordinary engineering materials (such as metals and polymers), are consistently much less remarkable than those measured for the individual nanostructures themselves. For example, simple geometric predictions, which are very accurate for most nanocomposite materials, predict a 50-fold increase in thermal conductivity for polymer composites with only a 1% (by volume) addition of carbon nanotubes, but experimental results show an increase of less than a factor of 2. These lackluster results for nanotube-based assemblies and composite materials are typical, and the community generally agrees that the disappointing numbers are the result of unfavorable interfacial coupling—that is, the tubes are such unique materials, the mismatch of properties between the tubes and whatever they make contact with inhibits their synergistic performance. The question then becomes how do we modify the nanotube interfaces to improve mechanical, thermal or electrical coupling at their intersections with neighboring tubes and with other materials? Nanotechnologists are proficient when it comes to attaching molecules to surfaces to tailor the interfacial properties of many materials, but the unique challenge with nanotubes becomes effective enhancement of interfacial coupling without disruption of the, intrinsic nanotube properties. Strong (covalent) chemically bound molecules can help improve interfacial properties, but their alteration of the stiff carbon-carbon bonds results in negligible, or even negative, property enhancement. In fact, a single, simple molecule bound to a carbon nanotube sidewall can impede total heat flow along a nanotube by more than 10%.

Our theoretical and experimental work has been aimed at overcoming the interfacial barriers limiting the utility of carbon nanotubes in macroscopic assemblages. We are particularly focused on maximization of thermal and electrical energy flow through carbon nanotube assemblies. For our experiments we use macroscopic carbon nanotube yarn, spun like wool from nanotube arrays composed of billions of carbon nanotubes. These materials have considerable potential, and our aim has been to see how closely we can match the mechanical, thermal and electronic properties of our three dimensional structures to a single nanotube as an indicator of the quality of our interfacial engineering efforts. Our results indicate that we are indeed finding effective ways to significantly enhance the properties of carbon nanotube-based interfaces through tailoring of their interfacial architecture and chemistry, and simultaneously expanding the lists of both "Properties" and "Applications" for these remarkable materials.