Quantum-chemical Studies of the Mechanical and Optical Properties of Functionalized Carbon Nanotubes

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Carbon nanotubes (CNTs) have many attractive mechanical, electrical, and optical properties leading to their numerous potential applications, including the design of fibers. For over a decade, attempts have been made to utilize the properties of individual CNTs at macroscopic scales. One of the ways to manipulate and improve the physical and chemical properties of CNTs is by chemical functionalization, which can either be covalent attachment of chemical groups or the noncovalent adsorption or wrapping of various functional molecules. Modifying the composition of CNTs leads to the creation of novel materials such as CNT-polymer composites and fibers, which are appealing for their potential use in the next generation of flexible armor systems where lightweight robust materials are needed. However, it has been extremely challenging to design fibers of sufficient length with consistently high strength, stiffness, and toughness. This is due in part to a lack of fundamental understanding of the mechanisms which contribute to efficient hierarchical structures and in part to the limited available methods to synthesize hybrid fibers which control structural features at multiple length scales.

This research seeks to exploit quantum-chemical methods in order to provide important insights into the fundamental understanding of the CNT-polymer interactions, cross-linking effects, and bond-breaking mechanisms. Here, we show our recent research efforts in modeling the effects of functionalization on CNTs' mechanical properties using MM3 force fields and DFTB method. We also investigated using DFT level of theory how a single functional defect on a carbon network affects the electron density distribution which in turn affects the propagation of the reaction. Lastly, we present our results for the IR and Raman modeling of CNTs which may provide enough information to allow the understanding of the fundamental interactions of CNTs and polymers as well as the mechanisms of load transfer and failure.