Summer 2016 URP Proposal

Nanostructural Stability and Interactions of Carbon Allotropes and Molecular Linkers

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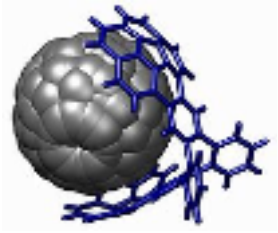
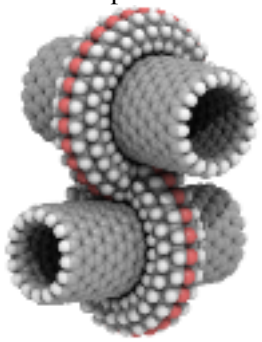
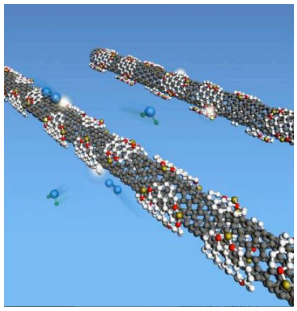
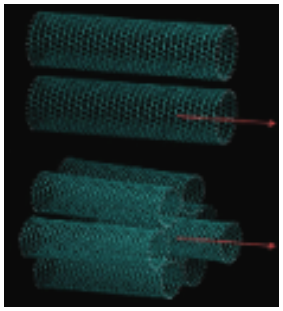
Nanotechnology refers to materials having at least one dimension in the 1 to 100 nm size range. One aspect of nanotechnology and more broadly nanoscience is the possibility of devices or materials that self-assembly from components that combine together. A related area of study is supramolecular chemistry that deals with systems made of assembled molecular subunits. A supramolecular structure is something beyond a regular molecule or collection of molecules. Such structures may be held together by noncovalent forces such as hydrogen bonding or intermolecular van der Waals (vdW) forces. A large supramolecular structure could be in the nanoscale range.

Our interest is in using molecular mechanics software to computationally build and study nanostructures of hundreds to thousands of atoms. These structures would be formed by combinations of carbon allotropes and molecular linkers. Carbon allotropes examples include single atom thick graphene, carbon nanotube (CNT), or C_{60} Buckyball. While the individual carbon allotropes and the individual linker molecules would be held by covalent bonds, the larger nanostructures formed by their combination could be held together by noncovalent interactions. These noncovalent forces would hold adjacent carbon allotropes and molecular linkers together. Noncovalent forces such as vdW forces are normally weak relative to covalent bonds. However, as larger surface areas of contact are involved, then the vdW forces can be significant. For example, layers of two-dimensional graphene are held together in a three-dimensional structure of graphite by the vdW forces between adjacent layers.

Both the flat sheets of carbon in the form of graphene and the rolled tube form of carbon nanotubes have unique and desirable properties of electrical conductivity, thermal conductivity, optical transparency (graphene) or electromagnetic absorption (CNT), high strength to density ratio, etc. Carbon nanotubes can form ropes and bundles. Pure bundles and modified bundles of CNT could have unique and useful applications as filters, molecular wires, chemical sensors, transport agents, electromagnetic receivers, drug carriers, nanotechnology structural building blocks, etc.

In prior work, my students and I have used computer-based models of graphene surfaces, rough surfaces, porous surfaces, and carbon nanotubes in conjunction with molecular mechanics to calculate molecule-surface binding energies. These calculated values compared well to experimental values obtained from gas-solid chromatography and thermal desorption so they should also function well for predictions of CNT bundling and the interactions of other carbon nanostructures composed of carbon allotropes with organic molecules and linkers. We have begun an exploration of bundles of carbon nanotubes and predictions of the binding energies holding different size and shape bundles together. In addition, under consideration is a linker molecule ($C_{80}H_{30}$ saddle-shaped warped nanographene molecule) that may be able to hold together CNTs in a perpendicular arrangement rather than in the normal parallel structure.

The objective of this work is to model possible stable and useful nanostructures, find the interactions, and determine the binding energies (how strongly these structures are held together). With this computational and modeling approach, we will explore new nano-architectural designs that we create.

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