Computational Simulations of Carbon Materials

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Introduction

Carbon materials and nanostructures (fullerenes, nanotubes) are promising building blocks of nanotechnology. Potential applications include optical and electronic devices, sensors, and nano-scale machines. The controlled growth of single-walled carbon nanotubes and furthermore the ability to control of assembling of smaller carbon nano-blocks into larger units with a specific physico-chemical properties is a major challenge in nanotechnology for material science and carbon nano-tube research [1]. Our computational efforts concern improving understanding of processes related to the fabrication of carbon nano-materials, especially focusing on the possibility of reactions between nano-particles. We investigate collision induced coalescence of carbon nanostructures by means of direct molecular dynamics in which electrons are treated quantum mechanically via self-consistent-charge density-functional tight-binding (SCC-DFTB) method[2]. We particularly focus on explaining a mystery of very high stability and low reactivity of C_{60} fullerene comparing to C_{70} fullerene [3,4].

Methods

We are attempting to see if there is a correlation between dipole polarizability of C_{60} and C_{70} fullerenes and the relative cross section. That is, we hope to observe trend similar to those shown in Figure 1 [3], with a significantly larger value for polarizability for C_{70} than the polarizability from C_{60}.

We are also interested in how the polarizability changes when approximate electronic excitation is accounted for, as well as the dynamics of the structure.

Methods cont.

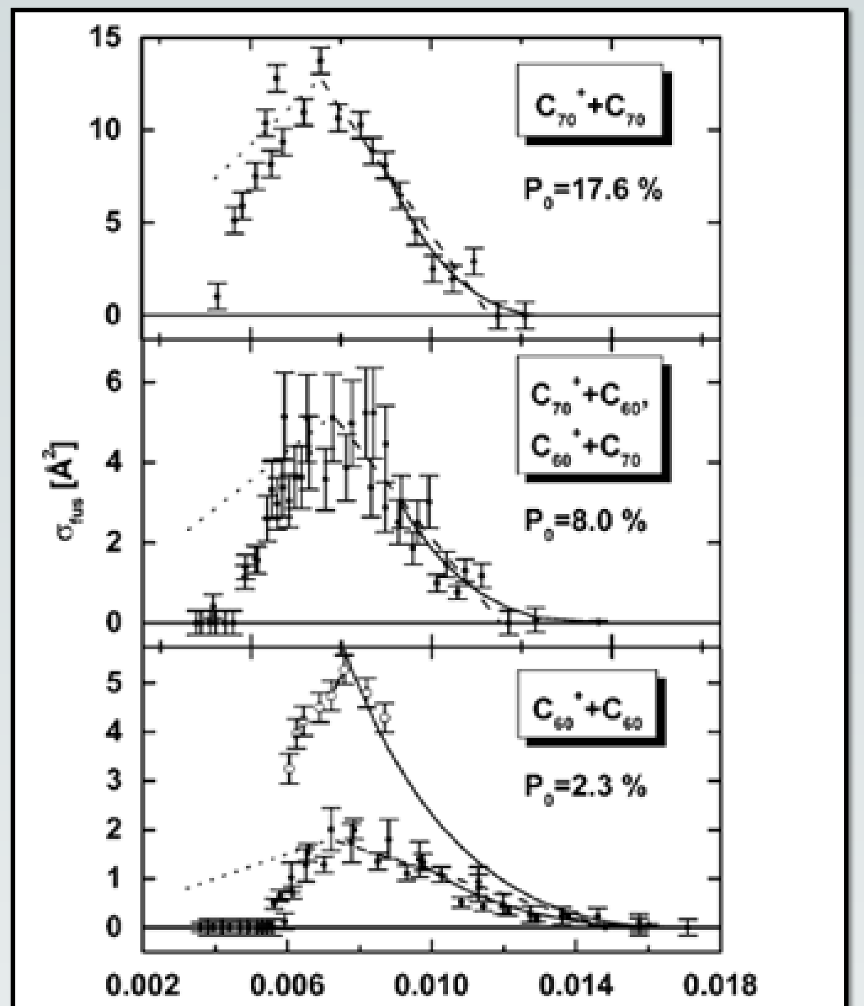

Figure 1. Absolute fusion cross section as a function of the inverse collision energy for three collision systems.

When carbon materials collide, there are six main collision paths that we are considering, as shown in Figure 2: (a)nonreactive elastic scattering, (b)(b) dimerization/polymerization, (c) collision-induced internal reorganization/inelastic scattering, (d) partial coalescence, (e) full coalescence, and (f) fragmentation [4]. We are simulating controlled collisions of carbon material in which we manipulate certain variables in order to determine what conditions will make these carbon structures most inclined towards fusion.

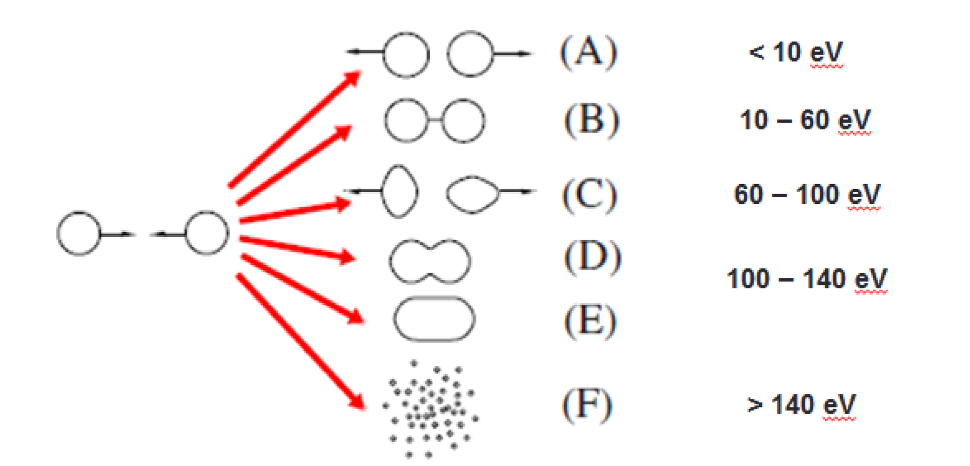

Figure 2. Schematic outcomes of collision between fullerenelike structures [4].

Procedure

- Programs: DFTB+, Xming
- Machines: Kraken
- Simulations: 5 ps, Nose-Hoover thermostat, T = 2000 K, finite difference evaluation of polarizability

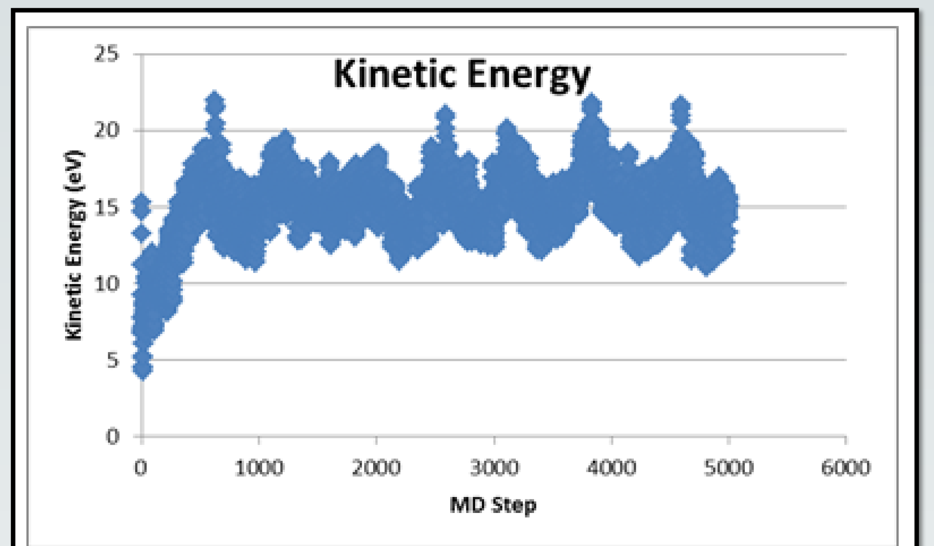

Figure 3. Plot of kinetic energy versus steps at 2000 K.

- Codes: Bash scripting
- PBS script, queuing, parallel scripting
- Created data structures

Preliminary Results

Before running our code with dynamics, we calculated the optimized polarizability, which can be seen in Table 1. This value was calculated using the following equation: $\mu = \alpha\vec{E}$, where μ is dipole moment, α is polarizability, and $\vec{E}$ is electric field.

Method	C_{60}	C_{70}	C_{70}/C_{60}	References
Tight binding	77.00	91.60	1.19	[5]
TDDFT/SAOP	83.00	101.00	1.22	[6]
DFTB	56.00	67.90	1.21	Experimental

Table 1. Experimental vs. theoretical comparison of polarizability (Å³)

Direction

- Observe a general trend of the effect of polarizability on collision pattern
- Create a visual model of collision
- Run collision simulations on various structures

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