Computational Simulations of Carbon Materials

Erin Yancey, Nicholas Wang, Shiquan Su, Jacek Jakowski
Henderson State University, Arkadelphia, AR; Georgia Institute of Technology, Atlanta, GA; National Institute for Computational Sciences, Knoxville, TN; National Institute for Computational Sciences, Knoxville, TN

Introduction

Carbon materials and nanostructures (fullerenes, nanotubes) are promising building blocks of nanotechnology. Potential applications include optical and electronic devices, sensors, and nanoscale machines. The controlled growth of single-walled carbon nanotubes and furthermore the ability to control of assembling of smaller carbon nanomaterials into larger units with a specific reactivity of C60 fullerene [3,4].

Methods

We are attempting to see if there is a correlation between dipole polarizability of C60 and C20 fullerene 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 C20 than the polarizability from C60.

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.

When carbon materials collide, there are six main collision paths that we are considering, as shown in Figure 2: (a)nonreactive elastic scattering, (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.

Procedure

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

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: \( \mu = aE' \), where \( \mu \) is dipole moment, \( a \) is polarizability, and \( E' \) is electric field.

<table>
<thead>
<tr>
<th>Method</th>
<th>C60</th>
<th>C20</th>
<th>C60/C20</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tight binding</td>
<td>77.00</td>
<td>91.40</td>
<td>1.19</td>
<td>[5]</td>
</tr>
<tr>
<td>TDDFT/4AOCP</td>
<td>73.00</td>
<td>101.00</td>
<td>1.22</td>
<td>[6]</td>
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<tr>
<td>DFTB</td>
<td>56.00</td>
<td>67.90</td>
<td>1.21 (Experimental)</td>
<td></td>
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Table 1. Experimental vs. theoretical comparison of polarizability (A³)

Acknowledgements

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References