COMPUTATIONAL SIMULATIONS OF CARBON MATERIALS

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Purpose

- Nanotechnology: carbon materials promising building blocks

- Applications: optical and electronic devices, sensors, and nano-scale machines

- Dipole polarizability of $C_{60}$ fullerene comparing to $C_{70}$ fullerene

- Effect of electronic excitation & structural dynamics on polarizability


**Figure 1.** Absolute fusion cross section as a function of the inverse collision energy for the three collision systems indicated in the figure.
Figure 2. Schematic outcomes of collision between fullerene-like structures: (a) nonreactive elastic scattering, (b) dimerization/polymerization, (c) collision-induced internal reorganization/inelastic scattering, (d) partial coalescence, (e) full coalescence, (f) fragmentation.

Procedures

- Programs: DFTB+, Xming
- Machines: Kraken
- Simulations: 5000 MD, 100 electric field
- Codes: Bash scripting
- PBS script, queuing, parallel scripting
- Created data structures
- Calculation of dipole moments and polarizability

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

- Observe a general trend of the effect of polarizability on collision pattern
- Create a visual model of collision

Figure 4. Time dependence of kinetic and potential energy during collision MD between two $C_{60}$ with $T_e=2000$ K.