COMPUTATIONAL SIMULATIONS OF CARBON MATERIALS

Erin Yancey
Nick Wang

Mentors:
Jacek Jakowski
Shiquan Su

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

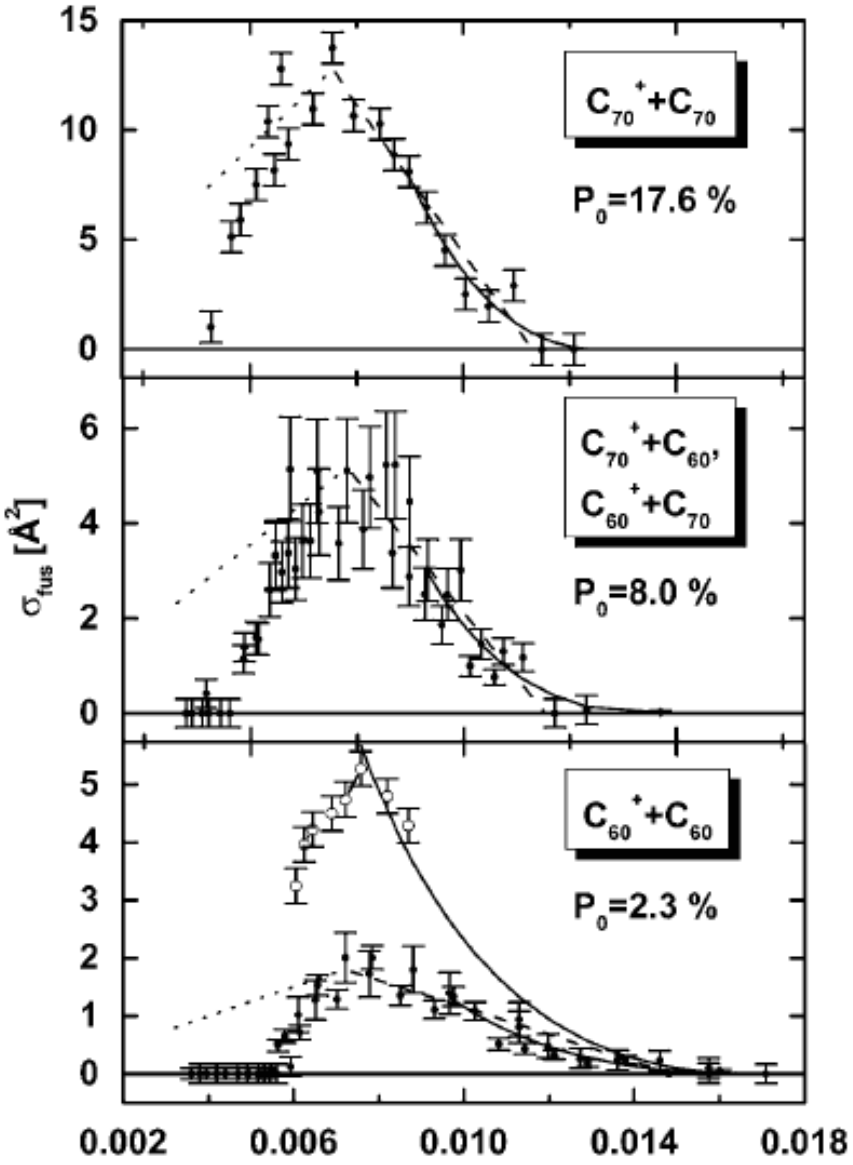


Figure 1. Absolute fusion cross section as a function of the inverse collision energy for the three collision systems indicated in the figure.

E.E.B Campbell and F. Rohmund, Rep. Prog. Phys. **63**, 1061 (2000).

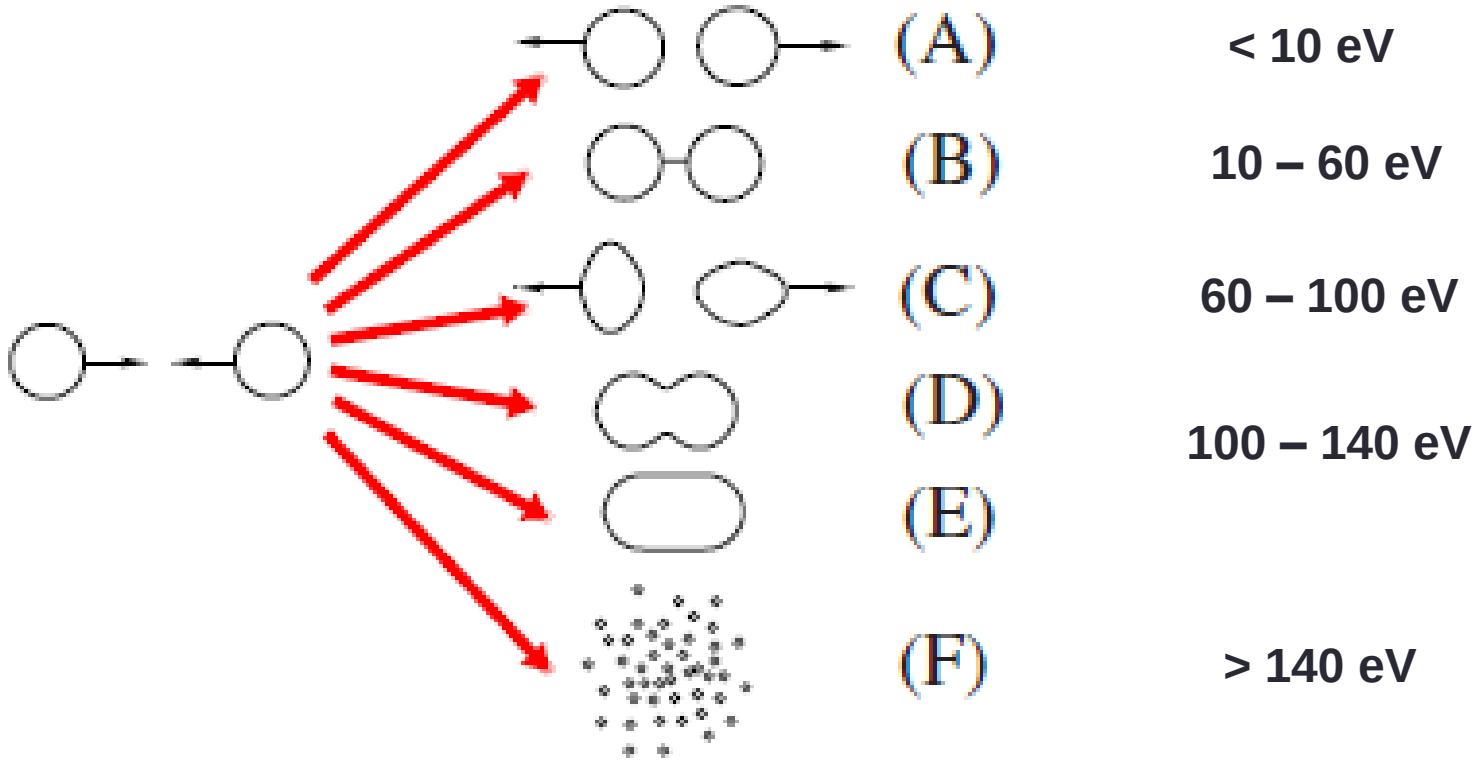


Figure 2. Schematic outcomes of collision between fullerenelike structures: (a) nonreactive elastic scattering, (b) dimerization/polymerization, (c) collision-induced internal reorganization/inelastic scattering, (d) partial coalescence, (e) full coalescence, (f) fragmentation.

J. Jakowski, S. Irle, and K. Morokuma, Phys. Rev. B **82**, 125443 (2010).

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

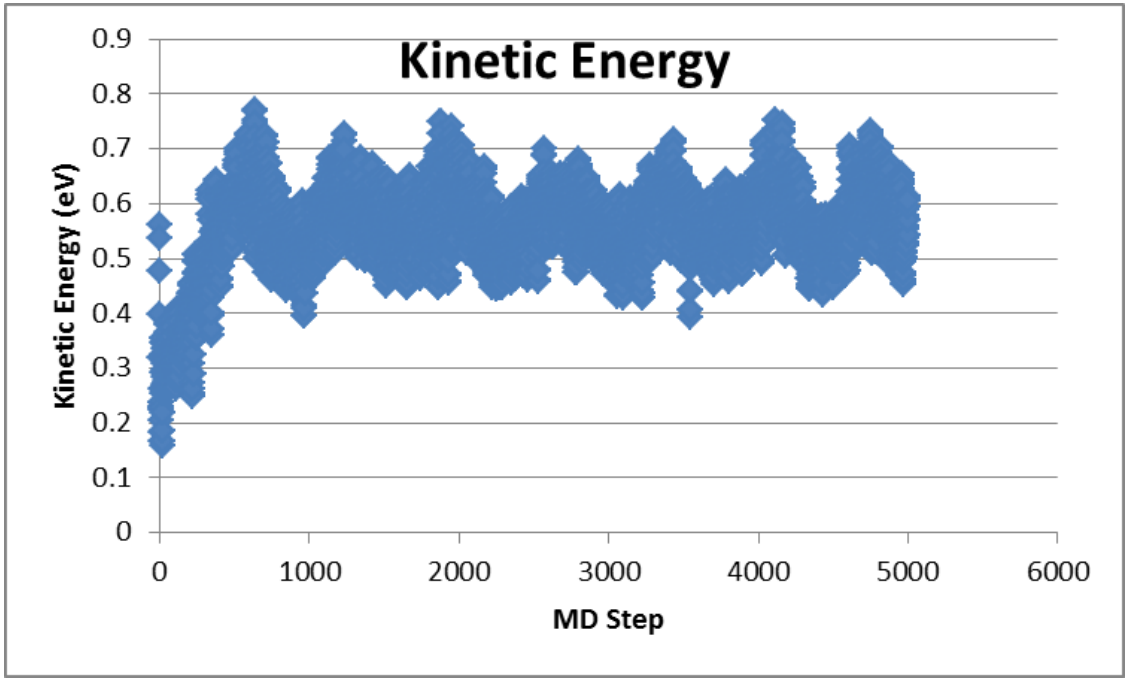
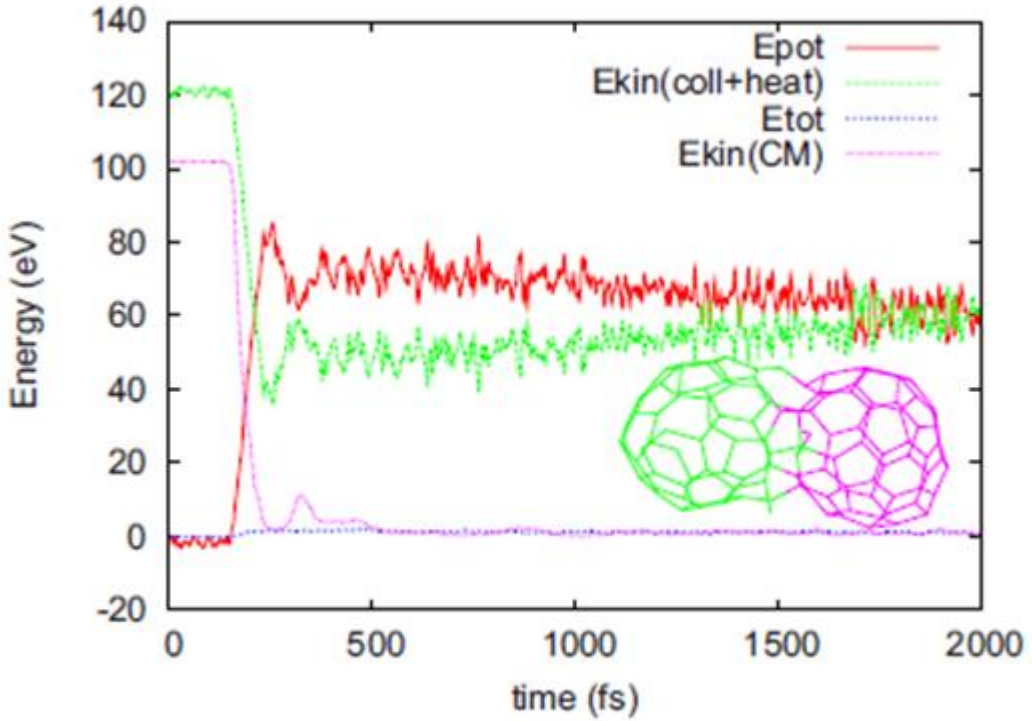


Figure 3. Plot of kinetic energy versus steps at 2000 K.

Direction

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



$$\mathrm{Ekin} = 102\ \mathrm{eV}$$

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

J. Jakowski, S. Irle, and K. Morokuma, Phys. Rev. B **82**, 125443 (2010).