COMPUTATIONAL SIMULATIONS OF CARBON MATERIALS

Erin Yancey
Nick Wang

Mentors:
Shiquan Su
Jacek Jakowski

Purpose

Nanotechnology: carbon materials promising building blocks.

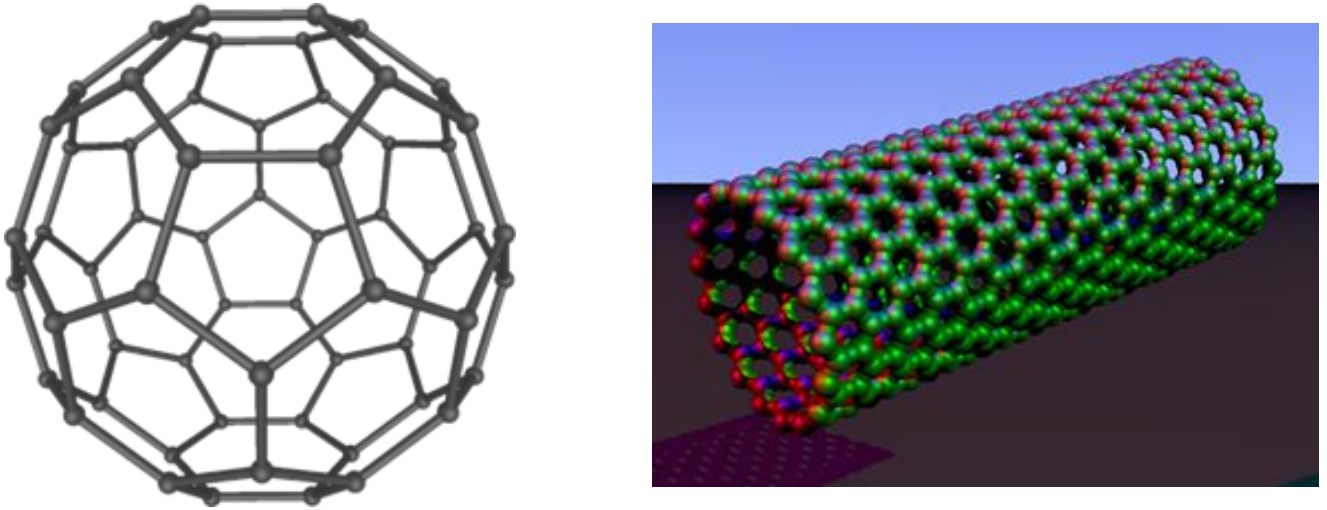


Figure 1. Members of the fullerene family: C_{60} and a carbon nanotube.

Strock, Michael. Members of the fullerene family. Graphic. 6 Feb. 2006. Fullerene. Wikipedia Commons. *Wikipedia, the Free Encyclopedia*. 2 Aug. 2013.

Purpose

- Applications:
  - Optical and electronic devices
  - Sensors
  - Nano-scale machines

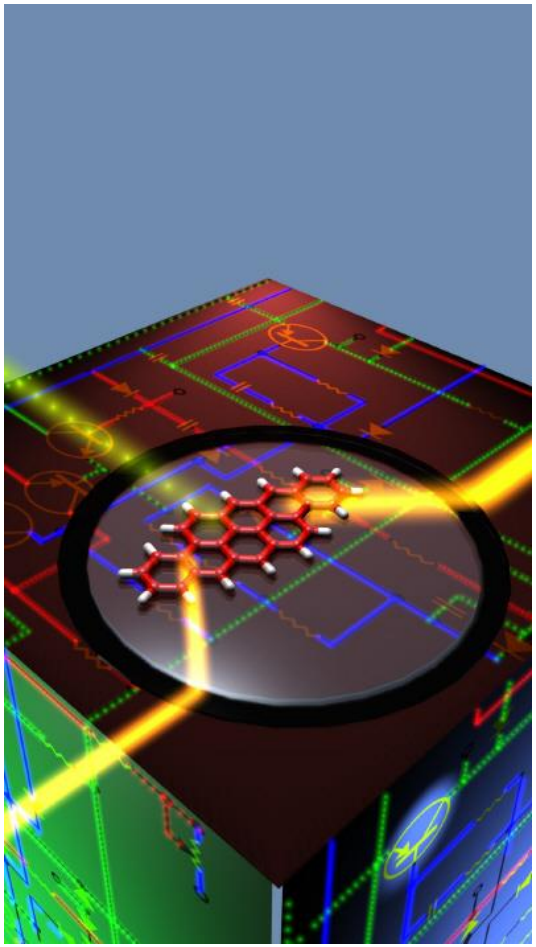


Figure 2. View of a photonic circuit with molecular building blocks.

Lettow, Robert. Optical Transistor. Illustration. 2 July 2009. Optical transistor breaks size record. *Nanotechweb.org.* 2 August 2013.

Methods

- Dipole polarizability of C_{60} fullerene comparing to C_{70} fullerene
- Effect of electronic excitation & structural dynamics on polarizability

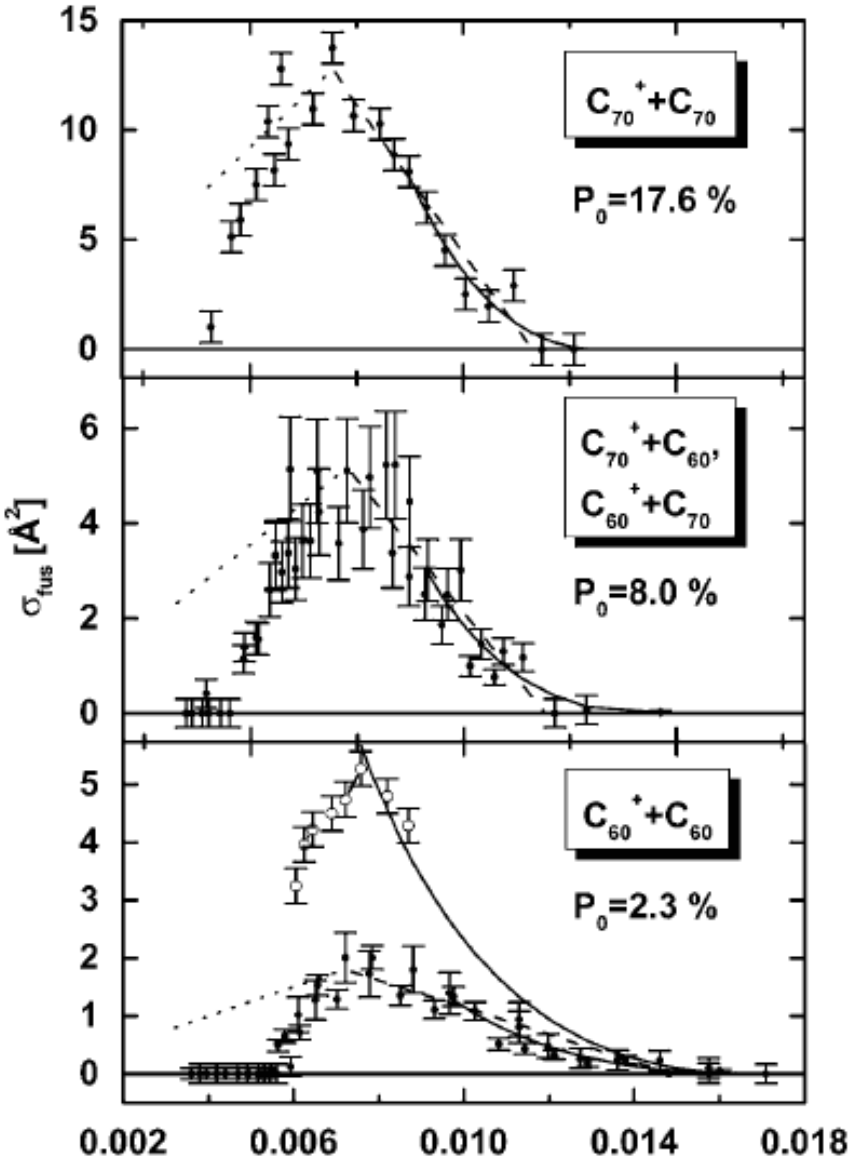


Figure 3. Absolute fusion cross section as a function of the inverse collision energy for the three collision systems indicated in the figure.

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

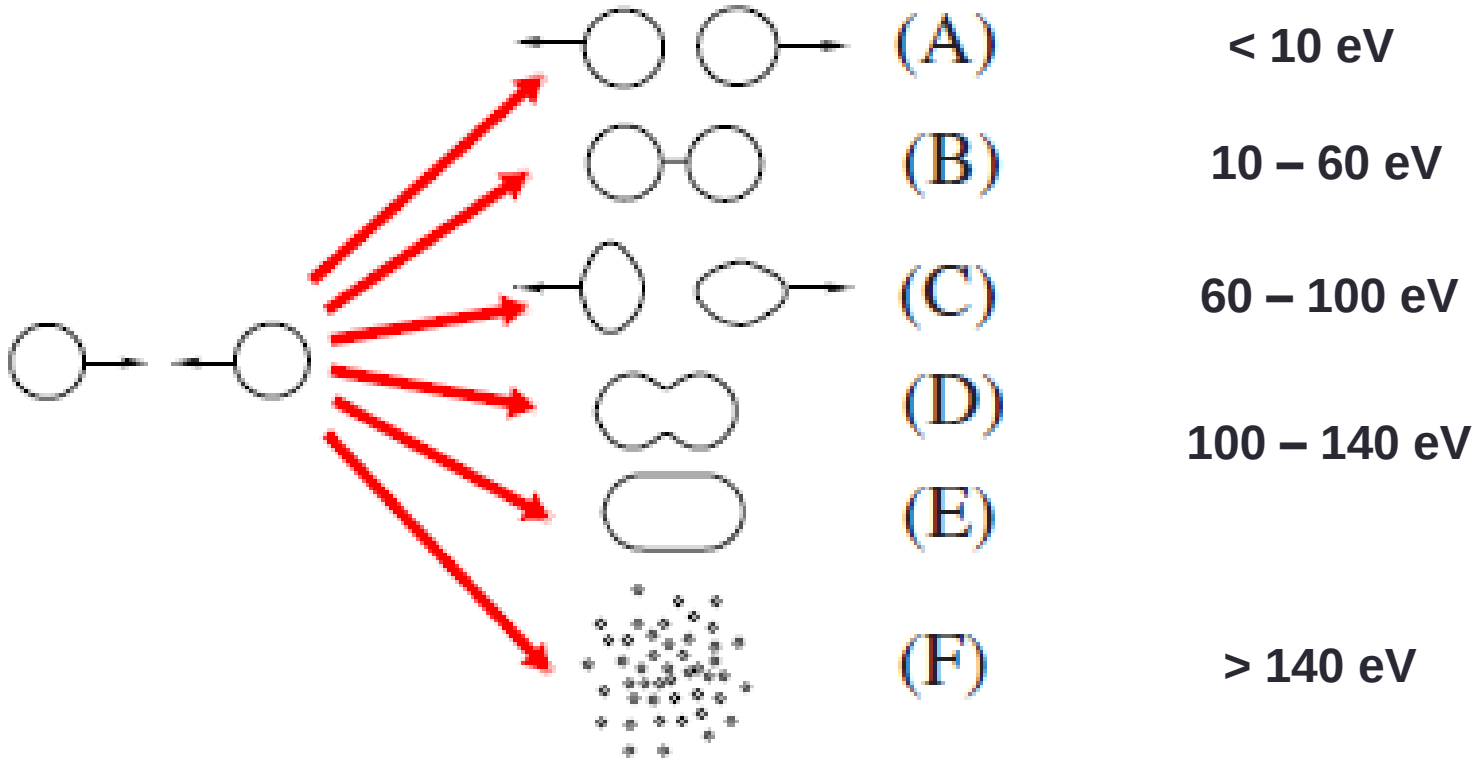


Figure 4. Schematic outcomes of collision between fullerene like structures: (a) nonreactive elastic scattering, (b) dimerization/polymerization, (c) collision-induced internal reorganization/inelastic scattering, (d) partial coalescence, (e) full coalescence, (f) fragmentation.

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

Procedure

- DFTB+:
  - Approximate density functional theory
  - Quantum mechanical modeling method approach
  - Employs slater type orbitals
  - Minimal basis set
  - Only treats valence electrons

```
Fermi energy:                      -0.1830372076 H           -4.9807 eV
Band energy:                     -107.5973090636 H        -2927.8717 eV
TS:                                 0.0055345700 H            0.1506 eV
Band free energy (E-TS):         -107.6028436336 H        -2928.0224 eV
Extrapolated E(0K):              -107.6000763486 H        -2927.9470 eV
Input/Output electrons (q):    240.00000000    240.00000000

Energy H0:                       -107.2052588543 H        -2917.2035 eV
Energy SCC:                         0.0019067085 H            0.0519 eV
Total Electronic energy:         -107.2033521458 H        -2917.1516 eV
Repulsive energy:                   4.4549430585 H          121.2252 eV
Total energy:                    -102.7484090873 H        -2795.9265 eV
Total Mermin free energy:        -102.7539436573 H        -2796.0771 eV

SCC converged

Dipole moment   :     0.27195375   -0.06805678    0.15923616 au
Dipole moment   :     0.69123754   -0.17298309    0.40473797 Debye
```

Figure 5. Example DFTB+ “detailed.out” file.

Procedures

- Programs: DFTB+, VMD
- Machines: Kraken
- Codes: Bash scripting
- PBS script, queuing, serial scripting
- Created data structures

Figure 6. The UT supercomputer Kraken located at Oak Ridge National Laboratory.

"Kraken XT5." Photograph. n.d.. Computing Resources: Kraken. *The National Institute for Computational Sciences.* Web. 25 July 2013.

Procedures

- Molecular dynamics (MD) simulation of C_{60} and C_{70}
- 5 ps
- Nose-Hoover thermostat
- 2000 K
- Produced 5000 geometry steps
- Used every 50th step from 1000 to 5000

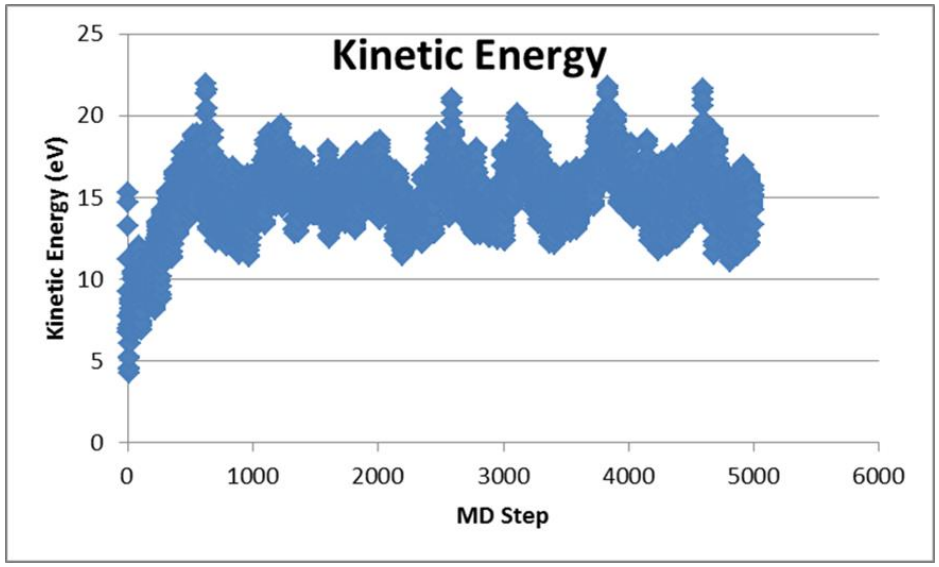
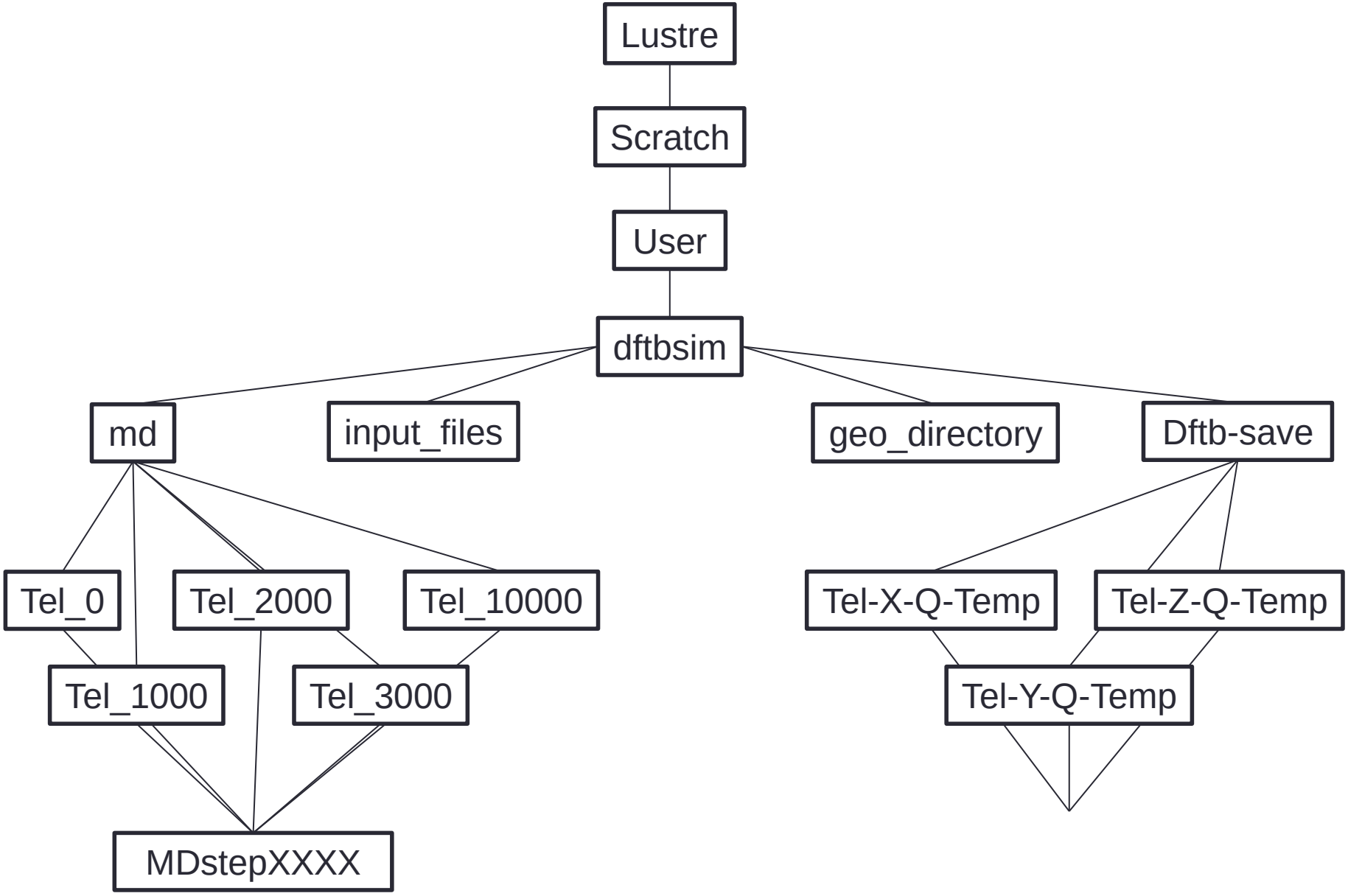


Figure 7. Plot of kinetic energy versus steps at 2000 K.


Lustre
Scratch
User
dftbsim
md
input_files
geo_directory
Dftb-save
Tel_0
Tel_2000
Tel_10000
Tel-X-Q-Temp
Tel-Z-Q-Temp
Tel_1000
Tel_3000
Tel-Y-Q-Temp
MDstepXXXX

Results

- Calculated optimized polarizability
- $\mu = \alpha\overrightarrow{E}$
  - μ = dipole moment
  - α = polarizability
  - $\overrightarrow{E}$ = electric field

Method	C_{60}	C_{70}	C_{70}/C_{60}
Tight binding	77.00	91.60	1.19
TDDFT/SAOP	83.00	101.00	1.22
DFTB	56.00	67.90	1.21

Table 1. Experimental vs. theoretical comparison of polarizability (Å^3).

Zope, Rajendra R., J. Phys. B: At. Mol. Opt. Phys. **40**, (2007).

Results

- Goal: examine how polarizability is affected when electronic temperature and electric field are manipulated

- Ran simulations on geometries:

  - Electronic temperatures: 0, 1000, 2000, 3000,10000 K

  - Point charges: 0.0, 0.1, 0.4, 0.6, 1.0 C.

Results

- Polarizabilities calculated using “awk”

```
#for 0.0-0.1

        paste dipoleFileZ_0.0 dipoleFileZ_0.1 |awk '{b2a=0.529177249;   printf("
%s %16.8f  %16.8f  %16.8f \n", $1, ($13-$5)*b2a, ($14-$6)*b2a, ($15-$7)*b2a)}'
 |   awk '{Q=0.1; sc= 5000/Q ;  alx= $2*sc; aly = $3*sc;  alz =$4*sc; av+=alz;
printf("%s  :: %12.6f  %12.6f %12.6f         %12.6f  \n", $0, alx,aly,alz,av/NR)
 } '  |tail -1 > avepolar_0.0-0.1

        awk '{printf("%16.8f \n", $9)}' avepolar_0.0-0.1 > valAve

        paste dipoleFileZ_0.0 dipoleFileZ_0.1 valAve |awk '{avg+=$17; printf("%s
 %16.8f %16.8f %16.8f %16.8f %16.8f %16.8f %16.8f \n", $1, $5, $6, $7, $13, $14,
 $15, avg)}' | awk '{b2a=0.529177249;   printf("%s %16.8f %16.8f %16.8f %16.8f \
n", $1, ($5-$2)*b2a, ($6-$3)*b2a, ($7-$4)*b2a, $8)}'   |   awk '{Q=0.1; sc= 5000
/Q ; alx= $2*sc; aly = $3*sc; alz =$4*sc; av+=alz; av0=$5; s+=(alz-av0)**2; prin
tf("%s :: %12.6f %12.6f %12.6f av = %12.6f rms=%12.6f \n", $0, alx,aly,alz,av/NR
, sqrt(s/NR))}' > Z_0.0-0.1
```

Figure 8. Script using “awk.”

Results

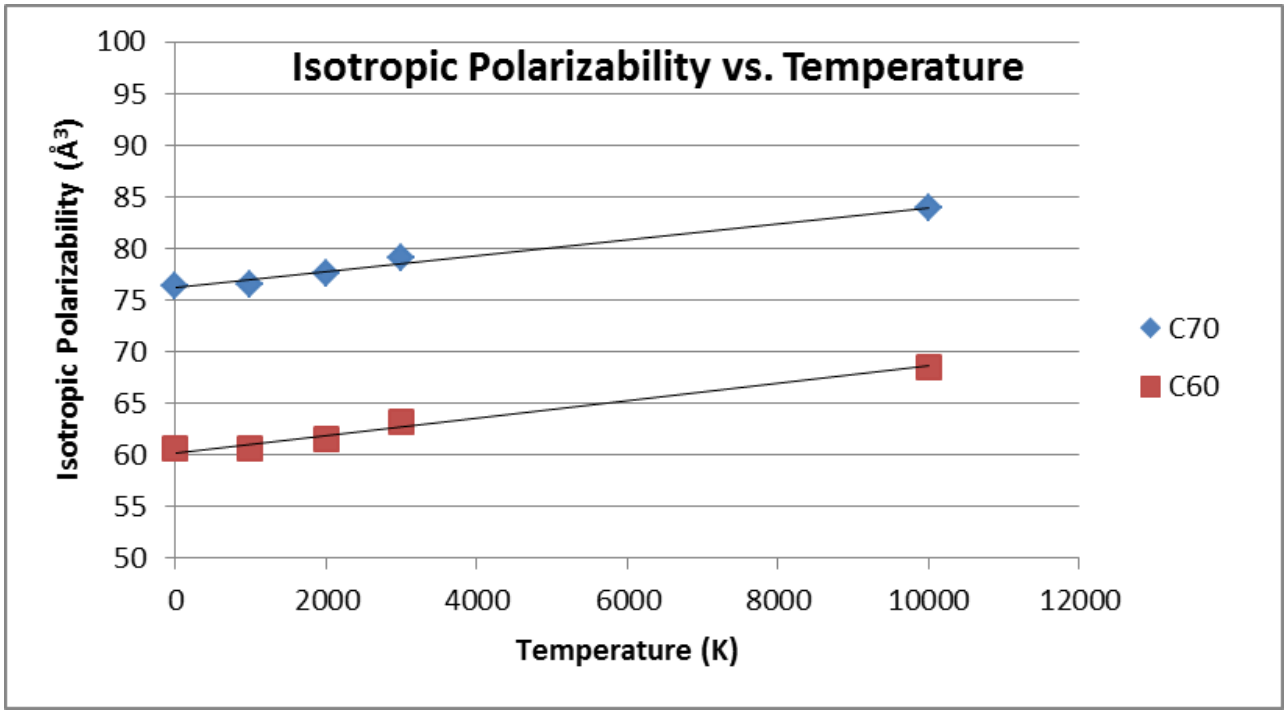


Figure 9. Isotropic polarizability versus temperature change for C_{60} and C_{70} at a charge of 0.1 C.

Results

- Simulation in VMD of dynamic structure of C_{60} and C_{70} under the following conditions:
  - Charge: 0.1 C in the x direction
  - Temperature: 2000 K

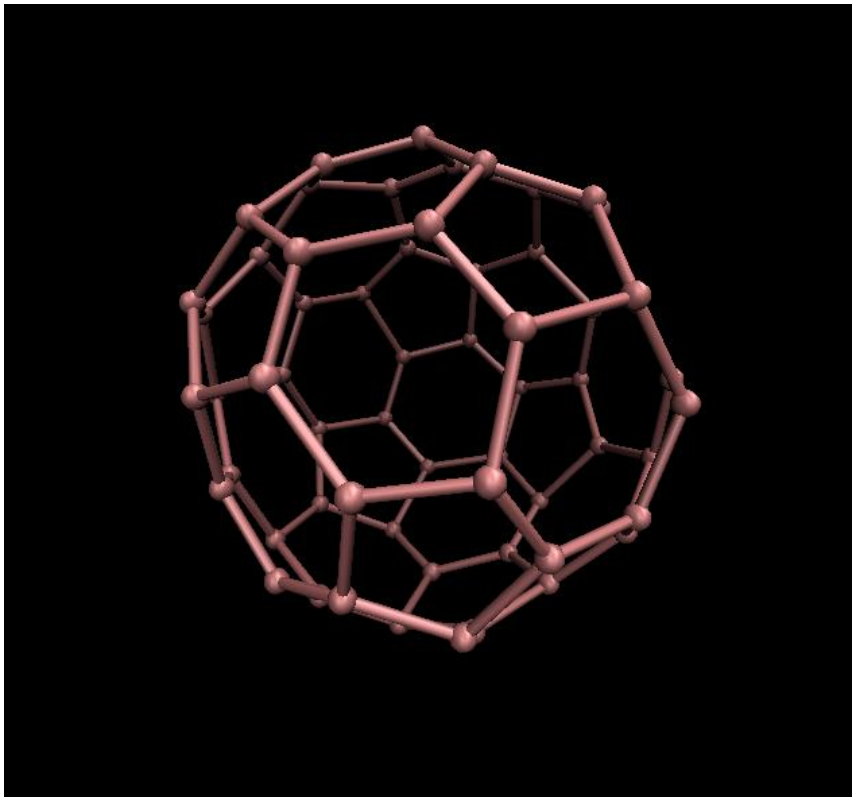
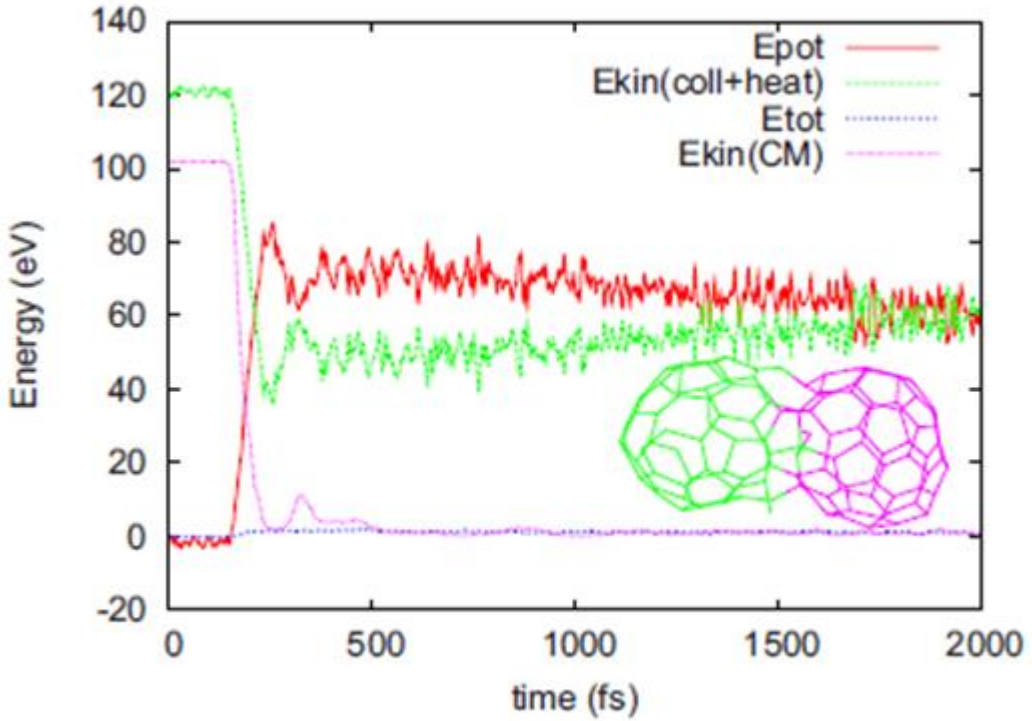


Figure 10. Still shot from VMD simulation of C_{60}.

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 11. 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).

Acknowledgements

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