Group Meeting

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OUTLINE

- Molecular Dynamics
- LAMMPS
- Reaxff
- Microporous Structures of Carbide-Derived Carbon-Based Supercapacitors
- MD simulations in the constant potential ensemble

Molecular dynamics

- MD is a computer simulation method for analyzing the physical movements of atoms and molecules
- The atoms and molecules interact for a fixed period of time
- The trajectories of atoms and molecules are determined by numerically solving Newton's equations of motion for a system of interacting particles

Molecular dynamics

Goal of the molecular dynamics method?

- Given number of atoms, you want to simulate and predict how atoms will be moving according to time

- Firstly, You need a initial conditions of the molecules such as position, velocity depends on temperature

- Secondly, You need inter atomic energy for each atom, forces and their distances: Coulomb interaction, Van der Waals, standard 12/6 Lennard-Jones potential

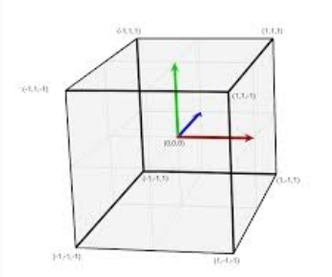
- Minimization of energy, energy and geometry optimization

LAMMPS

- Acronym for Large-scale Atomic/Molecular Massively Parallel Simulator.
- A molecular dynamics code, but can be used for energy minimization and Monte Carlo Simulations.
- Can model systems from a few particles up to billion of particles – slower simulation

LAMMPS

- Freely available, open-source code
- Current version is written in C++
- Presently maintained by the Sandia National Lab
- Can run on single-processor laptop/desktop, but optimized for clusters
- Can be installed on MacOS, Linux, Windows



Cubic Box

- Define the geometry, the simplest a cubic box

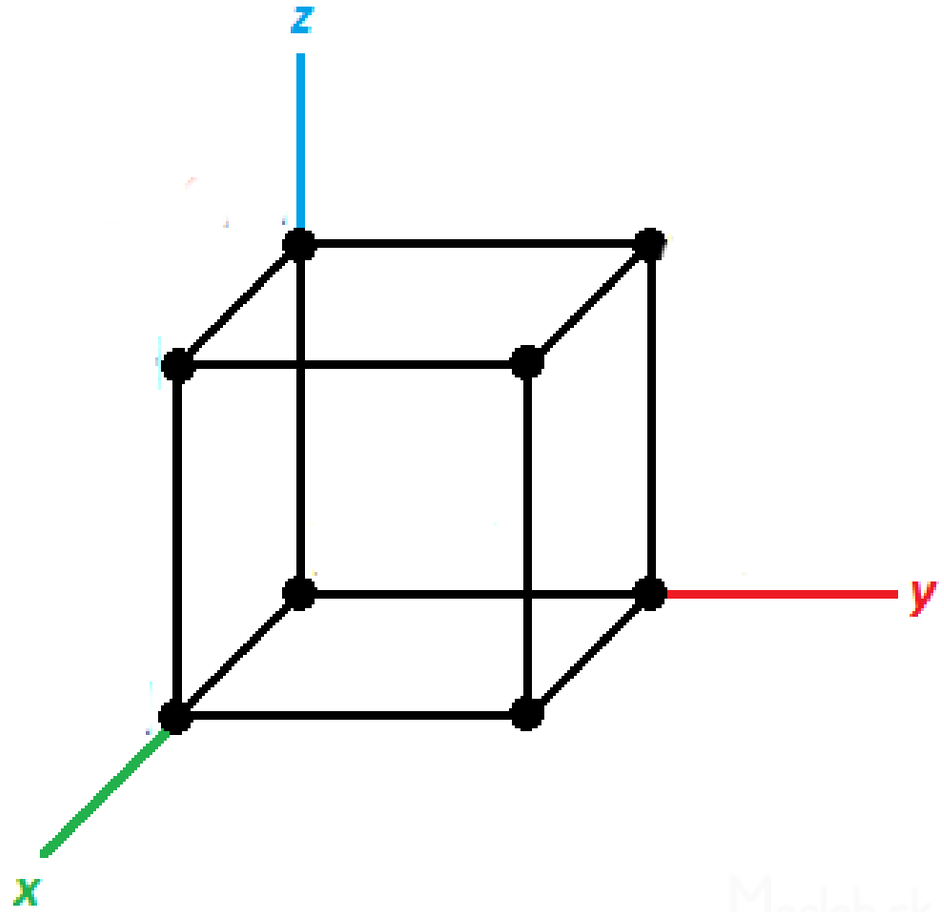
  xlo= 0, xhi = a

  ylo= 0, yhi = a

  zlo= 0, zhi = a

p : periodic, infinite replication

f : non-periodic



Thermodynamic ensemble

Define dynamics

- NVE : micro canonical ensemble
- NVT : canonical ensemble
- NPT : isobaric ensemble

N	V	E	→ extensive property
μ	P	T	→ intensive property

Chemical potential

Input Files

- structure.dat – data file: contains the size of the system, the number of atoms, mass of the each type, the position of each atom (potential velocities)

- in.file – input file: contains the instructions of the tasks to perform, potential force-field parameters

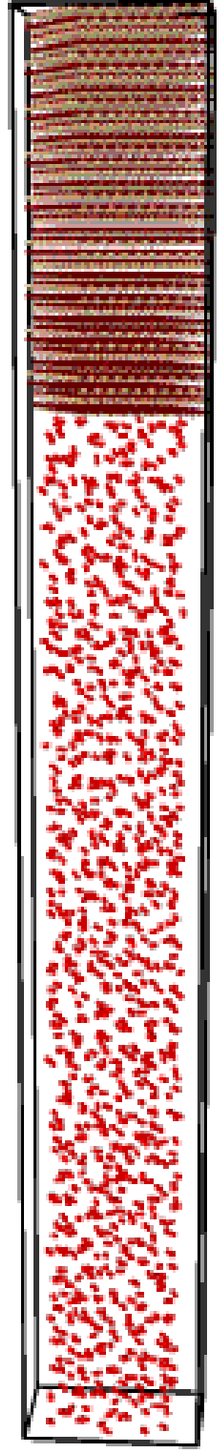
- pod.mod – potential file: if necessary
  ex: tersoff potential, classic MD

Reaxff

- ReaxFF, a force field for reactive systems

- ReaxFF uses distance-dependent bond-order functions to represent the contributions of chemical bonding to the potential energy.

- Fix NVE, Silicon carbide with O2 → SiO2



Microporous Structures of Carbide-Derived Carbon-Based Supercapacitors

- Molecular dynamics simulations for modeling microporous amorphous carbon.

- The crystal structure of SiC was used as initial structure and follow a pseudo-mimetic approach using quenched molecular dynamics (QMD).

- The SiC Tersoff potential is used

Microporous Structures of Carbide-Derived Carbon-Based Supercapacitors

1. 50 ps NVT @ RT
2. 200 ps NPT @ 2500 K
3. Quenching from 2500 K to RT with quench rate of 2.2 x 10^12 K/s in NPT ensemble
4. Removal of all Si atoms
5. 200 ps NVT @ RT

50 ps = (run x timestep /1000) time

2500K/2500ps = 1 K/ps

Simulation of Double Layer Capacitors

Carbide-Derived Carbon-Based Supercapacitors

MD simulations in the constant potential ensemble

→ to break down the effects of microscopic correlations on electrochemical response

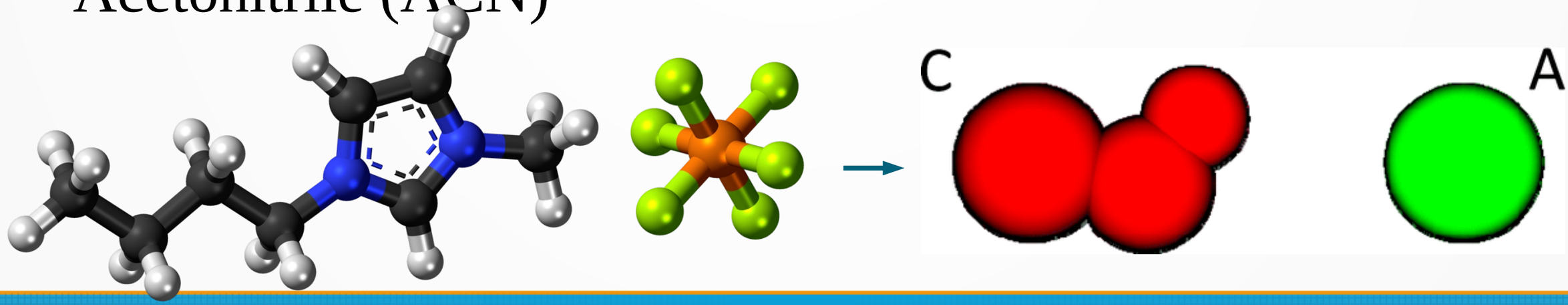
- fixed potential difference $\Delta\Psi$
- temperature T
- system volume V
- the number of electrolyte molecules N

Carbide-Derived Carbon-Based Supercapacitors

- Interactions are present in this coarse-grained representation leads to a huge computational savings
- Ionic liquid-solvent mixture is used as electrolyte

1-Butyl-3-methylimidazolium hexafluorophosphate

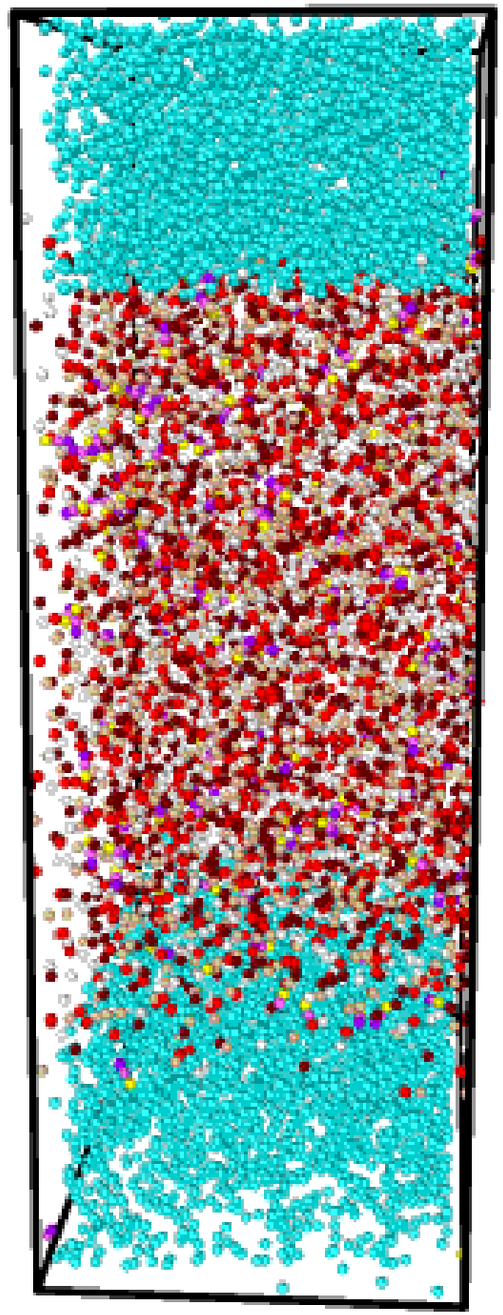
Acetonitrile (ACN)



Carbide-Derived Carbon-Based Supercapacitors

- T → 400 K
- P → 1-600 atm
- Porosity → 4.5 - 6.1 - 6.5 and 6.6 ångstrom
- Electrolyte concentration →0.12 - 0.47 - 0.63 and 0.89
- 2 different type of solvent

Total = 32 simulations



Carbide-Derived Carbon-Based Supercapacitors

Measurements:

- Porosity
- Capacitance
- Electrolyte Molecular Distribution
- Probability Density Distribution
- Mean Square Displacement (MSD)

Thank you for your listening!