Task A: Melting point of a model of NaCl

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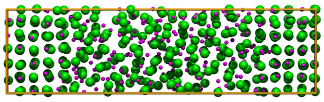

Aim: Determine the melting point of a model of NaCl by direct equlibrium in the slab geometry

Model: Lennard Jones + charges [S. Joung and T.E. Cheatham, III: *J. Phys. Chem. B* **112**, 9020 (2008)]

Simulation details: Verlet/leap-frog integrator, Andersen thermostat, Ewald summation, Berendsen barostat, linked-cell list.

Steps:

- Replicate Na_4Cl_4 3 × 3 × 3 times and simulate the crystal $Na_{108}Cl_{108}$ in the periodic boundary conditions.
- Determine the equilibrium box size, radial distribution function, and running coordination numbers.
- Melt and analyze the same quantities.
- Replicate crystal $Na_{108}Cl_{108}$ 1 × 1 × 3 times and melt half of the box.
- Simulate at given temperature and determine whether the crystal melts or grows.

Task B: Structure around a solute in water

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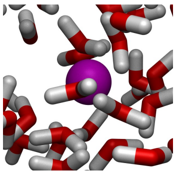
sw2/1



Aim: Study the stucture of water around a solute molecule.

Models: water: SPC/E (classical model, Simple Point Charge/Extended)
solute: Lennard-Jones (+ charge, fulleren: CHARMM21)
(Na^+, Cl^-, Li^+, Ca^{2+}, noble gases, endofullerenes)
Warning: the simulations with endofullerenes are slower!

Simulation details: Verlet/leap-frog integrator, SHAKE, smoothed cutoff (10–12 Å) electrostatics, Berendsen thermostat and barostat

Steps:

- Prepare (by random shooting) a configuration of the solute in about 200 waters.
- Equilibrate.
- Simulate at constant T, p.
- Show the radial distribution function and the running coordination number.
- Observe the orientation of the water molecules around the solute.
- Observe the hydrogen bond network in the solvation shell.

Task C: Coealescence of small water droplets

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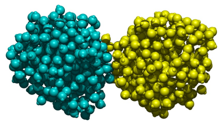

Aim: Prepare two small water droplets and let them coalesce. Observe a possible increase of temperature caused by decreasing the surface energy.

Water model: SPC/E (Simple Point Charge/Extended).

Simulation details: Verlet/leap-frog integrator, SHAKE, Berendsen thermostat, smoothed cutoff electrostatics to 12 Å, direct pair sum.

Steps:

- Prepare a box of $N = 200$ to 400 water molecules and equilibrate a bit.
- Place it into a large box and simulate: a spherical droplet will be created.
- Replicate twice and add small velocity to both droplets so that they will meet.
- Simulate in the microcanonical ensemble and observe the coalescence.
- Try to determine the potential energy and temperature increase during the coalescence from the temperature convergence profile.
- Calculate the increases theoretically (you will need the surface tension, density, and heat capacity; use the data for real water).