Final exam 18.12.2019.
Molecular Dynamics Simulations 2019

No electronic devices (incl. calculators) or notes allowed. Time for exam 4 hours.
Max score (8+6+4) 18 p

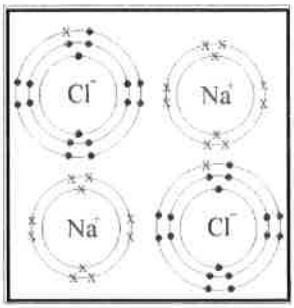
1) Explain briefly the following terms (a few sentences each, max. two pages in total):

a) Molecular dynamics and its differences with Monte Carlo (1p)
b) NVE and NPT ensembles (1p)
c) Ergodic hypothesis (1p)
d) Neighbour list skin thickness (1p)
e) Periodic boundary conditions (1p)
f) Ehrenfest MD (AIMD) (1p)
g) Gradient minimization methods (1p)
h) Group-based cutoff (1p)

2) Answer all questions (roughly max. half a page each.)

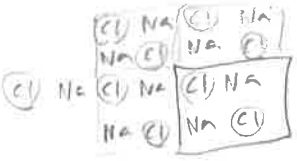
a) How (and why) to select the time step? How does using constraints & constraint algorithms affect the speed of calculation? (2p)
b) Explain briefly why most materials cannot be accurately modelled by a pair potential (2p)
c) Explain the principle and properties of the Berendsen vs. Nosé-Hoover thermostats (2p)

3) A periodic cell of NaCl is shown on the right.



a) Describe the type of bonding that dominates the atomic interaction.
b) What is the potential energy of the top-left atom if looking only the atoms in this cell in classical MD? Give attractive and repulsive components separately (no numerical value needed.)
c) How does the sum of potential energy behave (qualitatively) if you start summing the neighbouring cells (periodic images) to improve the value?
d) Explain briefly, what methods can be used to circumvent the problem and their basic ideas.

(roughly one page) (4p)



$d_1 = 2\sqrt{2}\,a$

$(2a)^2 + a^2 = d^2$

$d = \sqrt{4a^2 + a^2} = \sqrt{5a^2}$

$= \sqrt{5}\,a$