Worksheet 3: Diffusion processes and atomistic water model properties

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1 Short Questions - Short Answers

What are the main differences between various atomistic water models?

- Geometry - some are planar, some tetrahedral, also the location and size of partial charges can differ
- Polarizability - some models take it into account some don't
- Rigidness - some have fixed atom positions, others model atoms connected by "springs"

What is the difference between the SPC and the SPC/E water model?

The SPC/E model takes the averaged polarization effects into account, SPC doesn't.

What are the typical terms in an atomistic classical force field?

Typical terms for the potential are: E_{bond},$E_{torsion}$,$E_{angular}$,$E_{van-der-Waals}$, E_{LJ} and $E_{coulomb}$

How is the Pauli exclusion principle incorporated into a classical force field?

It is incorporated into the energy expression of the Lennard-Jones interactions E_{LJ}. If two (non-bonded) atoms get too close to each other their electron clouds overlap which results due to Pauli repulsion in a very strong repulsive force between these atoms. In the Lennard-Jones potential the r^{-12}- term describes this strong (Pauli -) repulsion.