Test questions in Computational Chemistry

Andriy Zhugayevych, Sergei Tretiak

October 27, 2015

§2. Lecture 2. Molecular mechanics

1. (5) What is the major caveat of gradient-based optimization?
2. (5) Interpret a given force field parameter file.
3. (5) Show examples when the convergence criteria for geometry optimization must be tightened.
4. (10) Geometry optimization is not converging. Suggest possible solutions.
5. (10) Molecule has a lot of conformations. Suggest possible approaches to find the global minimum.

§3. Lecture 3. Molecuar dynamics

1. (5) Give an example of PES for which a high-temperature quench will give highly nonequlibrium structure.
2. (5) Why enthalpy is used as a "standard" thermodynamic energy in thermochemistry?
3. (20) Ergodicity of all real materials is well established but not proven fact. Explain.
4. (5) How velocities are distributed for a classical gas of interacting particles in a thermal bath?
5. (15) Why periodic boundary conditions are commonly used for MD instead of hard walls?