C7790/Sample of the final test

Name:

1) The concept of potential energy surfaces is based on:

- ☐ molecular mechanics methods
- ☐ Born-Oppenheimer approximation
- ☐ molecular dynamics methods
- ☐ exact solution of the Schrödinger equation

2) Which of the above relations can be used to calculate the energy E(r) of a covalent bond in molecular mechanics:

- ☐ $E(r) = \frac{1}{2}K(r - r_0)^{-2}$
- ☐ $E(r) = \frac{1}{2}K(r - r_0)$
- ☐ $E(r) = K(r - r_0)^2$
- ☐ $E(r) = \frac{1}{2}K(r - r_0)^3$

where r is the bond length, r_0 is the equilibrium bond length and K is a force constant.

3) A typical integration step length in molecular dynamics is:

- ☐ 10 s
- ☐ 1 ps
- ☐ 0.01 ps
- ☐ 1 fs

4) The PM3 quantum mechanical method belongs to

- ☐ empirical methods
- ☐ semiempirical methods
- ☐ ab initio methods
- ☐ DFT methods

5) Wave function

- ☐ describes the state of a molecular system
- ☐ describes the size of the molecular system
- ☐ describes the wavelength of the molecular system
- ☐ defines the composition of the molecular system

6) Finding a local minimum on the potential energy surface in comparison to finding a global minimum is:

- ☐ easier
- ☐ equally difficult
- ☐ harder

7) Fluctuation of kinetic energy of a system in molecular dynamics:

- ☐ is independent of its size
- ☐ decreases with increasing number of atoms
- ☐ increases with its size

8) Potential energy calculated using molecular mechanics methods is a function of:

- ☐ the spin of the system
- ☐ the position of the electrons of the atoms
- ☐ the mass of the system
- ☐ the position of the atoms

9) The Leap-Frog integration algorithm provides the velocities and positions of the atoms:

- ☐ at the same time
- ☐ shifted by half of an integration step
- ☐ shifted by an integration step
- ☐ velocities are not available

10) The thermodynamic temperature of the simulated system is proportional to:

- ☐ its size
- ☐ the mean potential energy of the system
- ☐ the kinetic energy at time t
- ☐ the mean kinetic energy of the system

11) Molecular dynamics using molecular mechanics is based on the solution-of:

- ☐ the time-dependent Schrödinger equation
- ☐ Newton's equations of motions
- ☐ the time-independent Schrödinger equation
- ☐ Hooke's law equations

12) To calculate electrostatic energy in molecular mechanics, it is necessary to know:

- ☐ proton number
- ☐ the distance between atoms
- ☐ the number of electrons
- ☐ the distance between electrons

13) Which approximation is the Hartree-Fock method based on?

- ☐ one-electron
- ☐ two-electron
- ☐ one-spin
- ☐ two-spin