Computational Chemistry and Materials Modeling
Homework 3, due date is set in Canvas LMS
Topic: computational chemistry

***Notes**: In multiple choice problems explain your answer. Add references if needed. Upload solution as a single file "YourName.pdf" or "YourName.zip".*

1. Which methods (including basis set) you would likely use to study dispersive interactions in a naphthalene dimer?

2. In which case solvent effects result in the largest change of the total energy: (A) Neutral singlet ground state, (B) Neutral singlet excited state, (C) Neutral triplet state, (D) Anion/cation ground state?

3. The calculations of vibrational normal modes of some molecule gave the following frequencies (cm^{-1}, negative means imaginary): -50.6, -15.1, -3.2, 4.5, 106.7. How do you interpret these results?

4. Which nuclei of paracetamol molecule produce no strong NMR signal for their most abundant isotope?

5. Which method(s) you would likely use to study energy gaps in bulk semiconductors?

6. If you increased the size of your nearly orthorhombic simulation cell by two times along x direction, how will you change the number of k-points along x and in total to ensure the same k-point density?

7. What method of orbital occupation cannot be used for insulators:

(A) All states below Fermi-level are fully occupied, all others are empty
(B) Fermi–Dirac distribution
(C) Gaussian smearing
(D) Methfessel–Paxton smearing
(E) Linear tetrahedron smearing with Blochl corrections

8. Provide the minimum reasonable parameterization of water in an all-atom force field, i.e. how many atomic types, charges, bond types, vdW types etc. What is the number of independent force field parameters to optimize?

9. Identify misuse of empirical potential or force field: (A) EAM for Se; (B) EIM for NaCl; (C) COMB for SiO_2; (D) OPLS for polythiophene; (E) MM3 for benzene; (F) ReaxFF for Si surface oxidation.

10. A thermodynamic system can take three different discrete microscopic states S1, S2 and S3. The system was put into an MD simulator and allowed to propagate for 1 ns, taking a snapshot of the system every 1 ps. It was observed that 20% of time the system was in the microstate S1, and stayed in the microstate S3 only for the last 100 snapshots. Can we say that the statistical weight of the microstate S2 is 7/10?