

Computational Chemistry and Materials Modeling

Homework 3, due date is set in [Storion](#) web page

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

2. (2 pts. in total) Lysozyme (A) can irradiate in hydrogen peroxide (H_2O_2) dissolved in thiourea (B), at a wavelength where thiourea does not absorb. This process can be may be characterized by the list of reactions:

1. $\text{A} + h\nu \longrightarrow \text{A}^\bullet$
2. $\text{A}^\bullet \xrightarrow{k_2} \text{A} + h\nu'$
3. $\text{A}^\bullet \xrightarrow{k_3} \text{A} + \Delta$
4. $\text{B}^\bullet \xrightarrow{k_4} \text{B} + h\nu''$
5. $\text{B}^\bullet \xrightarrow{k_5} \text{B} + \Delta$
6. $\text{A}^\bullet + \text{B} \xrightarrow{k_6} \text{A} + \text{B}^\bullet$

(1 pt.) Name reactions 1 – 6, using Figure 1 as a reference.

(1 pt.) Illustrate these reactions, drawing your own Jablonski diagram. The processes should be marked with labels (1 – 6) and rate constants (k_i) from the reactions above.

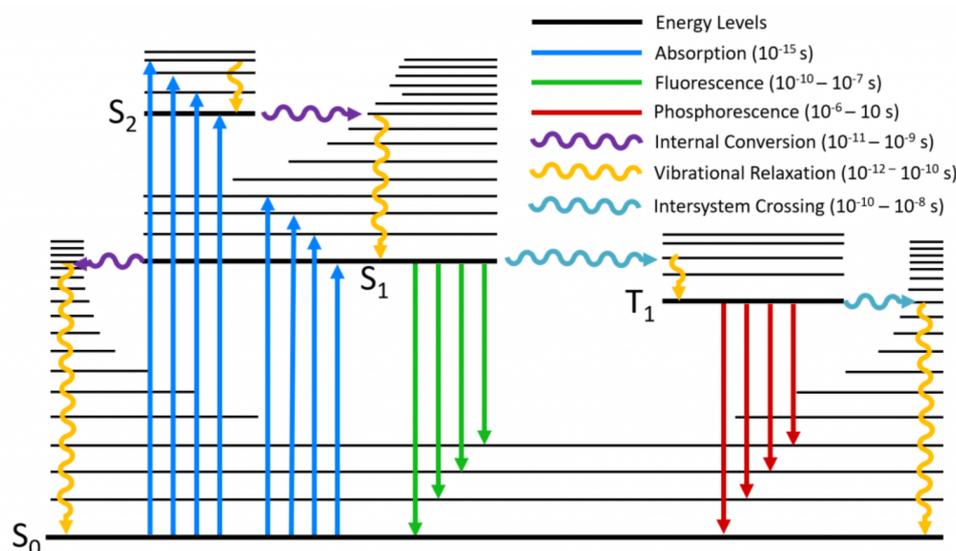


Figure 1: An example of Jablonski diagram.

3. (1 pt.) 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?

4. (1 pt.) 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?

