Electron Transfer in Protein
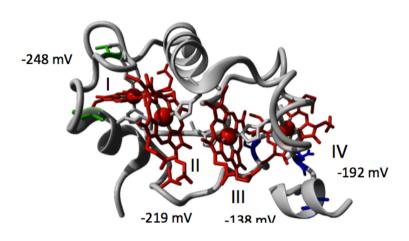
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➡ Respiration process

➡ Technological application

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r}, \mathbf{R}, t) = \hat{\mathcal{H}}\Psi(\mathbf{r}, \mathbf{R}, t)$$

➡ Mixed quantum-classical MD

➡ Non Adiabatic Dynamics:

Surface Hopping

$$\begin{matrix} \mathcal{H}^{aa} & \mathbf{F}^{adiab} \\ \mathcal{H}^{ab} & C_i \end{matrix}$$

➡ Use CP2K Mixed Force Mod.

➡ Analytic Overlap Method