

Simulation of Biological Systems

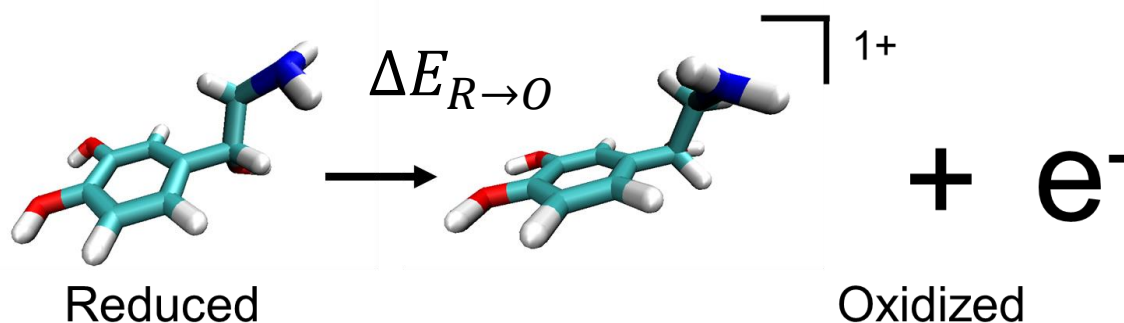
Day 7 – Computer Exercises: Computation of Redox Potentials

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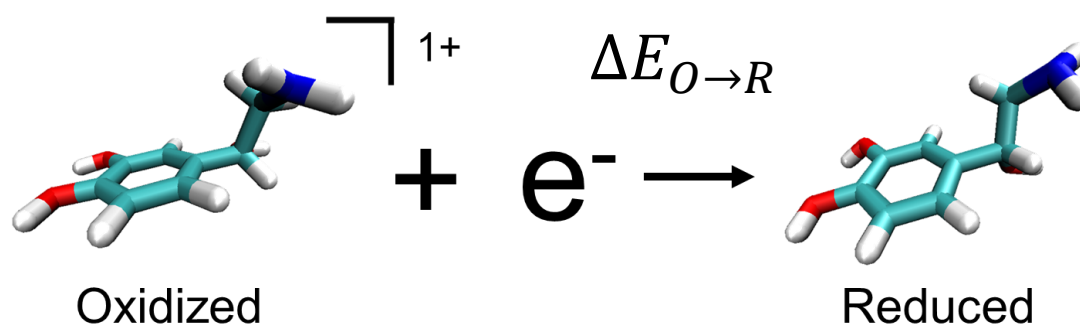
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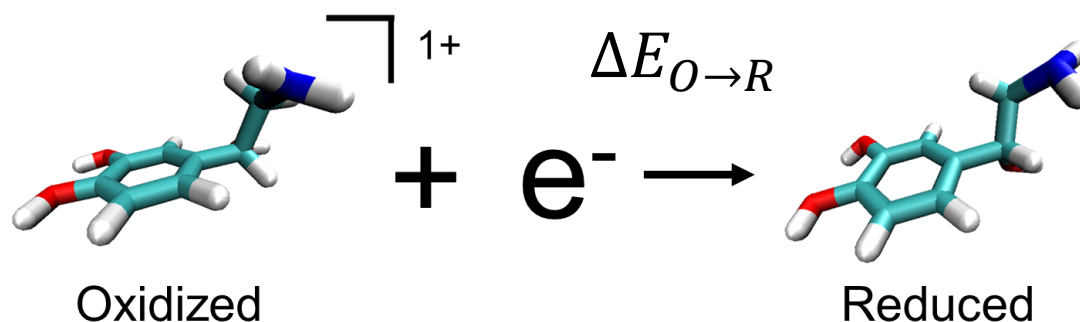
Oxidation half reaction



In practice, report the
Reduction Potential



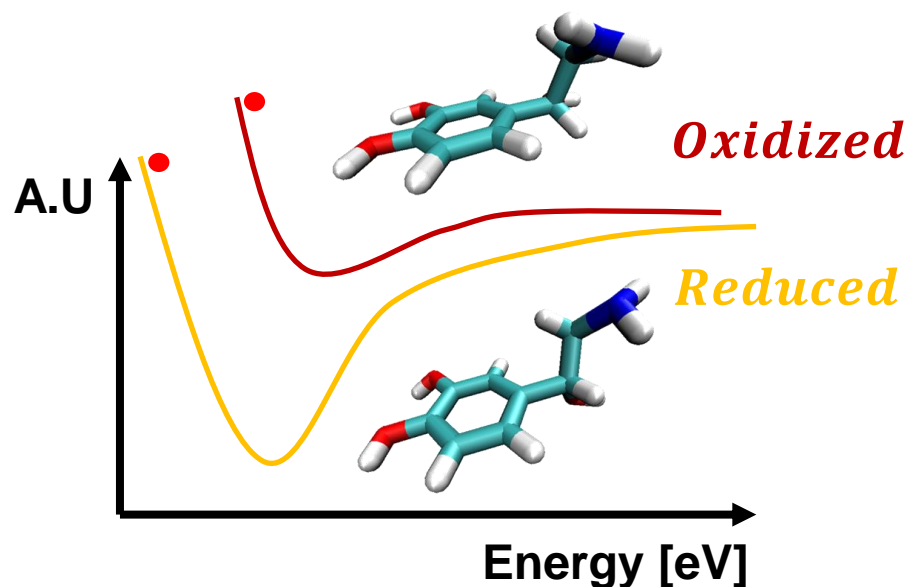
In practice, report the
Reduction Potential



$$\Delta E_{O \rightarrow R} = \Delta E_{red}$$

$$\Delta G_{red} = -nF\Delta E_{red}$$

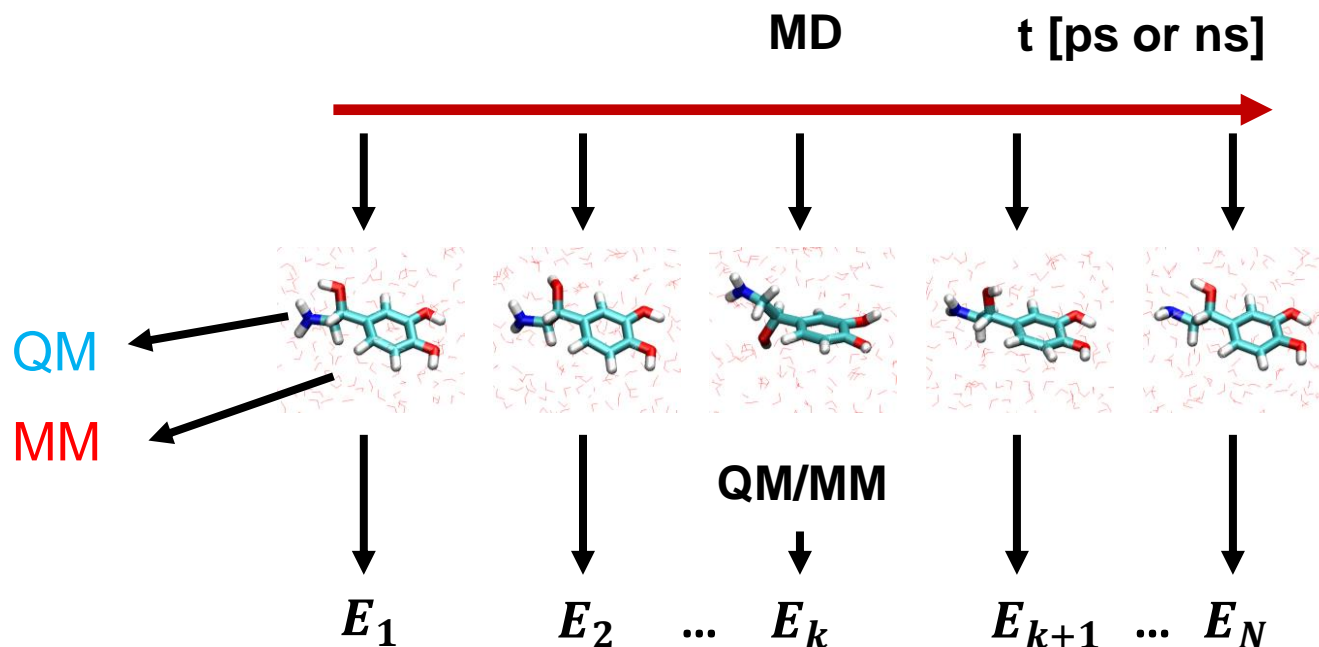
$$\Delta G_{red} = -nF\Delta E_{red}$$



Sampling on both
the oxidized and the
reduced states!

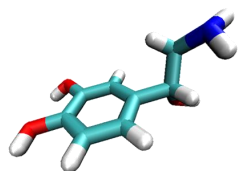
$$\Delta G_{red} = \langle E_R \rangle - \langle E_O \rangle - [\Delta G_{e,solv}]$$

Ensemble Averages Solvated e^-

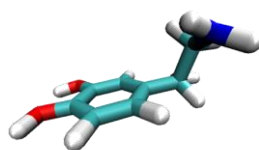


Part 1: QM/MM MD [ps]

Part 2: Classical MD,
then QM/MM [ns]



Reduced



Oxidized

Charge 0

+1

Spin Mult. 1

2

$$V_{\text{AMBER}} = \sum_i^{n_{\text{bonds}}} K_{r,i} (r_i - r_{i,\text{eq}})^2 + \sum_i^{n_{\text{angles}}} K_{\alpha,i} (\alpha_i - \alpha_{i,\text{eq}})^2 + \sum_i^{n_{\text{dihedrals}}} V_i (1 + \cos(n_i \phi_i - \gamma_i)) + \sum_{i < j}^{n_{\text{atoms}}} \sqrt{\epsilon_i \epsilon_j} \left[\left(\frac{r_{i,\text{min}} + r_{j,\text{min}}}{2r_{ij}} \right)^{12} - 2 \left(\frac{r_{i,\text{min}} + r_{j,\text{min}}}{2r_{ij}} \right)^6 \right] + \sum_{i < j}^{n_{\text{atoms}}} \frac{q_i q_j}{4\pi \epsilon_0 r_{ij}}$$

FF(Reduced) ≠ FF(Oxidized)