Glassy protein dynamics and gigantic solvent reorganization energy of plastocyanin

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Fast, inefficient $\sim 10^{12} \text{s}^{-1}$

Slow, efficient $\sim 10^4$-$10^9 \text{s}^{-1}$

But we will show that $\lambda$ is large.

$\Delta G = -\lambda$

$\Delta G = 0$

Marcus model's restriction:

$\Delta x_{st} = 2\lambda$

Tradition shows that $\lambda$ is small.

$E^{\text{act}} \propto \lambda/4$, $\lambda \sim 0.8 \text{ eV}$ requires a very close approach.

$\lambda$ must be small to not lose energy, $\sim 0.1$ - $0.2 \text{ eV}$
Solution Electron Transfer

\[ \lambda_2 = 2 \lambda_1 \]

Protein Electron Transfer

\[ Y = X + \gamma q \]

Proteins have glassy conformational dynamics.

Our model shows that \( \Delta X_{st} \) is frozen.
For protein ET, there is a clear breakdown of the link between $\lambda$ and $\Delta X_{st}$.

Now, when reorganization energy rises, the activation barrier drastically lowers.
Our model describes biological electron transfer including a huge $\lambda$ and a frozen $\Delta X_{st}$.

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Supplemental Data Section

(a) $G_i(X)/eV$

(b) $G_i(Y)/eV$
Supplemental Data Section
Supplemental Data Section

(a) $\tau_{ET} \ll \tau_q$

$\lambda = \lambda_p$

(b) $\tau_{ET} > \tau_q$

$\lambda = \lambda_p + \lambda_q$