# Efficient Energy Transfer in Light-Harvesting Systems, III: The Influence of the Eighth Bacteriochlorophyll on the Dynamics and Efficiency in FMO

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As mentioned in the main text, the Hamiltonian for FMO is constructed from the crystal structure recently deposited in the protein data bank (pdb code: 3eoj).[1] The site energies are taken from those computed in Ref. 4 and the coupling element between sites $n$ and $m$ is calculated from the dipole-dipole approximation,

$$V_{nm} = C\left(\frac{\mathbf{d}_n \cdot \mathbf{d}_m}{|\mathbf{r}_{nm}|^3} - 3\frac{(\mathbf{d}_n \cdot \mathbf{r}_{nm})(\mathbf{d}_m \cdot \mathbf{r}_{nm})}{|\mathbf{r}_{nm}|^5}\right) . \tag{1}$$

Following the prescriptions used previously for constructing the dipole-dipole interactions,[2–4] the unit vectors, $\mathbf{d}_n$, in Eq. (1) point along the axis connecting the $N_b$ and $N_d$ atoms of the $n$-th Bchl and $\mathbf{r}_{nm}$ is the vector connecting the Mg atoms of Bchl $n$ and $m$. Setting the constant $C = 155000$ cm$^{-1}$Å$^3$ leads to an effective dipole strength of 30 D$^2$. With these specifications the system Hamiltonian (in cm$^{-1}$) for the eight site model is

$$H_{\mathrm{FMO}} = \begin{pmatrix}
310.0 & -97.9 & 5.5 & -5.8 & 6.7 & -12.1 & -10.3 & 37.5 \\
-97.9 & 230.0 & 30.1 & 7.3 & 2.0 & 11.5 & 4.8 & 7.9 \\
5.5 & 30.1 & 0.0 & -58.8 & -1.5 & -9.6 & 4.7 & 1.5 \\
-5.8 & 7.3 & -58.8 & 180.0 & -64.9 & -17.4 & -64.4 & -1.7 \\
6.7 & 2.0 & -1.5 & -64.9 & 405.0 & 89.0 & -6.4 & 4.5 \\
-12.1 & 11.5 & -9.6 & -17.4 & 89.0 & 320.0 & 31.7 & -9.7 \\
-10.3 & 4.8 & 4.7 & -64.4 & -6.4 & 31.7 & 270.0 & -11.4 \\
37.5 & 7.9 & 1.5 & -1.7 & 4.5 & -9.7 & -11.4 & 505.0
\end{pmatrix} , \tag{2}$$

where the zero of energy is 12195 cm$^{-1}$. Note that there is an error in the sign of the coupling between sites 1 and 2 in the table provided in Ref. 4. Aside from this, these values reproduce all of the couplings listed therein to within 3 cm$^{-1}$.

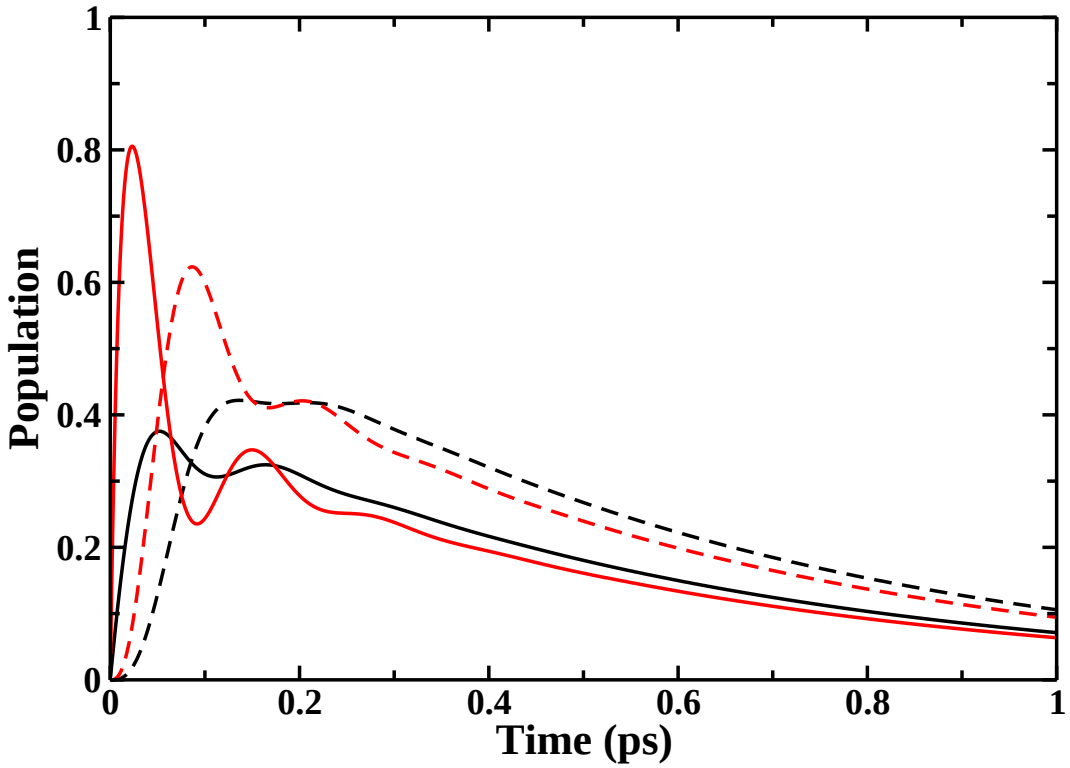


Figure 1: The site populations of the dimer calculated using the NIBA discussed in the main text. The solid and dashed lines correspond to the populations of site 1 and 2, respectively. The black lines are calculated with a decay rate from site 8 of $\gamma = 15$ ps$^{-1}$ and the red lines with $\gamma = 100$ ps$^{-1}$. In both cases, the temperature is 300 K with a reorganization energy of 35 cm$^{-1}$ and cutoff frequency of $\omega_c^{-1} = 50$ fs. Note in particular, the onset of oscillations in the dynamics of site 2 when $\gamma = 15$ ps$^{-1}$ (dashed black) and the recovery of the dynamics in Figure 2(c) of the main text when $\gamma = 100$ ps$^{-1}$ (red).

## References


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