Supporting Information

Importance of Inter-monomer Couplings of the FMO Complex in Coherently Initiated Dynamics

Davinder Singh* and Shubhrangshu Dasgupta

Department of Physics, Indian Institute of Technology Ropar, Rupnagar-140001, Punjab, India

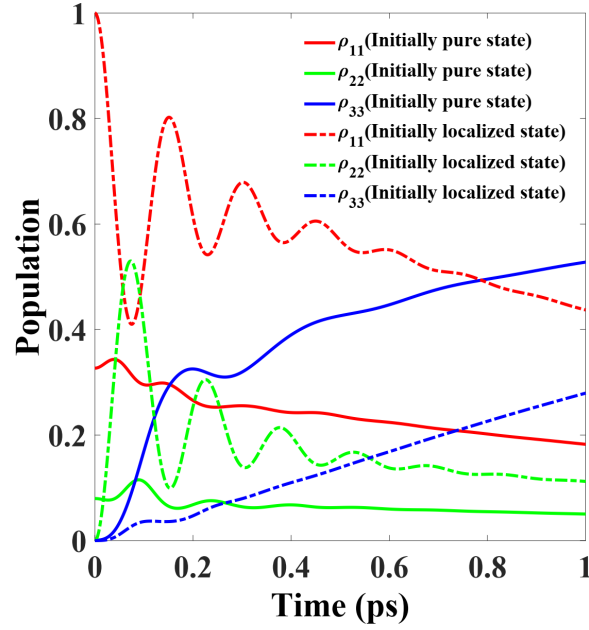E-mail: davinder.singh@iitrpr.ac.in

Role of the initial condition

The energy transfer dynamics has been compared for two different initial conditions, i.e., an initial pure state and initial localized state (when bacteriochlorophyll-a (BChla) 1 is assumed to be initially excited as has been assumed on the basis of closeness of the baseplate linker pigmet[1]). Following Ishizaki and Fleming,[1] the energy transfer dynamics has been studied for the 7-site monomer of the FMO complex, and the homogeneous protein environment is assumed with $\lambda = 35$ cm^{-1} and $\gamma = 106$ cm^{-1} for all the BChla sites. The following initial pure state has been used to study the energy transfer dynamics.

$$
\begin{aligned}
|\psi\rangle &= \sqrt{0.3268}|1\rangle + \sqrt{0.0797}|2\rangle + \sqrt{0.0005}|3\rangle + \sqrt{0.2648}|4\rangle \\
&+ \sqrt{0.0322}|5\rangle + \sqrt{0.0127}|6\rangle + \sqrt{0.2833}|7\rangle \ .
\end{aligned} \tag{S1}
$$

It is evident from Fig.S1 that in both cases, the BChla 3 has negligible excitation initially. However, with the initial pure state, the BChla 3 gets populated quickly, i.e., almost 35 % population is transferred to BChla 3 at $\sim$200 fs. While the transfer of population is comparatively slow to the BChla 3 when initially localized state is assumed, i.e., it took almost 1000 fs to transfer the 35% population to BChla 3. It implies that with the use of an initial pure state, the population is distributed quickly among the different BChla sites as compared to the initially localized state. Which further implies that the initial condition plays an important role in the dynamics of energy transfer, and a realistic initial condition needs to be considered for the more accurate study of the dynamics.

References

(1) Ishizaki, A.; Fleming, G. R. Theoretical Examination of Quantum Coherence in a Photosynthetic System at Physiological Temperature. *Proc. Natl. Acad. Sci.* **2009**, *106*, 17255–17260.

(a)

Figure S1: Comparison of the coherent oscillatory population dynamics in the 7-site monomer of the FMO complex for the initial pure state (i.e., Eq.(S1)) and the initially localized state when BChla 1 is assumed to be initially excited. The solid (dash-dotted) lines illustrate the population dynamics for the initial pure (localized) state. Here we have used a time step of 1 fs and 4 hierarchy levels with 3 exponential bath terms.