

Abstract Submitted  
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**Excitation Energy Transfer in Peridinin-Chlorophyll *a*-Protein Complex Using Förster Resonance Energy Transfer** WILLIAM BRICKER, CYNTHIA LO, Washington University — Peridinin-Chlorophyll *a*-Protein (PCP) is a trimeric light-harvesting protein complex containing peridinin and chlorophyll *a* pigment molecules, and the excitation energy transfer (EET) efficiency within this system is estimated at close to 90%. To study the EET in PCP, we use the Förster Resonance Energy Transfer (FRET) model, assuming that energy transfer occurs incoherently. We calculate the FRET coulombic coupling and spectral overlap terms using multi-reference configuration interaction (MR-CI) with semi-empirical basis sets in MOPAC. The two dominant EET pathways within PCP are from the  $S_2$  state of peridinin to the  $Q_x$  band of chlorophyll *a*, and from the  $S_1$  state of peridinin to the  $Q_y$  band of chlorophyll *a*. In peridinin, absorption in the visible spectrum is due to the strongly allowed  $S_0$  to  $S_2$  transition, while the  $S_0$  to  $S_1$  transition is optically forbidden and has double excitation character. To more accurately describe the FRET coulombic coupling term, we are working on an extension to the MOPAC source code, which will provide transition densities for all transitions. Our EET study of PCP using FRET reveals the interplay of pigment geometry and environment on the EET rates and efficiencies within the complex.

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