Quantum coherences and dephasing in biological systems

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Excitation energy as well as charge transfer processes are important and ubiquitous in biological systems but at the same time complicated to model at the molecular level. In a multiscale approach classical molecular dynamics simulations and electronic structure calculations need to be combined. The results of such a treatment can subsequently be employed in quantum approaches to determine the respective charge and energy transfer scenarios as well as optical responses. As examples, excitation energy transfer in light-harvesting systems and charge transport through a DNA molecule are detailed. The experimental observation of long-lived quantum coherences in the Fenna-Matthews-Olson light-harvesting complex has steered considerable effort to explain these findings. Results of the above envisioned multiscale scheme are presented. In the second example, the charge transport through a DNA molecule is detailed with a special emphasis on the time-dependent effects caused by the liquid environment.

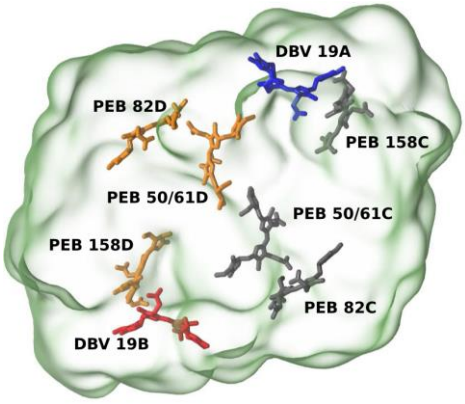

Figure 1- Distribution of bilin molecules in the PE545 light-harvesting complex.

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[3] C. Olbrich, T.L.C. Jansen, J. Liebers, M. Aghtar, J. Strümpfer, K. Schulten, J. Knoester, and U. Kleinekathöfer, J. Phys. Chem. B 115, 8609-8621 (2011).