Photoactive molecular complexes

Research opportunities 2016-2017 *Dr. Arend G. Dijkstra (a.g.dijkstra@leeds.ac.uk)*
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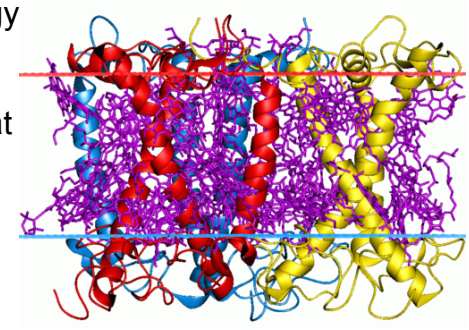
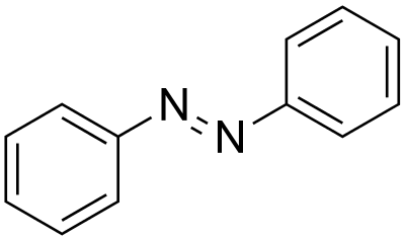
In our group, we use models to understand how molecular systems use light to function. These models are compared with state of the art optical experiments, which allow us to probe the fundamental motions of electrons and nuclei that take place on femtosecond to picosecond time scales. Inspiration for our work comes from biological systems. Our work uses mathematics and computer programming. The projects are suitable for chemistry, physics and mathematics graduates.

The first project is about ***photosynthesis*****.** How is the energy that is collected by plants and bacteria from sunlight transported? It turns out that answering this question requires a detailed description of the pigment molecules that interact with the light, as well as of the protein and solvent environment. In this project, you will build a new model of the energy transport mechanism. The model will be based on quantum mechanics of an electronic system interacting with vibrations. A main goal of the project is to accurately determine the parameters that describe real systems, from either simulation or comparison to experiment.



Light harvesting complex II from green plants (source: Wikipedia)

The second project is about ***photo switching.*** Some of the fastest events in biology occur within the eye. As in photosynthesis, electrons are excited by light absorption, However, in the primary step in vision the nuclear motion induced by electronic excitation is very large. Cis-trans isomerization in the rhodopsin molecule completely changes the structure. The system clearly explores parts of the potential energy surface far away from equilibrium, such that a harmonic description is completely invalid. This is also the case in man-made photo switches. This is a challenging regime for models that treat both the electronic and the nuclear motion under the influence of the protein environment. This project aims at developing a new theory to describe quantum decoherence and friction outside the harmonic approximation.



Azobenzene, a photo switching molecule (source: Wikipedia)

References

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[3] Dijkstra, A. G., Wang, C., Cao, J. and Fleming, G. R., J. Phys. Chem. Lett. **6**, 627 (2015).