PhD Project

Molecular Dynamics of Supramolecular Aggregation

Materials for highly efficient organic solar cells require excellent light harvesting capabilities but at the same time need to be efficient charge transporters. Both properties are intimately linked to intra- and intermolecular arrangements, which often feature the so-called π-π stacking. How exactly the link between this supramolecular aggreation and light harvesting is established and whether there exist novel possibly even more efficient configurations, however, is not clear at present.

The aim of the project is to understand this connection using Molecular Dynamics computer simulations. Various candidate materials such as perylene bisimides and others are being synthesized by our collaborators in chemistry and spectroscopically analyzed in the experimental physics department. The current project will connect to the latter epxeriments and provide key information in order to understand light harvesting processes which is not directly available from the measured spectra.

Simulations will be run using the GROMACS Molecular Dynamics package on local as well as national supercomputing facilities. Analysis tools using advanced sampling techniques such as Umbrella Sampling or Replica Exchange will be written by the candidate in C/C++.

The successful candidate must possess a strong background in theoretical physics, numerical mathematics, computational chemistry or a similar discipline. Interest in writing and using computer codes (C/C++) is required.

Research will be conducted in the Biofluid Simulation and Modeling group at the University of Bayreuth. Bayreuth is a lively city with a large student population situated in a beautiful natural setting between the mountains of the Fränkische Schweiz and Fichtelgebirge.

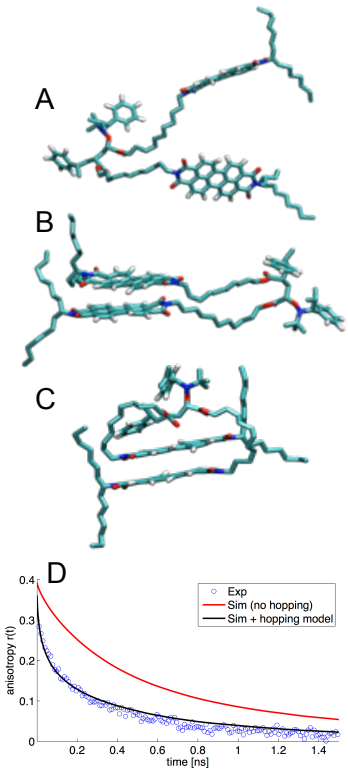

Fig. 1: A perylene bisimide dimer in its open (A) and stacked (B+C) molecular conformations. Comparison between theoretical and experimental spectrum (D).

For applications or further information please contact:

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