PhD position available in the Molecular Dynamics Group, University of Groningen, The Netherlands

Topic: Multiscale modeling of self-assembled molecular nanotubes

Where: The PhD candidate will be placed at the Molecular Dynamics Group (supervised by Prof. Siewert-Jan Marrink), and work in a collaborative research project between the Molecular Dynamics Group, the Theoretical Physics Group, and the Optical Condensed Matter Group at the University of Groningen, embedded within the world-famous Zernike Institute for Advanced Materials.

Background: We study electronic excitation energy transport in self-assembled molecular nanotubes that are inspired on tubular chlorophyll aggregates occurring as light-harvesting systems in nature. Tubular aggregates combine a wire-like structure with a built-in robustness against the detrimental effects of disorder characteristic for truly one-dimensional wires. As specific example we focus on double-walled tubular aggregates of the cyanine dye C8S3, which, similar to natural light-harvesting systems, have energy transport taking place at different hierarchical scales. Experimental tools include manipulation of C8S3's chemical structure to incorporate excitation traps and/or launchers into the system, recently developed two-dimensional (2D) correlation spectroscopy, and single-molecule microscopy. Experiments will be compared with an unprecedented level of theory, where we aim to be the first team worldwide to establish a first- principles modelling of exciton states and energy transport in large self-assembled systems. The project should lead to a detailed understanding of the nature (coherent vs. incoherent) and range of energy transport in these bio-inspired materials, indications for design principles for materials with better transport properties, and, in general, opening the horizon for first-principles modelling of the optical functionality of large self-assembled systems. The role of the prospective PhD candidate is to provide the large scale models for the nanotube aggregates, based on multiscale (all-atom, coarse-grained) molecular dynamics simulations.

Qualifications:
- solid background in biophysics or physical chemistry
- experience with computational modeling

When: the sooner, the better; September 2015 at the latest

How to: Interested candidates should send an email with motivation letter, two recommendation letters, and CV to Prof. S.J. Marrink: s.j.marrink@rug.nl