

## Open PhD project:

### Femtosecond time-resolved imaging of the elementary steps of organic solar cells studied in a 0.4 K cold nanolaboratory

Where: Femtolab, Aarhus University

When: Application GSST, Aug 1, 2018. Expected start: Nov 1, 2018 - possibly later

Program: Chemistry, Physics, or Nanoscience

Requirement: Bachelor in Physics, Chemistry, Nanoscience

Supervisor: Henrik Stapelfeldt

Before applying: Contact Henrik Stapelfeldt, [henriks@chem.au.dk](mailto:henriks@chem.au.dk) for more information

#### Project description:

*The scientific goal of this PhD project is to explore the fundamental molecular processes in polycyclic aromatic hydrocarbon molecules that underlie organic solar cell applications. In particular, the aim will be to obtain an atomistic view of how the molecules change during photoinitiated reactions with femtosecond time-resolution.*

Polycyclic aromatic hydrocarbons (PAHs) are conjugated molecules, composed of multiple aromatic rings that promise to be attractive candidates for materials to build the next generation of optoelectronic devices.

As a unique approach the PAHs will be studied inside helium nanodroplets. The helium droplets are created by expanding a cryogenically cooled, high pressure gas of helium into vacuum. They consist of about 10,000 He atoms, have a diameter of ~ 10 nm and a temperature of 0.4 K. The droplets move with a few hundred meters per second and when they pass through a doping cell, containing a gas of molecules, they can pick up one or several molecules. The pressure of the gas determines how many molecules each droplet pick up. Thereby, it becomes possible to study either single molecules, using a low doping cell pressure, or dimers (or larger oligomers) of molecules, using a higher doping cell pressure, since two (or more) molecules inside a droplet will bond due to intermolecular interactions, primarily van der Waals (vdW) interactions. Dimers of PAHs, notably tetracene and pentacene, are of special interest for organic solar cells.

The experimental methodology to be applied is laser-induced alignment and femtosecond time-resolved imaging using ultrashort laser pulses. The latter includes Coulomb explosion and linear dichroism. The project will initially aim at determining the static structure of PAHs dimers. These structures have been calculated theoretically but hardly anything is known experimentally. The next step is fs time-resolved imaging of the vdW dimers upon photoexcitation of one of the monomer units. This excitation leads to a strong increase of the intermolecular interaction and formation of an exciplex. The ultimate goal is to directly image the structural rearrangement from the initial vdW complex to the exciplex. Finally, we want to study singlet fission (SF), which is a competing mechanism to the exciplex formation.

Singlet fission can occur when a PAH molecules in an excited singlet state, created by absorption of light, shares its excitation energy with a neighboring ground state molecule resulting in conversion of both molecules to excited triplet states. The interesting solar cell perspective is that SF leads to two electron-hole pairs rather than only one as in a conventional Si-based solar cell. This doubling of charge carriers may be

exploited to strongly enhance the solar-to-electrical power conversion. The ambitious goal in this project is to obtain insight about the coupled motion of electrons and nuclei and thus about the flow of charge and vibrational energy that underlies the fundamental SF mechanisms.