

## **Research Plan:**

Dr. Seyhan Salman is a computational/theoretical chemist interested in photophysical and charge transport properties of optoelectronic materials used in organic electronic devices. By using density functional theory, she investigates the geometric, electronic and optical properties of pi-conjugated molecules and based on theoretical calculations tries to develop structure – photophysical property relationships of these materials.

Recently, she has been involved in the calculations of the ground and excited state electronic and optical properties of donor-acceptor type organometallic chromophores and investigates reliable theoretical methods for the description of the energetics and nature of the low-lying electronic excitations responsible for the near-infrared/visible absorption spectra of these donor-acceptor type chromophores (*Organometallics* 2013).

She is also interested in modeling electronic processes taking place where materials (organic, inorganic and metals) come into contact at interfaces in organic electronic devices (*J. Phys. Chem. Lett.* 2012). Therefore, part of the work in collaboration with LPPI at the University of Cergy-Pontoise will focus on the electronic and optical properties of pi-conjugated donor-acceptor type molecules synthesized at LPPI. The experience of Dr. Seyhan Salman originating from her studies in collaboration with the group of Prof. Jean-Luc Brédas at Georgia Tech', Atlanta, Georgia, USA, will be very helpful for a deep understanding of these properties. Another aspect of the common work with Dr. Salman will focus on the electron transfer processes at (bio)organic interfaces, which constitutes another theme at LPPI (Dr. Philippe Banet). For modeling the electronic processes at (bio)organic interfaces, the common expertise on bioelectronics of our lab and of Dr. Salman will be extremely useful. As a result, the overall work at University of Cergy will help us to develop a fundamental understanding of the photophysical and transport mechanisms in bio-conjugated optoelectronic materials.