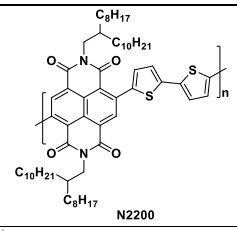
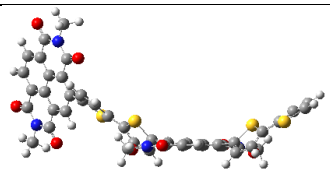
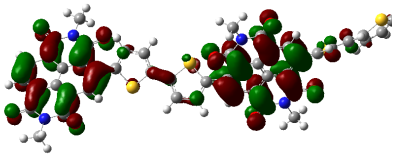
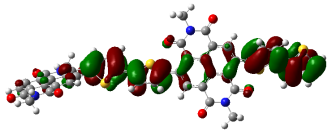
30/60 Credits Master's Thesis Project:

Computer Modelling for the Design of Conjugated Polymers

All-Polymer solar cells (All-PSCs), which consist of p-type semiconducting donor polymers and n-type semiconducting acceptor polymers have become the popular topic in the field of organic solar cells due to their tunable chemical and electronic properties as well as better stabilities. Despite the advantages mentioned above, n-type conjugated copolymers, which could act as electron acceptors in all-PSCs are rather underdeveloped. One of the challenges of developing new n-type acceptor polymer for efficient all-PSCs is having a suitable offset in the frontier molecular orbital (highest occupied molecular orbital (HOMO)/lowest unoccupied molecular orbital (LUMO)) energy levels of the donor polymer / acceptor polymer.

Therefore, we are looking for a highly motivated student who is highly interested in both computer modelling and all-PSCs.

Table 1: The typical chemical structure n-type acceptor polymer, side view, and energy level distributions of two repeating units

Chemical Structure	 N2200
Side view	
LUMO distribution	
HOMO distribution	

During this project you will be able to learn the following techniques:

- Computational software such as: Chem 3D, Gauss View 09, Materials Studio
- Design rules of n-type acceptor polymers for all-PSCs
- Density functional theory (DFT) calculation aided polymer design and analysis

For more information, please contact:

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