Computational characterisation of donor-acceptor polymer properties for solar cell applications

PhD project proposal for EPSRC/NPIF Funding in materials science, 2018

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Industrial Collaborator: Merck Chemicals Ltd., University Parkway, Chilworth, Southampton, SO16 7QD, UK

Background:

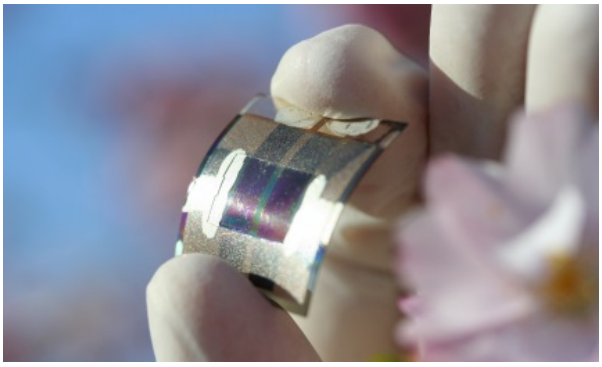

Figure 1 Mechanically flexible polymer-based organic solar cells are slowly reaching marketable efficiencies beyond 10% [1]. Their versatility and cost-effectiveness will enable much easier deployment than conventional silicon-based solar cells.

Organic solar cells based on polymers have attracted great attention. They are mechanically flexible, light, and cost-efficient (see Fig. 1). Polymers that comprise both electron donor and acceptor moieties are specifically interesting as energy-harvesting materials as they contain a large number of light-absorption and charge-separation centres in one macromolecule and enable versatile synthesis with a variety of molecular building blocks. However, a major remaining challenge is the molecular-level characterisation of the structure and the optoelectronic properties of this type of materials, both in solution and inside a photovoltaic thin-film where the polymer is in contact with a conductive charge extraction layer (see Fig. 2). First-principles computational modelling has the ability to predict the structure and optoelectronic properties of molecules in photovoltaic devices and, in synergy with controlled polymer synthesis and atomic-resolution characterisation experiments, can provide a bottom-up route to the rational design of polymer-based organic solar cells. This is the goal of this project.

Programme of work of PhD project:

We will use computational condensed matter simulation methods based on Density Functional Theory (DFT) and approximate DFT-based tight-binding methods to predict the charge donor and acceptor properties of polymers as a function of their structure. This will guide experimental development of new polymeric solar cell materials. The student will work in tight collaboration with experimental and industrial partners to achieve the following goals:

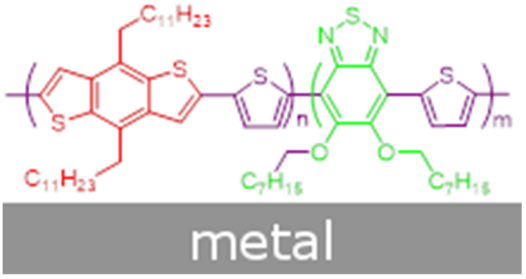

Figure 2 A charge-donor polymer adsorbed to a metallic contact enables single-molecule characterisation and provides a simple lab-based model for organic solar cell devices.

- A computational prediction of charge donor-acceptor properties of polymers as a function of the degree of polymerisation and different building blocks that will guide the synthetic development of new materials by the group of Prof. David Haddleton.
- A computational prediction of structure and donor-acceptor properties of selected polymers adsorbed at metallic contacts to support the sub-monomeric structural characterisation and sequencing of conjugated polymers by scanning probe microscopy and spectroscopy, performed by the group of Prof. Giovanni Costantini. These simulations will furthermore provide insights into important device parameters such as electrode-polymer charge injection and extraction barriers.

Training and Environment: This PhD project will be embedded in a unique experiment-theory collaboration that encompasses polymer synthesis (Prof. Haddleton), experimental on-surface characterisation and sequencing of single polymer molecules (Prof. Costantini), and quantum theoretic simulation of structural and optoelectronic properties of polymers in solvent and when adsorbed on metallic electrodes. Based on the experience of the supervisor on modelling complex organic materials [2] and hybrid organic-metallic interfaces [3], the student will be trained in state-of-the-art computational materials modelling techniques and in scientific computing on national-scale high-performance computing infrastructure.

Industrial Collaboration: The industrial collaborator Merck will be continuously consulted on the economic and industrial relevance of newly identified polymers and the student will be involved in industrial knowledge exchange that will guide the progress of their research.

References:

[1] Lichttechnisches Institut, Karlsruhe Institute of Technology. https://www.lti.kit.edu/7003.php
[2] Mortazavi et al., J. Phys. Chem. Lett. 9, 399-405 (2018), [3] Maurer et al., Progr. Surf. Sci. 91, 72-100 (2016)