

## Structure and Dynamics of conjugated polymers for energy and optoelectronic applications

Conjugated polymers are solution-processed semiconductors that can be used in thin-film electronic devices such as organic light emitting diodes, organic photovoltaic (OPV) devices, organic field-effect transistors or biosensors. The optoelectronic properties of the polymers are controlled by the conformation of the relatively stiff backbones, which is in turn influenced by the more flexible side chains. The polymer chains fluctuate in shape, and this strongly affects electronic processes such as charge carrier transport in electronic devices or charge separation in solar cells. The performance of OPV devices depends dramatically on the fine tuning of the microstructure of such blends and the underlying structural fluctuations. Thus, the structural dynamics of the donor-acceptor components forming the blends is a fundamental aspect affecting the lifetime of the OPV devices, and one of the common degradation mechanisms to deal with at the microscopic level.

One of the most powerful probes of molecular structure and dynamics is neutron scattering (NS), which allows a direct microscopic probe of matter. Quasi-elastic neutron scattering (QENS) enables probing the chain dynamics of polymers on various time scales. Inelastic neutron scattering (INS) enables probing lattice and molecular vibrations relevant to chemical bonding behavior in molecular system. On the other hand, small angle neutron scattering (SANS) offers the possibility to probe the conformation of chains in solution. Neutron scattering can be used as a master method to probe or to complement structural X-ray investigations by making use of the deuteration technique to resolve individually side chains, backbones and solvent/small molecule in the case of co-crystallization. Atomistic simulations can synergistically be used for the sake of the analysis and interpretation of the neutron data, as well as serving as a prediction tool in some cases.

This PhD project builds on an ongoing active collaboration between Imperial College London and the ILL, bringing together a wide range of complementary expertise in synthesis, structural, dynamical, optical and electronic characterization, as well as *ab-initio* and molecular dynamics calculations to support the study of organic electronic materials.

The scientific aim of this project is to investigate the underlying microscopic mechanisms and the effect of blending on the dynamics of conjugated polymer(s): small molecule(s) blend, in order to establish how molecular diffusion is influenced by the polymer environment. The scope of the study includes other multi-component systems such as ternary blends using alternative acceptors. The impact of different polymer conformers in selected conjugated polymers, influencing both optical properties through appearance of extra vibronic bands and electronic properties such as charge transport, will be also studied. Establishing the relationship between structure and dynamics is vital for tailoring the above-mentioned targeted properties. Neutron scattering studies, supported by numerical simulations, will play a key role in this investigation.

The techniques to be used in this project include: (i) different solution-processing synthesis methods, (ii) a variety of structural, electronic and vibrational characterization measurements, (iii) neutron scattering techniques, and (iv) quantum chemistry and molecular dynamics simulations.