

*Molecular Photovoltaics Research in the Physics Department, Imperial College London.*

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Research into molecular photovoltaic materials and devices in the Physics Department at Imperial College encompasses the following themes: (1) material and device characterisation for polymer / fullerene bulk heterojunctions; (2) characterisation and optimisation of hybrid organic / metal oxide heterojunction devices; (3) measurement and simulation of charge transport in conjugated materials; and (4) scalable deposition processes for large area device fabrication. (1) In the area of polymer/fullerene bulk heterojunction devices, current research is focused on the monitoring and control of blend and molecular morphology, determination of the relationship between morphology, transport properties and device performance, and improvements to device structure and design. In particular, optical probes such as spectroscopic ellipsometry and Raman spectroscopy have been used to probe the dynamics of phase segregation and the degree of vertical and lateral phase segregation in blend films. Novel routes to multi-layer device fabrication are used with the aim of enhancing device performance through electrode selectivity. (2) In the area of hybrid organic/ metal oxide structures, recent studies have addressed the dependence of open circuit voltage on the electronic properties of materials, the modification of the organic / metal oxide interface using molecular monolayers to control material compatibility and charge transfer, improved infiltration of polymers into metal oxide nanostructures using techniques such as in-situ polymer growth, and improved charge separation yields through enhanced energy transport in self-organized donor films. (3) Recognising that charge transport is a major factor limiting the performance of organic photovoltaic devices, we have developed expertise in the measurement of charge mobilities in organic films as a function of chemical structure, composition and processing conditions, and in the correlation of charge transport properties both to the physical and chemical structure of the materials, and to the performance of resulting devices. The group offers particular strengths in the modelling of charge transport, having developed a multi-scale approach incorporating atomistic molecular dynamics, quantum-chemical methods and kinetic Monte Carlo simulations, which together offer the capability to predict transport properties from details of chemical structure and molecular packing. (4) Large area device fabrication on flexible substrates is being studied via gravure printing and other techniques. This work builds on the recent demonstration of high performance, fully printed organic field-effect transistors fabricated by gravure printing.

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