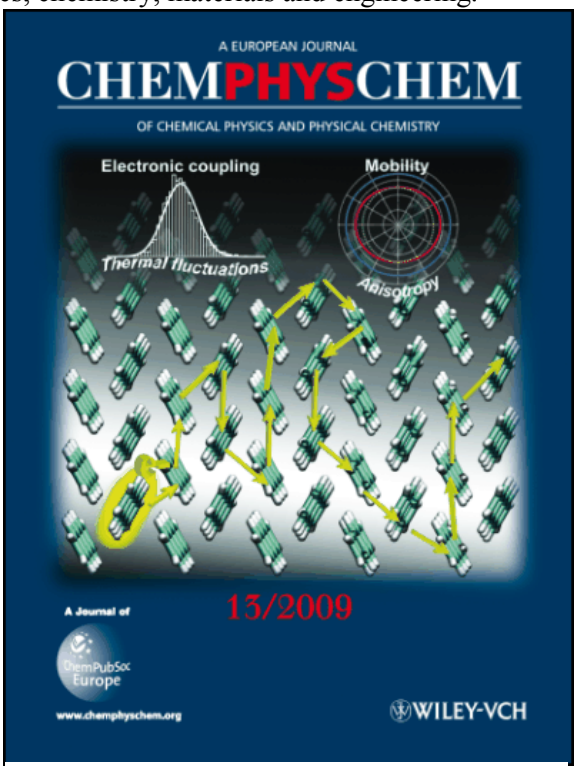
Publishable Executive Summary

This research project was targeted towards a fundamental understanding of charge and energy transport properties in pi-conjugated materials. Devices can be made cheaply from these materials and this is a disruptive technology with applications in displays, lighting, printed electronics, photovoltaics and sensors including biosensors. The originality and feasibility of the project came from the unique possibilities afforded by combining the expertise of six EU, one Chinese groups complemented by six US partners. Modecom has been highly successful, producing 49 refereed publications in international level journals, listed on the Modecom website. They have attracted much attention as shown by an excellent citation record and two journal covers. We have demonstrated significant progress towards the goal of understanding electroactive conjugated materials at the multiscale through combining state of the art techniques from physics, chemistry, materials and engineering.

The goals in the Project summary are shown in italics.

(i) Provide accurate estimates of all basic microscopic parameters that control electron and energy transfer processes.

- A software package to compute geometric, electronic and optical properties of isolated molecules and polymer chains at the microscopic level was extended and enhanced. It has predicted rectification ratios crucial for the assessment of the technological usefulness of single molecule junctions as diodes.
- Quantum chemical theories of oligomers and molecules employing state of the art many body theories were developed.
- Molecular parameters governing charge and exciton transport were studied in organic crystals (one study is illustrated), host-guest systems, and 1dimensional arrays.
- Studies were made of the electronic structure at organic/organic interfaces as interface phenomena have a major influence on device behaviour.



Journal cover showing Modecom research

(ii) Develop theoretical models establishing a coherent connection between the microscopic parameters and the macroscopic description verified by data from ultrafast spectroscopy, photoelectron spectroscopy and transport measurements

- A molecular to mesoscale model for temperature dependent exciton transport in conjugated oligomers was developed. Predictions of packing arrangements were validated through comparison with experimental data.
- The spectroscopy of acene solids was analyzed to obtain information about electronic delocalization and domain sizes
- An explanation for low charge mobilities measured for transport in pentacene layers on dielectrics was provided.

(iii) Find reliable structure-transport property relationships that bridge the molecular scale, mesoscale and the macroscopic device scale.

- Strategies to improve exciton diffusion lengths based on changing the chemical structure were shown to yield cancelling effects in studies of energy transport along polymer chains.
- Microscopic and macroscopic device simulation models that include the effects of morphology were proven to be useful tools to experimentalists in analyzing organic device performance.
- Devices were fabricated to study the temperature dependence of charge mobilities in fluorene-based copolymers and this data was interpreted using a numerical model allows for the effects of the carrier concentration and energetic disorder on transport.