Project Publishable Report

UHMOB

Ultra-high Charge Carrier Mobility to Elucidate Transport Mechanisms in Molecular Semiconductors

Project Number: 811284

Period covered by the report: from 01/05/2019 to 30/04/2021

I. Project context and objectives

Organic electronics is an active field of research that aims to replace Silicon by organic semiconductors. The former is energy- and cost-intensive whereas the later are cheap to produce and allow additive manufacturing of electronic circuits. The UHMob objective is twofold. On the one hand, the project aims to design, synthesise, and assess performances of a novel generation of organic semiconductors creating a favorable environment for industrial innovations. On the other hand, UHMob delivers the finest quality research training and transfer of knowledge in an interdisciplinary, inter-sectoral, and emerging supra-disciplinary field, to 15 early-stage-researchers to educate them to become future scientific leaders.

II. Work performed from the beginning of the project to the end of the period covered by the report and main results achieved so far

A series of innovative semiconductors has been successfully synthesised. Based on particular: (a) two isomers of a fused-ring compound (DN4T and isoDN4T). On the basis of their crystal structures, theory has demonstrated that a subtle change in molecular topology can lead to a radically different behaviour for charge transport; (ii) linear conjugated rods substituted by chiral side chains to promote a helicoidal-like interlayer packing; and (iii) a series of rylene derivatives of increasing size to be exploited in the experiments on vacuum coupling whose design has been optimized in parallel. Theory has also focused on the characterisation of the phonon modes in different crystals to be confronted to experimental Raman and neutron scattering spectra and to be used for the analysis of the impact vibrations on charge transport. A strong theoretical focus has also been given to the structural packing properties of an asymmetric BTBT derivative substituted on one side by a phenyl group and by a saturated chain on the other side; note that asymmetric compounds are scarcely investigated at this stage in the field. For a selected set of organic semiconductors, the study of the bulk and surface polymorphism has been completed allowing also the isolation of several single crystals. Crystalline structure determination has been achieved by single crystal and powder diffraction measurements. The thermodynamic and kinetic stability of different polymorphs have been studied both for bulk material than for thin films.

Deposition and characterisation with different techniques have been also considered to evaluate the quality and properties of the obtained crystal forms. With state-of-the-art spectroscopic methods like time-resolved sum frequency generation and optical pump THz probe spectroscopy, dynamics on picosecond timescales of charge-transport in materials varying from polymers to aqueous solution has been studied. It could be concluded that in polymer films electron-phonon scattering plays an important role. We have to date investigated and optimised OFET devices with several novel molecular semiconductors developed in the programme. Good device performance with high field-effect mobility and low contact resistance has been achieved for DN4T deposited by vacuum sublimation onto heated substrates. We have also developed novel deposition techniques, such as bar-assisted solution shearing, that allow the controlled deposition of blends of molecular semiconductors and insulating binder polymers from solution. Optimisation of deposition conditions has allowed the fabrication of high performance OFETs, which are now available for in-depth transport studies. 1 Ref. Ares(2021)5444653 - 03/09/2021 Significant progress has been made on achieving the technical conditions needed to study charge carrier mobility under strong coupling to the vacuum field from the mid-infrared to the THz region. In this process, it was serendipitously found that the supramolecular assembly could be significantly modified by coupling simultaneously the solute and solvent vibrations, turning gels into flakes. This provides insight into the fundamental changes induced by such coupling and will help other aspects of the project research. Fifteen talented young researchers have been hired. An individual Personal Career Development Plan (PCDP) has been established for each of them. They are continuously being trained in different interdisciplinary technical issues related to scientific objectives of the project as well as in a large variety of soft skills. The young researchers are collaborating together intensively and are presenting their results in meetings. Each partner has been actively involved in advertising open positions to recruit the young researchers, promoting the project, and participating to online events. In parallel, all ESRs have been actively committed in disseminating through papers and online events. Project media channel has been regularly updated with the ESRs social media campaign via the Twitter and LinkedIn accounts.

III. Progress beyond the state of the art, expected results until the end of the project and potential impacts

In a concerted research effort, UHMob contributes to advance the field of organic electronics by developing molecular semiconductors with improved charge transport characteristics for industrial applications. The project develops also revolutionary concepts, such as the coupling with vacuum states that is widely applicable to control structure and reactivity across chemistry. Fundamental understanding of charge transport mechanisms in organic materials, by an integrated theoretical and experimental

approach, constitutes an important achievement, too. Finally, the control of polymorphism of organic compounds, which remains an unsolved scientific problem notably for the pharmaceutical sector, is actively pursued. The largest and most noticeable societal impact of UHMob is the cross-sectorial and interdisciplinary education of 15 young scientists, through research. They will be part of the next scientific elite that Europe needs to for its administration, governments, industries, and universities.

For more information about the project, please visit the project public website www.uhmob.eu

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This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 811284.