CECAM Workshop Scientific Report – ESF/Psik

Workshop: Charge transport in organic materials

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I. Summary

Charge transport modelling of organic materials is an extremely challenging and interdisciplinary field. This is due to the wide variety of transport regimes, the crucial role played by defects, chemical environment, thermal fluctuations, mesoscopic and microscopic morphology of the material. The electronic states themselves can be delocalized (bandlike or small polaron models), strongly localized (hopping models, or big polaron) or dynamically localized by the adiabatic coupling with the nuclear structure and the surrounding environment (DNA, Liquid Crystals). Building a solid theoretical framework to describe charge transport in such materials is still a challenge, and it is of fundamental importance to support the engineering of optoelectronic devices with reliable simulation tools.

The main objective of the proposed workshop was to bring together research groups with expertise in cutting edge simulation and experimental techniques to stimulate mutual collaboration between experiment and theory, but also to encourage a critical discussion regarding the application of different methods, their precision, their computational limit and hence their ability to reproduce experimental measurements or to provide an effective support to device and material engineering.

The workshop hosted 98 participants coming from Argentina, Algeria, Australia, Austria, Belgium, Denmark, Finland, France, Germany, UK, Ireland, Italy, Saudi Arabia, Serbia, Slovakia, South Korea, Sweden, Switzerland and the USA.

The programme consisted of 32 invited talks of 40 minutes (35+5) each and one poster session presenting 44 posters. In addition, many social events (reception and conference dinner) to allow for informal exchange were held. The invited talks were given by well-established scientists from the different communities, both theoretical and experimental, which acted as platform for interesting cross-interdisciplinary discussions. The invited talks were followed by a poster session where the participants could show they scientific work and exchange of ideas with a broad knowledge in oxide chemistry/physics. The organization was very compact with the scientists accomodated in the same hotel fostering exchange and discussion between the participants also outside the meeting room.

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II. ***Scientific content, main outcome of presentations, selected discussions***

The workshop succeeded in the following objectives:

1) To define the range of application, inner limitations, advantages and eventual complementaries between different charge transport models for describing the electronic structure and the charge transport process depending on the amount of static and dynamic disorder and the localized/unlocalized nature of charge. Particular emphasis has been given to the assumptions behind the models and the class of materials/devices they're expected to successfully model.

2) To set up, share and investigate current and novel multiscale approaches combining atomistic description of the charge transfer process, classical force field dynamics, Monte Carlo and Finite Element description of the material, in order to develop methodologies towards the simulation of realistic structures, estimating and possibly including the effects of thermal fluctuations, configurational and statistical disorder.

3) To intensify the interaction between experimental and theoretical communities. Of particular interest has been exchanging knowledge about the available experimental technique for the characterization of structural, electronic and optical properties of disordered polymeric and composite structures, the typical footprints of different transport processes, the direction in research needed to optimize and engineer these novel class of materials and devices.

4) To promote the creation of international collaboration networks in order to improve the interdisciplinary approach and connect scientists coming from chemical physics, quantum chemistry, and electronic engineering communities.

Scientific advances expected for the next 4 years on which facilities

he talks and discussion during coffee breaks identified that in order to advance the field one needs

(i) to develop methods capable of assessing self-assembling properties of soluble organic semiconductors. (2,3)

(ii) to develop methods for quantitative description of electrostatic and polarization effects (0.1eV accuracy) in large-scale molecular morphologies. (3)

(iv) to develop techniques for constructing diabatic (localized) states in large and partially ordered morphologies (3,4,5).

(v) to develop charge/exciton transfer theories beyond semi-classical high-temperature limits.

Note the number meaning: 1) desktop computing, 2) departmental machines, 3) national supercomputers, 4) Current European Supercomputers (PRACE resources) 5) Leading edge peta-flop or exa-flop machines.

II. Assessment of the results and impact on future direction of the field

Assuming sufficient administrative support to be in place, has the workshop identified research areas that might be funded by the EU 2020 program ?

The workshop identified three main aspects to be related to current and future funding opportunities:

1) The topic calls for highly interdisciplinary approaches, ranging from basic theoretical physics to organic chemistry to electronic engineering. All these communities were represented by several speakers during the workshop.
2) A strong effort is devoted to efficient peta-scale numerical simulation schemes and most of the computational results shown can only be obtained on HPC systems.
3) The technology transfer process between academy, spinoff enterprises, small medium enterprises (SMEs) and large enterprises (LEs) is short, a fact proved by the participation of industrial representative from US and Europe.

All these points are well represented in the funding scope of the HORIZON2020 European Framework Program. Interdisciplinarity and involvement of SMEs calls especially for large collaborative projects. The most relevant research opportunities may include:

1) Multiscale modelling of organic electronic devices from ab-initio to mesoscopic simulation. This is not only relevant to academy, but to SMEs active in the industrial field of scientific modelling and SMEs and LEs developing materials and devices.
2) Advances in ab-initio and QM/MM simulation of time-dependent excited states, which is more closely related to academic activity.

These concepts are relevant to the 2014-2015 HORIZON2020 calls (FETPROACT1, FETHPC1) and to two pillars (out of three) of the HORIZON2020 funding scheme: ‘emphasis on excellent science’ and ‘industrial innovation and leadership’.

May 20th 2014

The Organizers