Scientific report

"2nd TYC Conference: Charge Transfer for Energy Applications"

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1 Summary

Charge transfer underlies the function of many devices ranging from transistors to light-emitting diodes, and from solar to biofuel cells. It is often the limiting factor for the performance of these devices. As such it is absolutely vital to understand the mechanism, thermodynamics and kinetics of this important physical process on a molecular level. Although the time and length scales of the charge transfer that occurs in these devices may be rather different, the inherent dynamics may be similar and indeed be described by similar theoretical approaches. The aim of this workshop was to bring together experimentalists, theorists and computational scientists working on charge transfer within and between (i) organic semiconductors, (ii) thermo-electrics, (iii) dye-sensitised solar cell materials and (iv) semiconducting oxides.

The workshop took place from 6. to 8. June 2012 at King's College London, UK. There were 4 half-day sessions, each dedicated to one of the above topics. The program started with a reception in the evening of June 6. On the following morning the workshop was officially opened by Prof David Richards, Head of Research at King's College London, followed by the morning session on organic semiconductors and the afternoon session on thermo-electrics. A poster session and buffet was organised for the evening of 7. June. The following day started with a session on dye-sensitised solar cell materials followed by the last session on semiconducting oxides. After the award of a poster prize, Prof Mark Van Schilfgaarde of King's College, closed the workshop and gave an inspiring outlook into the future of energy research. Workshop papers by invited speakers are currently under peer-review and will be published in a special issue of the journal Phys. Chem. Chem. Phys. (RSC Publishing) prospectively in early 2013.

We were fortunate that a number of world-leading researchers followed our invitation to deliver talks of exceptional quality, among them Profs Siebbeles, Rossky, Rubio, Galli, Prezhdo, Wolf, Dupuis and Nitzan. We also gave researchers on a more junior-level the opportunity to present results in form of a contributed talk. The quality of these talks was generally very high, which we explain by the large number of applications that we have received and the possibility to select from excellent abstracts. Participants that were not selected for a talk had the opportunity to present a poster. There were 17 invited talks and 9 contributed talks (3 female and 23 male speakers from 9 European countries and the US) as well as 48 poster presentations.

The event certainly fostered the dialogue and, as we hope, also the collaboration between experimentalists and theorists on the particularly relevant topic of charge transfer in energy materials, at a time where energy research is more important than ever. Several key issues for future developments were identified in each of the four sub-themes, for instance the need to go beyond hopping models in organic semi-conducting materials, to develop density functionals that go beyond the adiabatic approximation for the description of photo-induced processes and the need to modify existing models for charge transfer in metal-oxide materials. With 124 participants from 13 European countries, the US and Japan attending, this workshop was a successful event that met the objectives set out in our proposal.

2 Scientific Content and Discussions

Organic semiconductors. Prof. Siebbeles presented a talk entitled *Photogeneration and mobility of charges in photovoltaic materials based on conjugated polymers and covalent organic frameworks*. He reported on the mechanism of charge carrier photogeneration in blend films of the polymer P3HT and the electron accepting fullerene PCBM by ultrafast optical and terahertz spectroscopy. Photoexcitation led to direct formation of free mobile electrons and holes with a yield that was independent on temperature. This implied that the Onsager-Braun model with an initial electron-hole distance of the order of nanometers was inadequate. This was attributed to charge delocalization causing the electron-hole Coulomb attraction to be negligible. Prof. Siebbeles also presented results on a new class of materials with great promise for application in organic opto-electronics consists of Covalent Organic Frameworks (COFs). He studied the dynamics of excitons and charges within COFs consisting of phthalocyanine units that are strongly coupled by pi-pi stacking in an eclipsed configuration. The charge mobility was virtually independent on temperature, which is typical for a band-like mechanism of charge motion, in contrast to hopping via localized states. According to quantum mechanical simulations, eclipsed stacking of the phthalocyanine units can lead to a high charge mobility of 100 cm^2/Vs, which largely exceeds that for conventional organic semiconductors.

Prof. Troisi presented a talk entitled *Charge separation and recombination in organic photovoltaics interfaces*. The electronic and geometric structure of the prototypical polymer:fullerene interface (P3HT:PCBM) was investigated theoretically using a combination of classical and quantum simulation methods. It is shown that the electronic structure of P3HT in contact with PCBM is significantly altered compared to bulk P3HT. Due to the additional free volume of the interface, P3HT chains close to PCBM are more disordered and, consequently, they are characterized by an increased band gap. Excitons and holes are therefore repelled by the interface. This provides a possible explanation of the low recombination efficiency and supports the direct formation of quasi-free charge separated species at the interface. Prof. Troisi discussed how and when a combination of computational and theoretical models can truly contribute to organic electronics and he provided a few examples of genuine material properties predictions based on computational chemistry methods.

Dr. Dabo presented a talk entitled *Electronic structure of organic photovoltaic compounds from first principles*. In his presentation, he demonstrated that orbital dependent DFT (OD-DFT) based upon Koopmans condition1 is apt at describing donor and acceptor levels within 0.1-0.4 eV and 0.2-0.6 eV relative to experiment, which is comparable to the predictive performance of many-body perturbation theory methods. Furthermore, Koopmans-compliant dielectric responses for semiconducting polymers were predicted in close agreement with more expensive wave-function methods. This level of predictive performance allows the physically accurate and computationally tractable electronic-structure description of photoactive donor-acceptor materials from first principles.

Prof. Rossky presented a talk entitled *Exciton and charge transfer dynamics at organic material interfaces*. In his talk Prof Rossky described recent progress in using a mixed quantum/classical non-adiabatic molecular dynamics simulation approach for simulation of exciton and charge transfer in organics employing an all-atom description of the intermolecular interactions coupled with a semi-empirical (PPP) electronic Hamiltonian. Results exploring several systems at ambient temperature were discussed. These systems included phenylene-vinylene and thiophene oligomers, as well as cyanine and fullerene components. The roles of molecular structural fluctuations and intermolecular electronic couplings, as well as the roles of donor and acceptor excited state alignments and of intrinisic interfacial fields was discussed.

Dr. Oberhofer presented a talk entitled *Simulating charge carrier mobilities in n-type semiconducting organic solar cell components*. In his contribution he briefly discussed a density functional theory based techniques for estimatation of electron mobilities from computer simulations. He presented applications to C60 and modified fullerene crystals and concluded that the results can represent a starting point for a microscopic understanding of structure-mobility relationships in these important materials.

Prof. Cornil presented a talk entitled *Theoretical Modelling of the Key Electronic Processes in Organic Solar Cells*. He illustrated that theoretical modelling at the atomistic scale can prove very useful to under-

stand and optimize key electronic processes governing the operation of organic solar cells. Quantum-chemical calculations were exploited to tailor the optical properties of the materials in order to optimize the absorption of the solar light and to describe the parameters controlling energy transfer processes in supramolecular architectures, excitation dissociation into charge carriers, and charge transport properties. Monte-Carlo simulations were then used to propagate excitations and charges in supramolecular architectures on the basis of the parameters obtained at the quantum-chemical level and estimate exciton diffusion range and charge mobility, respectively.

Prof. Cacialli presented a talk entitle *Threaded molecular wires as model conjugated polymers with controlled interstrand interactions*. In this experimental contribution, Prof Cacialli reported on threaded molecular wires made with conjugated-polymers-based polyrotaxanes, which offer an example of a bottom-up approach to electroluminescent nanostructures. Such a supramolecular approach preserves the fundamental semiconducting properties of the conjugated wires, and is effective at both increasing the photoluminescence efficiency and blue-shifting the emission of the conjugated cores, in the solid state, while still allowing charge-transport and thus electroluminescence (EL). He showed that control of the threading ratio was possible, thereby resulting in fine tuning of the excitonic vs. aggregate contribution to the luminescence, as well as of the electro- and photo-luminescence efficiency.

Thermo-electrics. Prof. Galli presented a talk entitled *Atomistic simulations of thermal transport in nanostructured semiconductors*. She presented the results of atomistic simulations of heat transport in realistic models of ordered and disordered semiconductors. Specifically, the thermal properties of Si and SiGe at the nanoscale (nano-wires and nanoporous films) were discussed, as obtained from molecular dynamics simulations and Boltzmann transport equation calculations. Prof Galli also discussed recent results on disordered systems, including amorphous Si and SiO_2.

Dr. Cuenat presented a talk entitled *Nanoscale thermoelectric metrology: model requirement for accurate measurements*. In his contribution Dr. Cuenet presented his latest efforts to validate the metrology tools required to measure the distribution of local Seebeck coefficients in thermoelectric materials accurately enough to enable the integration of these new materials into commercial devices. A generalized driftdiffusion equation in the relaxation-time approximation was presented and numerically solved. Based on this model, he discussed how local measurement can reduce uncertainty in bulk measurements. He concluded by discussing further modelling requirements to enable the faster development of new improved thermoelectric materials based on energy-filtering.

Prof. D'Agosta presented a talk entitled *A dynamical approach to thermoelectric energy conversion*. In his talk, Prof D'Agosta presented a novel way for a direct evaluation of the Seebeck coefficient for thermoelectric energy conversion, without reverting to any approximation. He casted the theory in the framework of time-dependent dynamics, which in principle allows also for the calculation of the electrical and thermal conductance of the electrons. He discussed a possible extension for the calculation of the vibrational thermal contribution to show how one can build a complete theoretical and numerical approach to the investigation of thermoelectric energy conversion.

Prof. Sotomajor presented a talk entitled *Thermal conductivity in thin Silicon membranes: electrons and confined phonons contributions*. Thermal transport in Si nanowires (minimum width 100 nm) were studied experimentally as well as light scattering in Silicon-on-Insulator membranes (minimum thickness 8 nm) in order to: (a) ascertain the validity limits of the Wiedemans-Franz law and (b) determine the contribution of confined acoustic phonons to the thermal conductivity. It was found that already at feature size of 500 nm there is a decrease in the effective thermal conductivity, which dramatically depends on shape, interfaces, frequency and temperature.

Dr Madsen presented a talk entitled *Datamining High-Throughput DFT calculations in the search for new thermoelectric materials*. He introduced his talk by saying that new thermoelectric materials can be discovered by screening known structures for favourable thermoelectric properties by ab initio methods. However, there remain big challenges in discovering unknown phases computationally. Based on the data produced by the newly developed high throughput environment , and using the Ca-Zn-Mg-Si system as an example he showed how data-mining techniques can be used to predict the stabilities of unknown compounds.

Furthermore, he discussed how the correlations can be interpreted in terms of simplified models of the electronic structure, thereby leading to new insights into the chemistry of the system.

Dr Mathur presented a talk entitled *Electrocaloric cooling*. In his introduction Dr Mathur explained that a ferroelectric can be driven hot and cold by applying and removing a voltage near the Curie temperature. These electrocaloric effects are large in thin films, hence multilayer capacitor geometries have been proposed for cooling applications. In his talk he discussed recent progress in this area.

Dye-sensitised solar cell materials. Prof. Hupp presented a talk entitled *Interfaces and Architectures for Efficient Light-to-Electrical Energy Conversion with Dye-Sensitized Solar Cells*. His talk focused on: a) understanding what limits the efficiency of dye-sensitized solar cells, and b) illustrating how nanostructured molecular-dye architectures and semiconductor-electrode architectures, together with interface tailoring, might be used to circumvent these limits. The presentation drew upon recent studies that have utilized atomic-layer deposition (ALD) and related techniques to modify and define interfaces in a highly spatially resolved fashion. He also described the results of studies that have focused on boosting light-harvesting and subsequent charge collection and photocurrent production, without sacrificing photovoltage.

Dr. Tavernelli presented a talk entitled *Ab-initio methods in molecular design of dye-sensitized solar cells*. In his contribution, Dr Tavernelli discussed some such new theoretical developments for the design of novel organometallic dyes used in Graetzel-type solar cells. These were based on chemical modifications subjected to an appropriate selective pressure (in an evolutionary algorithm sense) or, to deterministic forces computed within TDDFT.

Dr Lamberti presented a talk entitled *High electron lifetime in transparent TiO_2 nanotubes-based photoanode for front-illuminated dye-sensitized solar cell*. The fabrication and characterization of non-curling, free-standing TiO2 nanotubes (nts) membranes and their integration in front-side illuminated dye-sensitized solar cells (DSCs) were reported. Dye loading on the metal-oxide surface was analyzed with UV-Vis spectroscopy, and the dependence of the cell efficiency on nts thickness and dye incubation time was studied by I-V electrical characterization, incident-photon-to-electron conversion efficiency and impedance spectroscopy measurements under AM 1.5 illumination. Compared to the standard nanoparticle-based DSCs, the TiO_2 nts-based devices showed an marked increase in electrons lifetime, yielding an overall power conversion efficiency up to 8.2%.

Prof Rubio presented a talk entitled *TDDFT for light-matter interactions in strong coupling regimes*. In this talk he addressed the problems and open questions related to the description of light-matter interaction with the goal of providing a sound description of laser-induced-population processes within TDDFT. He presented a description for dynamical induced charge transfer processes and many body tunneling and he showed recent advances in deriving a new memory-dependent functional. He emphasised that the description of photo-induced processes in chemistry, physics, and biology and the new field of attosecond electron dynamics and high-intense lasers all demand fundamental functional developments going beyond the adiabatic approximation.

Dr. Patrick presented a talk entitled *First-principles photoemission spectra of molecular photovoltaic interfaces*. He presented calculations of core and valence photoemission spectra of semiconductor/sensitizer interfaces and emphasised that determining the quasiparticle properties of these large interfaces represents a considerable computational challenge. He described a methodology, based on density-functional theory and post-DFT techniques, and showed that careful consideration of a wide range of physical effects is essential to understanding experimentally measured data.

Prof Prezhdo presented a talk entitled *Electron and energy transfer dynamics at TiO2 interfaces: Time-domain ab initio studies*. The talk focused on photoinitiated charge transfer at the interfaces of bulk TiO_2 with a variety of systems, including organic molecules, water, semiconductor quantum dots (QDs), and graphene using state-of-the-art non-adiabatic molecular dynamics techniques, implemented within time-dependent density functional theory. He gave evidence that his simulations provide a unifying description of quantum dynamics on nanoscale, resolved highly debated issues, and generated theoretical guidelines for development of novel systems for energy harvesting.

Semiconducting oxides. Dr Bersuker presented a talk entitled *Charge transfer to/from oxides: Roles*

of interfaces. In his presentation, Dr Bersuker focused on analyzing oxide structural features responsible for the charge transfer by combining a variety of electrical measurement techniques with high time and spatial resolution that allows capturing fast transient charging processes and differentiating signals from different regions through the depth of the multi-layer stack. These data were used to fit the results of modeling of the physical processes underlying the electrical measurements to extract spatial and energy profiles of electrically active centers. The extracted characteristics were then compared to the atomic-level material modeling data to identify atomic and energy characteristics of the material responsible for the electrical properties.

Dr McKenna presented a talk entitled *First principles modelling of electron transfer between point defects in MgO*. He summarised some of his recent work on modelling electron transfer between oxygen vacancy defects in MgO using first principles techniques. He showed that the rate of electron transfer between defects depends on both their separation and crystallographic orientation. He also predicted that as the separation between defects is increased, there is a crossover between delocalisation of electrons across defects, and activated transfer of localised electrons between defects, which occurs for defect separations in the range 7-10 . He concluded that these predictions have important consequences for modelling electron transport in wide-gap oxide materials, e.g. for simulating stress induced leakage current in metal oxide field effect transistors.

Prof. Wolf presented a talk entitled *Ultrafast Dynamics of Interfacial Electron Transfer*. He employed surface science techniques combined with time-resolved two-photon-photoemission (2PPE) spectroscopy to study the ultrafast dynamics of interfacial electron transfer at several hybrid interfaces: (1) Amorphous D_2O or NH_3 ice layers on a Cu(11) substrate were used as a model system to study in detail the ultrafast dynamics of electron injection, localization and solvation in the polar adlayer as well as charge transfer back to the metal substrate. In further experiments (2) he employed 2PPE spectroscopy to investigate the occupied and unoccupied electronic structure and the electron dynamics at the pyridine/ZnO(10-10) interface as an example for a hybrid system of inorganic and organic semiconductors.

Dr Pesci presented a talk entitled *Photocatalysis on metal oxide semiconductor electrodes*. He reported on transient absorption spectroscopy and electrochemical studies on photo-electrode materials such as WO_3, which provide insights into the dynamics of the charge carriers on WO_3. He was able to identify timescales of key processes and to provide important mechanistic insight into this widely studied material. Initial transient experiments that investigate the charge carriers dynamics on TiO_2 and Cu_2O were also reported.

Prof Dupuis presented a talk entitled *First Principles Approach to Polaron Transport in the Solid State*. In his presentation Prof Dupuis reviewed the computational characterization of polaron transport in the solid state using the Marcus/Holstein model and first-principles calculations. He discussed ideas to extend the modelling to the mesoscale with a multi-state empirical polaron model.

Dr. Botti presented a talk entitled *Electronic excitations in Cu-based materials for thin-film solar cells*. She discussed the type of theoretical approaches that allows one to gain insight into electronic excitations in materials for photovoltaics as well as their reliability and computational cost. She presented an example for an application in material design, that is presently a new frontier in the field of theoretical material science. Using the minima hopping method, she found and characterized new low-enthalpy phases of silicon with almost-direct band gaps and displaying strong absorption in the visible.

Prof Nitzan presented a talk entitled *Redox molecular junctions: Properties and functionalities*. The concept of redox molecular junctions was introducded. They are molecular conduction junctions that involve more than one oxidation state of the molecular bridge. This property was derived from the ability of the molecule to transiently localize transmitting electrons. He discussed the implications of this property in a system open to electron flux and their manifestations with regards to the nonlinear transport properties of such junctions.

3 Assessment of results and future directions

A range of different techniques was presented to investigate charge and exciton transfer in organics such as conjugated polymers or fullerene derivatives. They ranged from orbital dependent DFT methods focussing on the more fundamental problems such as electron self-interaction, to QM/MM methods with more approximate electronic Hamiltonians but including finite temperature effects of the environment, to Monte-Carlo and mesoscopic techniques which allows one to compute electron mobilities that can be compared to experiment. An important issue that still seems to be highly controversial is the nature of the excess charge in organic materials such as conjugated polymers and fullerenes, specifically its localisation length is unclear, as well as the transport mechanism of this charge. The latter is usually described by either band like conduction or thermally activated hopping. None of these limiting cases seems to provide a fully satisfactory description. The band-like mechanism relies on Bloch states and breaks down for higher temperatures where the mean free path becomes comparable to the intermolecular lattice spacing, whereas polaronic hopping seems to be incompatible with the absence of activated charge mobility in pure molecular crystals. In the past charge transport in organic semiconducting materials has often been described by charge hopping using Marcus or related electron transfer theories. However, in one contribution on fullerene materials it was clearly shown that the small polaron does not exist for a significant fraction of molecular orientations of the molecules constituting this material. Thus, a treatment that goes beyond the usual rate-based description is required for these materials. First developments in this direction on the level of idealised model Hamiltonians have been presented as well as direct dynamical methods such as non-adiabatic molecular dynamics simulation. This is clearly the way to go. We have seen first applications of such schemes even though with rather approximate electronic Hamiltonians. One of the main challenges for the future is to make these simulations more quantitative, e.g. by using better electronic Hamiltonians, using more rigorous non-adiabatic formalisms, and including nuclear tunnelling. One important aspect is also to work together with experimentalists to establish simulation protocols that allow for the calculation of observables that are accessible to experimental measurement.

The investigation of thermoelectric energy conversion summarises some of the problems we have seen discussed in the workshop. For the determination of the figure of merit - a way to quantify the maximum efficiency of the device - reliable information on the thermal and electronic transport of both the electrons and the atoms is mandatory. One key factor that enters into play is the thermal conductivity of the atoms. The common technique in this field is the molecular dynamics simulation and the Boltzmann Transport equation. Although, the first technique provides more reliable results and is less subject to approximations, the Boltzmann Transport equation might provide a predictive framework helping in designing novel thermoelectric devices. At the same time, a better treatment beyond the linear response theory of the electronic contribution is needed. Treating the electrons and the atoms on an equal footing seems the way to go for a full understanding of the thermoelectric energy conversion. From the experimental point of view, the measurement of the efficiency of thermoelectric materials is subjected to a large uncertainty. This is due to the complexity of fabricating devices, the measurement uncertainty and materials complications. For example, the Seebeck coefficient is currently measured at the macro-scale and induces in some case an uncertainty of up to 50% on the figure of merit measurement. As also has been pointed out in other experimental talks, the characterisation of these materials relies on the quality of the theoretical modeling. Improvements in this direction will not only provide efficient tools to search for the most apt materials, like improving the datamining/database available at the moment, given some requested properties, but will also help in understanding the admittedly scattered experimental results. We have witnessed a sincere interest from the experimental and theoretical communities in deepening their connection in the attempt to overcome the problems that are at the moment hindering the research in this field. This constitutes a novel direction: from this point of view we believe this workshop has been quite successful.

The problem of electronic excitations has been treated on several levels, ranging from simple Hueckel-type Hamiltonians in conjugated polymers, to time-dependent density functional theory (TDDFT) in the linear-response approximation to TDDFT descriptions in the nonlinear regime amenable to describe the interaction

with a strong laser field. It was shown that TDDFT offers a valuable framework for the calculation and the tuning of the spectroscopic properties of large molecular systems made of more than hundred atoms. Thanks to the recent advances in DFT/TDDFT functional design, a more accurate and reliable description of charge separated excited states (charge transfer excitations, and excitons) became recently available. This possibility opened new avenues in the field of ab-initio assisted molecular design, especially in the development of improved molecular dyes for solar cell devices. Particularly impressive was the ab-initio based design approach aiming to create a new dye that shows a broader absorption spectrum than conventional dyes. This was done in a rational way by suggesting substituents that would deform the molecule along the non-adiabatic coupling vectors computed using TDDFT. Future challenges are the development of functionals with minimal self-interaction error to permit more reliable predictions of charge transfer excited states as well as the inclusion of nuclear quantum effects in excited state molecular dynamics, which are particularly important at conical intersections. Another fundamental challenge that was highlighted is the development of functionals that go beyond the adiabatic approximation, as required for an improved description of photo-induced processes in chemistry, physics, and biology and the new field of attosecond electron dynamics in high-intense lasers fields.

We have seen that charge transfer in metal-oxide materials plays a critical role in an increasing number of technological applications in areas such as nanoelectronics, energy generation and photocatalysis. For example, electron transfer through point defects in thin metaloxide films gives rise to leakage currents in transistors which degrade the performance and reliability of devices. It is extremely challenging to probe ET in oxides experimentally. For this reason, first principles calculations can be invaluable, both to provide atomistic insights and for predictive modeling of materials. Present contributions relied mainly on hopping models with the relevant parameters obtained from density function theory based calculations. Successful applications to small polaron diffusion in TiO_2 were presented and validated by comparing to experimental rate measurements. Notably, first calculations for long range ET between oxygen vacancy defects in MgO were presented using constrained density functional theory. A key finding of this study was that there is a crossover between activated hopping and activationless, coherent electron transfer at a certain critical defect separation, suggesting that traditional models for charge transfer in these materials need modification. The qualitative picture established for MgO should be transferable to similar defects in other wide-gap oxide materials, such as HfO_2 or Al_2O_3, which needs to be investigated in future work. Future challenges include the quantitative modelling of charge transport in amorphous oxide materials, at grain boundaries and between oxide/oxide and metal/oxide interfaces. To accomplish this challenges it is necessary to develop methods that allow for the treatment of larger unit cells while maintaining a good level of the electron structure description (on the level of hybrid functionals) as well as the development of methods capable of simultaneously describing the delocalized charge carrier in the metal and the more localised carriers in the oxide material.

4 Annexes

4.1 Programme of meeting and list of speakers

Thursday June 7

9:00-9:05 Welcome

9:05-9:15 **Opening Address - Professor David Richards, Head of Research, King's College London**

Session 1: CT in organic semiconducting materials
Chair - Dr Feliciano Giustino, University of Oxford

9:15-9:45 **Professor Laurens Siebbeles,** Technical University Delft, The Netherlands
Photogeneration and mobility of charges in photovoltaic materials based on conjugated polymers and covalent organic frameworks

9:45-10:15 **Professor Alessandro Troisi,** University of Warwick, UK
Charge separation and recombination in organic photovoltaics interfaces

10:15-10:35 **Dr Ismaila Dabo,** Université Paris-Est, CERMICS, France (Contributed talk)
Electronic structure of organic photovoltaic compounds from first principles

10:35-11:05 Coffee Break

Chair – Professor Nikos Doltsinis, King's College London and University of Muenster

11:05-11:35 **Professor Peter Rossky,** University of Texas at Austin, USA
Exciton and charge transfer dynamics at organic material interfaces

11:35-11:55 **Dr Harald Oberhofer,** TU Munich, Germany (Contributed talk)
Simulating charge carrier mobilities in n-type semiconducting organic solar cell materials

11:55-12:25 **Professor Jerome Cornil,** University of Mons, Belgium
Theoretical Modelling of the Key Electronic Processes in Organic Solar Cells

12:25 -12:55 **Professor Franco Cacialli,** University College London, UK
Threaded molecular wires as model conjugated polymers with controlled interstrand interactions

12:55-15:00 Lunch and program committee meeting

Session 2: CT in thermoelectrics

Chair – Dr. Nicola Bonini, King's College London

15:00-15:30 **Professor Giulia Galli,** University of California at Davies, USA
Atomistic simulations of thermal transport in nanostructured semiconductors

15:30-15:50 **Dr Alexandre Cuenat**, NPL, UK (Contributed talk)
Nanoscale thermoelectric metrology: model requirement for accurate measurements

15:50-16:20 **Professor Roberto D'Agosta,** Universidad del Pais Vasco, Spain
A dynamical approach to thermoelectric energy conversion

16:20-16:50 Coffee Break

Chair – Dr. Arash Mostofi, Imperial College London

16:50-17:20 **Professor Clivia Sotomayor,** CIN Barcelona, Spain
Thermal conductivity in thin Silicon membranes: electrons and confined phonons contributions

17:20-17:40 **Dr Georg Madsen,** Ruhr-Universität Bochum, Germany (Contributed talk)
Datamining high-throughput DFT calculations in the search for new thermoelectric materials

17:40-18:10 **Dr Neil Mathur,** University of Cambridge, UK
Electrocaloric cooling

18:10-20:00 Poster session, buffet, poster prize selection

Session 3: CT in dye-sensitised solar cell materials

Chair – Dr. Martijn Zwijnenburg, UCL

9:00-9:30 **Professor Joseph Hupp,** Northwestern University, USA
Interfaces and Architectures for Efficient Light-to-Electrical Energy Conversion with Dye-Sensitized Solar Cells

9:30-10:00 **Dr Ivano Tavernelli,** Ecole Polytechnique Federale de Lausanne, Switzerland
Ab-initio methods in molecular design of dye-sensitized solar cells

10:00-10:20 **Andrea Lamberti,** Istituto Italiano di Tecnologia (IIT) (Contributed talk)
High electron lifetime in transparent TiO2 nanotubes-based photoanode for front-illuminated dye-sensitized solar cell

10:20-10:50 Coffee Break

Chair – Professor Michiel Sprik, University of Cambridge

10:50-11:20 **Professor Angel Rubio,** Universidad del Pais Vasco, Spain
TDDFT for light-matter interactions in strong coupling regimes

11:20-11:40 **Christopher Patrick,** University of Oxford, UK (Contributed talk)
First-principles photoemission spectra of molecular photovoltaic interfaces

11:40-12:10 **Professor Oleg Prezhdo,** University of Rochester, USA
Electron and energy transfer dynamics at TiO2 interfaces: Time-domain ab initio studies

12:10-13:10 Lunch Break

Session 4: CT in the solid state and in molecular junctions

Chair – Professor Mike Gillan, UCL

13:10-13:40 **Dr Gennadi Bersuker**, Sematech, USA
Charge transfer to/from oxides: Role of interfaces

13:40-14:00 **Dr Keith McKenna,** University of York, UK
First principles modelling of electron transfer between point defects in MgO

14:00-14:30 **Professor Martin Wolf,** Fritz-Haber Institute Berlin, Germany
Ultrafast Dynamics of Interfacial Electron Transfer

14:30-14:50 **Federico Pesci,** Imperial College London, UK (Contributed talk)
Photocatalysis on metal oxide semiconductor electrodes

14:50-15:20 Coffee Break

Chair – Professor Adrian Sutton, Imperial College London

15:20-15:50 **Professor Michel Dupuis,** Pacific Northwest National Laboratory, USA
First Principles Approach to Polaron Transport in the Solid State

15:50-16:10 **Dr Silvana Botti**, Ecole Polytechnique, France (Contributed talk)
Electronic excitations in Cu-based materials for thin-film solar cells

16:10-16:40 **Professor Abraham Nitzan,** University of Tel-Aviv, Israel
Redox molecular junctions: Properties and functionalities

16:40-16:45 Poster prize

16:45-17:00 **Closing remarks – Professor Mark Van Schilfgaarde, King's College London**

4.2 Full list of participants

Status*	Title**	Firstname	Surname	Nationality	Gender	Organisation
Participant	Mr.	Jawad	Alsaei	Bahrain	M	Imperial College London
Participant	Dr.	Francesco	Ambrosio	Italian	M	University of Warwick
Participant	Dr.	Jeffrey	Armstrong	British	M	Imperial College London
Convenor	Dr.	Francesca	Baletto	Italian	F	King's College London
Participant	Dr.	Wichard	Beenken	German	M	Ilmenau University of Technology
Participant	Mr.	Enrico	Berardo	Italian	M	UCL
Participant	Mr.	Daniel	Berger	German	M	TU Munich
Speaker	Dr.	Gennadi	Bersuker	American	M	SEMATECH
Participant	Mr.	Robert	Biele	German	M	Nano-bio Spectroscopy Group
Convenor	Dr.	Jochen	Blumberger	Austrian	M	UCL
Participant	Dr.	Nicola	Bonini	Italian	M	King's College London
Participant	Mr.	Dominic	Botten	British	M	King's College London
Participant	Dr.	Silvana	Botti	Italian	F	LPMCN, CNRS-University Lyon 1
Participant	Mr.	Samuel	Bradley	British	M	UCL
Participant	Mr.	Marian	Breuer	German	M	UCL
Participant	Mr.	Edward	Burke	American	M	US Army International Technology Center
Speaker	Prof.	Franco	Cacialli	Italian	M	UCL
Participant	Prof.	Markys	Cain	British	M	NPL
Participant	Miss	Clair	Chew	Malaysian	F	UCL
Speaker	Prof.	Jerome	Cornill	Belgium	M	University of Mons
Participant	Dr.	Tatiana	Correia	Portuguese	F	NPL
Participant	Mr.	Niccolo	Corsini	Italian	M	Imperial college London
Participant	Mr.	Stephen	Cox	British	M	UCL
Participant	Dr.	Ismaila	Dabo	French	M	CERMICS, Universite Paris-Est
Speaker	Prof	Roberto	D'Agosta	Italian	M	Nano-bio Spectroscopy Group
Participant	Mr.	Szymon	Daraszewicz	British	M	UCL
Participant	Mr.	Erlend	Davidson	British	M	UCL
Participant	Mr.	Peter	Davies	British	M	Imperial College London
Participant	Prof.	Alessandro	De Vita	Italian	M	King's College London
Participant	Dr.	Ivan	Duchemin	French	M	CEA
Speaker	Dr.	Michel	Dupuis	American	M	Pacific Northwest National Laboratory
Participant	Mr.	Al-Moatasem	El-Sayed	British	M	UCL
Participant	Prof.	Matthew	Foulkes	British	M	Imperial College London
Participant	Ms.	Fruzsina	Gajdos	Hungarian	F	UCL
Speaker	Prof.	Giulia	Galli	Italian	F	University of California, Davis
Participant	Mr.	David	Gao	British	M	UCL
Participant	Prof.	Michael	Gillan	British	M	UCL
Participant	Dr.	Feliciano	Giustino	Italian	M	University of Oxford
Participant	Dr.	Wolfgang	Gös	Austrian	M	TU Vienna
Participant	Miss	Gabriella	Graziano	Italian	F	UCL
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