E-MRS SPRING MEETING 2014

May 26th-30th - Lille Congress Center, France

CALL FOR PAPERS

Deadline for abstract submission: January 16th, 2014

Including Bilateral Energy Conference

E-MRS

MRS MATERIALS RESEARCH SOCIETY

Advancing materials. Improving the quality of life.

Symposium O:
Computational modelling of organic semiconductors: from the quantum world to actual devices

Modelling organic semiconductors plays a crucial role for advancing organic electronics. By now the used methods have become exceedingly divers, which calls for a platform where scientists from the various involved areas can discuss their findings and link their expertise in hither to unexplored ways.

Scope:
Using various types of advanced simulation approaches, tremendous insight into the properties of organic semiconductor materials and their application in devices has been generated. The great variety of the encountered problems requires the use of a very diverse pool of techniques ranging from highly-correlated quantum-chemistry approaches and band structure calculations (in many cases including many-body corrections) to more macroscopic techniques including molecular dynamics, coarse-grained, or micro-electrostatic modelling. For understanding the dynamics of charges and excitons or to analyze the formation of heterogeneous phases, statistical approaches including Monte-Carlo techniques are typically applied and, for understanding devices at their full level of complexity, drift-diffusion based calculations become necessary.
Recently, there has been a strong drive to combine these approaches in a hierarchical fashion, e.g., to use the results of molecular-dynamics modelling on complex structures as input for the quantum-mechanical simulation of electronic or optical properties. Beyond that, first attempts to establish tightly integrated multi-scale schemes are under way.
As a consequence, involved scientists typically have very diverse scientific backgrounds. This calls for the establishment of a platform for exchanging ideas, recent insights, and also the knowledge on specific computational tools. To aid in that, this symposium
(i) aims at providing an as comprehensive as possible overview of the strengths and limitations of modelling approaches used for describing organic semiconductors including the latest directly relevant methodological developments;
(ii) it will portray recent efforts in hierarchical and truly multi-scale modelling of these materials; and
(iii) above all, the symposium will provide a possibility for showcasing the insight into the intrinsic processes in organic semiconductors and devices that can be gained from computational studies.

Hot topics to be covered by the symposium:
spanning the length-scales:

- highly-correlated quantum-chemical and post density-functional theory methods
- quantum-mechanical techniques used for simulating complex structures
- molecular dynamics and coarse-graining applied to disordered and heterogeneous structures
- Monte Carlo techniques for simulating dynamics and growth
- simulation of device-structures at their full level of complexity by drift-diffusion based approaches
- hierarchical combination of simulations at multiple length-scales and true multi-scale modelling

phenomena in the focus of interest include (but are not limited to):

- understanding (charge-transfer) exciton formation/dissociation at hetero-interfaces
- modelling carrier injection/abstraction at electrodes
- quantifying the impact of disorder
- simulating dynamic processes from fs to minutes
- applying multi-scale approaches to charge-transport and exciton diffusion
- modelling film growth and phase dynamics
- understanding the impact of film heterogeneities on device performance

Proceedings:
Invited speakers will be asked to submit feature articles as contributions to a special issue of ***Advanced Functional Materials***. These will, naturally, be subject to strict peer reviewing.

Members of scientific committee (confirmed):

- Jean-Marie André, University of Namur, Belgium
- Jean-Luc Brédas, Georgia Institute of Technology, Atlanta, USA
- Gian Paolo Brivio, Universitá di Milano-Bicocca, Milano, Italy
- Paulette Clancy, Cornell University, Ithaca, USA
- Jerome Cornil, University of Mons, Belgium
- Claudia Draxl, Humboldt-Universität zu Berlin, Germany
- Dago de Leeuw, Max Planck Institute for Polymer Research, Mainz, Germany
- Elisa Molinari, CNRNano, Modena, Italy
- Mark Ratner, Northwestern University, Evanston, USA
- Zhigang Shuai, Tsinghua University, PR China
- Nobuo Ueno, Chiba University, Chiba, Japan

Invited speakers (confirmed):

- Denis Andrienko, Max Planck Institute for Polymer Research, Germany
- David Beljonne, Université de Mons, Belgium
- Clemence Corminboeuf, EPFL Lausanne, Switzerland
- Reinder Coehoorn, Philips Research Laboratories, The Netherlands
- Gianaurelio Cuniberti, TU Dresden, Germany
- Kristen A. Fichthorn, Penn State University, USA
- Geoffrey Hutchison, University of Pittsburgh, USA
- Hiroyuki Ishii, University of Tsukuba, Japan
- Jan Anton Koster, Rijksuniversiteit Groningen, The Netherlands
- Lingyi Meng, Xiamen University, PR China
- Jeff B. Neaton, Lawrence Berkeley National Lab, USA
- Chad Risko, Georgia Institute of Technology, USA
- Alice Ruini, Università degli Studi di Modena e Reggio Emilia, Italy
- Alexander L. Shluger, University College London, Great Britain
- Zoltán G. Soos, Princeton University, USA
- Alexandre Tkatchenko, Fritz Haber Institute of the Max Planck Society, Germany
- Claudio Zannoni, Universitá di Bologna, Italy

Symposium organizers:

Egbert Zojer
Institute of Solid State Physics
Graz University of Technology
Petersgasse 16
8010 Graz
Austria
Phone: +43 316 873 8475
egbert.zojer@tugraz.at

Leeor Kronik
Department of Materials and Interfaces
Weizmann Institute of Science
Rehovoth 76100
Israel
Phone: +972 8 9344993
leeor.kronik@weizmann.ac.il

Georg Heimel
Institut für Physik,
Humboldt-Universität zu Berlin
Brook-Taylor-Straße 6
12489 Berlin
Germany
Phone: +49 30 2093 7537
georg.heimel@physik.hu-berlin.de

Deadline for abstract submission: January 16, 2014

E-MRS 2014, May 26 - 30 – Grand Palais, Lille, France