

Welcome

The lifetime, reliability, and efficiency of organic light emitting diodes (OLED) are critical factors precluding a number of novel devices from entering the market. Yet, these stability issues of OLEDs are poorly understood due to their notorious complexity, since multiple degradation and failure channels are possible at different length- and timescales. Current experimental and theoretical models of OLED stability are, to a large extent, empirical. They do not include information about the molecular and meso-scales, which prevents their integration into the workflow of the industrial R&D compound design. It is the idea of this project to integrate various levels of theoretical materials characterization into a single software package, to streamline the research workflows in order for the calculations to be truly usable by materials engineers, complementary to experimental measurements. Towards this goal, this project brings together the academic and industrial expertise of the leading experimental and theoretical groups in the field of organic semiconductors.

Denis Andrienko

MOSTOPHOS Project Coordinator

Max Planck Institute for Polymer Research

Project Partners

■ Max Planck Institute For Polymer Research, Mainz



The current work of the group headed by Dr. Denis Andrienko is focused on three main topics: (i) enhanced sampling of soft matter systems, or systematic coarse-graining, (ii) charge and energy transport in organic semiconductors, and (iii) rational compound design for photovoltaic applications. All developed methods are implemented in an open-source software package, namely Versatile Object-oriented Toolkit for Coarse-graining and charge transport applications (VOTCA, www.votca.org). The purpose of the VOTCA-CTP toolkit is to simplify the charge transport simulations, providing a flexible platform to allow in silico prescreening of organic compounds.



■ Technische Universiteit Eindhoven



Peter Bobbert is associate professor in the group “Theory of Polymers and Soft Matter” in the Department of Applied Physics at Eindhoven University of Technology (EUT). His focus is on theoretical research into various aspects of Organic Electronics, such as the functioning of OLEDs and organic-field-effect transistors (OFETs), the opto-electronics of supramolecular aggregates, and organic spintronics. The group is specialized in the theoretical study of the effects of disorder on the charge-transport and optical properties of organic electronic materials and devices, investigated in three-dimensional systems using numerical Master Equation and Monte-Carlo methods. Recently Reinder Coehoorn joined TU/e with a professorship appointment. Reinder has led OLED research developments in Philips and will bring his expertise to the MOSTOPHOS project.

TU/e

■ BASF SE



The focus of the BASF team “Modeling of organic electronics” (C. Lennartz, F. May) is on multiscale modeling of thin organic films. So far the central point of research has been on understanding charge and energy transport in OLEDs, but recently, the group is also intensifying research on OFET systems. The group is linked to a broader synthetic/device fabrication activities on organic electronics located in Ludwigshafen (Germany), Basel (Switzerland) and Amagasaki (Japan) as well as to the cluster of excellence on organic electronics located in Heidelberg (Innovation Lab, www.innovationlab.de).



■ Consiglio Nazionale delle Ricerche - ISMN Institute



The Institute for the Studies of Nanostructured Materials (ISMN) is part of CNR, the largest public applied research institution of Italy. ISMN possesses state-of-art facilities for OLED fabrication and in-situ characterizations and expertise. The institute will participate in this project with its computational expertise, led by Dr. Alessandro Pecchia. Classical MD and DFT calculations will be performed in order to model electrodes morphologies, metal/organic interfaces and charge injection rates into the organic layers.



About us:

MOSTOPHOS addresses the problem of stability of blue emitting organic LEDs based on phosphorescent dyes in order to achieve all-organic white sources for lighting.

The consortium we set to tackle this problem comprises top experts in the fields of organics optoelectronics, from computational materials scientists to leading experts in OLED fabrication.

The challenge of the project is to provide a theoretical understanding of the dominant degradation mechanisms, that are at the basis of possible improvements.

Coordinator:

- Max Planck Institute Polymer Res. (D)

Project partners:

- Consiglio Nazionale delle Ricerche (I)

- BASF SE (D)

- Universidad Del Pais Vasco (S)

- Università di Roma 'Tor Vergata' (I)

- Technische Universiteit Eindhoven (NL)

- Technische Universitaet Dresden (D)

- sim4tec GmbH (D)

- COSMOLogic GmbH (D)



■ Universidad del Pais Vasco



The Nano-bio Spectroscopy Group, led by Prof. Angel Rubio, is developing novel theoretical tools and computational codes (the group host main developers of octopus, abinit and Yambo) to investigate the electronic response of solids and nanostructures. Research activities related to the project are: new developments within many-body theory and TDDFT, including ab-initio description of electron excitations, optical spectroscopy, time-resolved spectroscopies and lifetimes. The group also hosts the Chair of the European Theoretical Spectroscopy Facility (<http://www.etsf.eu>).



■ Institut für Angewandte Photophysik



Sebastian Reineke is assistant professor for organic semiconductors at the Institut für Angewandte Photophysik (IAPP) of the Technische Universität Dresden (TUD). His research interests include the fundamental understanding and improvement of OLEDs, the investigation of novel luminescent systems for application in optic and optoelectronic systems and the utilization of excitonic properties of organic semiconductors. Within MOSTOPHOS, he will lead experimental efforts to supplement the consortium partners with test devices and materials parameters.



■ sim4tec GmbH



sim4tec is an innovative, entrepreneurial company founded in January 2007 as a spin-off of the Institute of Applied Photophysics, University of Technology Dresden and CreaPhys GmbH. It focuses on advanced test equipment for organic material analysis and OLED design simulation tools. We help our customers to accelerate the organic material and OLED development cycles and to reduce quality cost by organic material analysis in production. The users of our products are industry experts doing complex designs of OLED's for Displays and Lighting. The organic material analysis portfolio serves all engineers with the need of a complete characterization of organic materials in research, device design and material quality control.



■ Università di Roma 'Tor Vergata'



The research activity of the group headed by Prof. Aldo Di Carlo at the Department of Electronics Engineering of the University of Rome "Tor Vergata" covers several topics of electronic device simulations. A variety of methods have been developed, ranging from Quantum transport, Boltzmann Monte Carlo simulations to drift-diffusion approaches. These have been applied to the analysis of organic and inorganic opto-electronic devices. In recent years the expertise matured in the development of a multiscale simulation tool called TiberCAD, based on finite elements and atomistic models.



■ COSMOlogic GmbH



Founded by Andreas Klamt in 1999 COSMOlogic introduced the COSMO-RS implementation COSMOtherm to the chemical engineering community from where it spread to many fields of science. COSMOtherm has changed the way people make predictions in fluid phase thermodynamics and is now established as a standard tool. In addition, COSMOlogic has developed a series of COSMOtools for special purpose applications such as micelle partitioning or 3D-alignment and QSAR. The product portfolio is completed by the quantum chemistry suite TURBOMOLE with applications ranging from chemical reactions to OLEDs.



Recent events & Scientific Highlights

MOSTOPHOS kickoff meeting took place in Mainz on June 8th, 2015. The main objective has been to set the bureaucratic aspects of the project. The first truly scientific meeting took place at Eindhoven on December 14th 2015, in occasion of the 6th month meeting of the project. The meeting has seen a lively discussion about all the modelling aspects of the BASF OLED stack and related progresses made by all groups. IAPP has started to grow the OLED stacks with materials provided by BASF reaching very good performances. Most of the other achievement reached so far are still confidential or under publication and will be communicated in future issues of this newsletter.

Upcoming events

The 12th month meeting of MOSTOPHOS will be organized in Rome at the beginning of June.

Publications & Conferences

MOSTOPHOS will be presented at the following upcoming conferences:

- VIII Multiscale Materials Modeling Conference, Oct 9-14 2016, Dijon

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