



PHYSIKALISCHES KOLLOQUIUM

Referent: **Dr. David Beljonne**
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Thema: **Modelling electronic and excitonic processes in organic semiconductors**

Zeit und Ort: Dienstag, 7.5.2019, 16:40 Uhr
Rechnagel-Bau, Hörsaal REC/C213, Haeckelstr. 3

Leiter: Dr. Frank Ortmann

Kurzfassung: Energetics of charge carriers in organic semiconductors: Implications for optoelectronics' A proper description of how semiconducting optoelectronic devices work starts with a quantitative assessment of the energy landscape explored by positive and negative charge carriers. In organics, this is controlled by the chemical nature of the molecular building blocks, but also by the way these organize into the solid state, which namely defines their classical electrostatic embedding and quantum-mechanical interactions. In addition, conjugated organic materials are 'soft' and coupling between their electronic and vibrational degrees of freedom is ubiquitous. In this presentation, we will first present a comprehensive review of the fundamentals of charged excitations in organic conjugated semiconductors based on a multifaceted modelling scheme combining a simple classical molecular dynamics micro-electrostatic scheme to a state-of-the-art perturbative many-body quantum approach. We will show applications of this computational machinery to ascertain the microscopic mechanisms of doping, singlet fission and charge photogeneration in the bulk and at interfaces between molecular materials.

Biographie: David Beljonne received his PhD in Chemistry with Professor Jean-Luc Brédas at the University of Mons-Hainaut in 1994. After post-doctoral stays at the Universities of Cambridge (with Professor Richard Friend) and Rochester (with Professor Shaul Mukamel), he became a research fellow of the Belgian National Science Foundation (FNRS) and is now FNRS Research Director. He is also a Visiting Principal Research Scientist at the Georgia Institute of Technology in Atlanta and serves as an associate editor for ACS Applied Materials & Interfaces. Co-author of about 400 scientific publications (more than 25000 citations; h index of 81, Scopus), his research activities deal with a multifaceted modelling of the opto- electronic processes taking place in the bulk and at interfaces of (semi)conducting organic, 2D and hybrid materials for electronics and energy applications.

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