Bereich Mathematik und Naturwissenschaften Fakultät Physik

PHYSIKALISCHES KOLLOQUIUM

Referent: **Prof. Dr. Alessandro Troisi**
Department of Chemistry & Materials Innovation Factory, University of Liverpool

Thema: **Designing organic semiconductors via model reduction**

Zeit und Ort: Dienstag, 20.11.2018, 16:40 Uhr
Recknagel-Bau, Hörsaal REC/C213, Haeckelstr. 3

Leiter: Prof. Dr. Karl Leo

Kurzfassung: We present a common strategy to design organic semiconducting materials based on the construction of reduced (predictive) models from (detailed) atomistic one. We will argue that, somewhat counterintuitively, by removing chemical detail from the model one can more easily perform non-trivial predictions. The topics considered in this lecture include (i) the definition of a map of all organic semiconductors for charge transport; (ii) the desirable properties of electron acceptors in organic solar cells; (iii) derivation of possible design rules for semiconducting polymers; (iv) uses and limitations of machine learning approaches for the same problems.

Biographie: Alessandro Troisi received his PhD in Bologna (2002) working on charge transfer reactions and performed postdoctoral work at Nortwestern working on single molecule junctions. He was appointed Assistant Professor at the University of Warwick (2005) where he became Professor of Physical Chemistry (2010). Since 2017 he works at the University of Liverpool (Dept. Chemistry and Materials Innovation Factory). His current interests include charge transport in organic semicondutors (molecular and polymeric), ultrafast phenomena in molecules and data based predictive methods. He is the recipient of the RSC Marlow Medal (2007), ERC Starting Investigator Award (2009) and ERC Consolidator Award (2013).

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