



Quantum Efficiency Seminar und Colloquium

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Modeling organic solar cells on the molecular and device level

ABSTRACT: Unlike traditional silicon solar cells, plastic solar cells can be made by simply printing layers of low cost conducting organic molecules onto flexible plastic substrates such as polyethylene. Consequently they offer the potential to be produced as cheaply as plastic food packaging. With recently reported energy conversion efficiencies of over 10% they offer the exciting prospect of a mass produced, low-cost, low-carbon energy source with the potential to solve the energy and carbon crisis. Despite this rapid increase in efficiencies there is still considerable debate surrounding the correct descriptions of the charge generation, transport, recombination and charge collection mechanisms. Understanding of these physical processes is essential if power conversion efficiencies are to be boosted to commercially viable levels.

In this talk we discuss organic solar cells both on the device level and on the molecular level. In the first half of the talk we use multi-scale modeling techniques to calculate the mobility of thin films of C60 derivatives from first principles using molecular dynamic (MD) simulations, Quantum Chemistry, Marcus theory and Monte-Carlo methods. In the second half of the talk we discuss organic solar cell device modeling and the application of Shockley-Read-Hall (SRH) recombination theory to this task. Using a combination of transient experimental methods and a numerical device model we extract both the HOMO and LUMO density of trapped states from a working solar cell. We find that the DoS of an organic solar cell can be described by a series of Gaussian deep traps.

Date: Tuesday, February 7th, 2012 16:15 pm
Location: Lecture Hall 1, Hermann-Herder-Str. 3, Freiburg

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