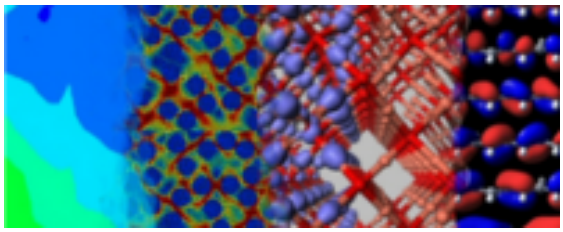

Contribution ID: **1** Type: **Talk**

Challenges for in silico design of organic semiconductors for photovoltaic applications

Thursday, November 8, 2012 3:40 PM (45 minutes)

Interest in the field of organic electronics is largely provoked by the possibility to fine-tune properties of organic semiconductors by varying their chemical structure. Often, compound design is solely guided by chemical intuition, even though material development would benefit from more rigorous structure-property relationships, which link the chemical structure, material morphology and macroscopic properties. To formulate such relationships, an understanding of physical processes occurring on a microscopic level as well as the development of methods capable of scaling these up to macroscopic dimensions are required. The aim of computer simulations is to facilitate this by zooming in on the behaviour of electrons and molecules and by bridging micro- and macroscopic worlds. Here, we describe the current status of methods which allow the linking of molecular electronic structure and material morphology to the mesoscopic/microscopic dynamics of charge carriers and excitons. Special attention is paid to the challenges these methods face when aiming at quantitative predictions.

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Session Classification: Session: Organic electronics, photovoltaics (Click for details or select 'Detailed view')

Track Classification: Organic electronics, photovoltaics