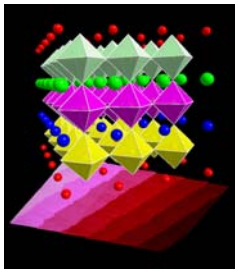
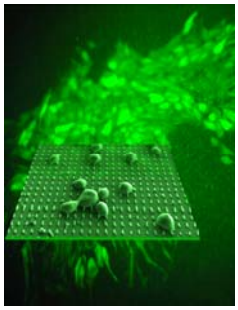
CNMS DISCOVERY SEMINAR SERIES

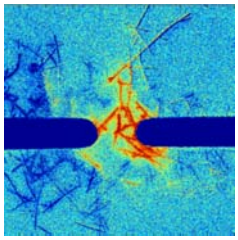
Friday, March 12, 2010
11:00 am
Iran Thomas Auditorium, 8600





Electronic and Optical Processes in Organic Solar Cells: Theoretical Description of Organic-Organic Interfaces

Jean-Luc Bredas
School of Chemistry and Biochemistry and
Center for Organic Photonics and Electronics
Georgia Institute of Technology



Abstract:

This presentation work seeks to provide a detailed theoretical description of the electronic and optical processes taking place in organic solar cells [1]. In particular, we report our recent results on:

(i) the description of the electronic structure of low bandgap polymers and the relationship between localization of the highest occupied and lowest unoccupied molecular orbitals (HOMO and LUMO levels) and the oscillator strength of the lowest-energy optical transition; and
(ii) the description of the donor-acceptor (D/A) interface in terms of: the electronic structure of the ground and excited electronic states; the polarization effects due to the inhomogeneous nature of the surrounding medium at the heterojunctions; and the role of interfacial molecular packing and of the intra- and inter-molecular geometry relaxations upon excitation.

Our goal is to provide a coherent quantum-mechanical characterization of the ultrafast charge-transfer (CT) and charge-separation (CS) processes occurring at D/A interfaces [2]. This requires the determination of the electronic couplings between the molecular (exciton) states and CT/CS states, which we calculate by using a computational approach recently developed in our group [3].

Host: Bobby Sumpter, sumpterbg@ornl.gov, 865.574.4973

Center for Nanophase Materials Sciences

References:

[1] J.L. Bredas, J. Norton, J. Cornil, and V. Coropceanu, *Acc. Chem. Res*. **42**, 1691 (2009).
[2] Y.Yi, V. Coropceanu, and J.L. Bredas, *J. Amer. Chem. Soc.* **131**, 5131 (2009).
[3] T. Kawatsu, V. Coropceanu, A. Ye, and J.L. Bredas, *J. Phys. Chem.* C **112**, 3429 (2008).