

Abstract Submitted  
for the MAR15 Meeting of  
The American Physical Society

**Computational Description of Donor-Acceptor pi-Conjugated Materials for Organic Photovoltaics Applications** JEAN-LUC BREDAS, King Abdullah University — This presentation will focus on the following topics, related to organic solar cell applications: 1) We will describe our recent work on the electronic structure and local morphology of donor-acceptor interfaces in bulk-heterojunction solar cells. 2) We will discuss how we can evaluate the polarization effects, which play a critical role in the charge-separation process at donor-acceptor interfaces in organic solar cells. 3) Finally, we will describe the peculiarities of the electronic structure of a new pi-conjugated polymer with very high hole mobilities over 20 cm<sup>2</sup>/Vs.

Jean-Luc Bredas  
King Abdullah University

Date submitted: 13 Nov 2014

Electronic form version 1.4