

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Organic solar cells: a theoretical study of the effects of polymer side-chains NICOLAS BERUBE, HELENE ANTAYA, MICHEL COTE, Université de Montreal — Organic photovoltaic cells received a great interest in the last few years as they offer an environmentally clean and low-cost solution to the world's rising energy needs. One of the main problems limiting the efficiency of an organic solar cell device is the strong binding energy of the excitons, typically situated about a few hundreds of meV, which is ten to one hundred times more than in inorganic devices. Another limiting factor can be the misalignment of the the HOMO (Highest Occupied Molecular Orbital) and the LUMO (Lowest Unoccupied Molecular Orbital) energy level of the different components of the solar cell. In this presentation, we will discuss how different modifications on organic polymers' side-chains can affect and improve their electronic properties. Our calculations, based on density-functional theory using the B3LYP functional, indicate a HOMO and LUMO lowering of more than 1 eV in various organic polymers like poly-isothianaphtene (pITN) and poly-thienothiophene (pTT), and various side-chains like aldehyde-based ones. Preliminary calculations on oligothiophenes also show a lowering of the exciton binding energy.

Nicolas Berube
Université de Montreal

Date submitted: 23 Nov 2010

Electronic form version 1.4