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Organic solar cells: How can the theory guide the experience? NICOLAS BERUBE, VINCENT GOSSELIN, HUGO LEPAGE, MICHEL COTE, Universite de Montreal — Research in organic photovoltaic applications are receiving 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 of a few hundreds of meV, which is ten to one hundred times more than in inorganic devices. Another limiting factor, persistent in P3HT:PCBM devices, can be the misalignment of the the HOMO (Highest Occupied Molecular Orbital) and the LUMO (Lowest Unoccupied Molecular Orbital) energy levels of the different components of the solar cell. Scharber's model (Scharber, M.C., Adv. Mater. 18, 789) is a simple yet interesting approach for predicting the efficiency of those devices, mainly based on the values of the HOMO and the LUMO and reasonable assumptions for the exciton binding energy. In this presentation, we will discuss how theoretical calculations based on density-functional theory can provide a guide to find promising polymers for photovoltaic cells. The accuracy, limits and possible expansions of Scharber's model will be examined, and a number of interesting polymer candidates to reach and perhaps break the well-known 10 % efficiency will be presented.

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