Theoretical Insights into the Phenomena of Exciton Creation and Charge Separation in Organic Solar Cells

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One of today's big challenges to Material Scientists is how to make cheaper and more efficient photovoltaic panels. Solar Cells that use organic molecules as active materials, known as Organic Solar Cells (OSCs), are promising candidates as they can be made lighter, cheaper, and semitransparent comparing to silicon-based cells. However, the Achilles heel of the OSCs is the efficiency, that is struggling to cross the barrier of 10% in practical applications.

Here, we discuss two theoretical models that can be applied to investigate the central problems of the OSCs: one deals with how excitons are created, from a molecular point of view; the other, shed light on how charges separate or recombine, from a phenomenological simulation.

Our first approach is based on a methodology, developed by Yi and coworkers, to compute rates of exciton creation and recombination in dimers formed by two organic molecules. Instead of using model dimers, we used Molecular Dynamics to simulate an interface of donor (Squaraine) – acceptor (C_{60}) molecules and computed the electronic couplings that describe the charge recombination and exciton dissociation at a donor-acceptor interface.

The second approach uses Kinetic Monte Carlo simulations to study the charge separation and charge recombination in a bilayer organic solar cell. In this later case, there are no molecules, as they are represented as a grid of points in which parameters, coming from Quantum Chemical calculations or from the experiment, are assigned. These parameters can consider important mesoscopic aspects of the device, such as the existence of an energy gradient at the donor-acceptor interface, energy disorder, and morphology.

Using a combination of Quantum Chemical calculations with Molecular Dynamics in one approach and a combination of experimental or theoretical data with a Kinetic Monte Carlo (KMC) model, we will show how theoretical modeling can be useful to guide Material Scientists in the design of more efficient Organic Solar Cells.