Public summary of PhD-thesis of Jens Wehner
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Modeling energy transport in an organic solar cell

In the future, a large portion of our renewable energy will be provided by the sun. Solar cells made out of polymers and small molecules, so called organic solar cells, are likely to supplant the current inorganic solar cell technology. Organic solar cells are tunable, transparent, flexible and lightweight, which opens up new areas and applications for solar cells. In my PhD research, I developed computer simulations to better understand how the energy absorbed by the solar cell is converted into electricity.

Organic solar cells consist of large amounts of organic molecules. When one of these molecules is hit by light, or more explicitly by a photon, there is a chance that the photon is absorbed by the molecule. If that happens, the photon transfers its energy to the molecules' electrons. This kicks the electrons into an excited state. If the photon has the right wavelength, it can eject an electron from the molecule and create a hole where the electron used to be. Unfortunately, the electron wants nothing more than to return to the hole and annihilate it. The objective of an organic solar cell is now to prevent this from happening and instead harness the energy of this ejected electron by moving it away from the hole it came from. Unfortunately, electron and hole are so attracted to each other, because of their opposite charge, that they stay very close. So close, that we treat them as one particle, called an exciton.

To help optimize our ability to move the electron away from the hole – to break the exciton up – we need computational techniques to model and understand exciton behavior. As electrons are really tiny, their behavior is governed by quantum mechanics. Simulations of quantum mechanical systems are possible but require a lot of computational resources, especially for systems larger than hundreds of atoms. Excitons inside an organic solar cell are influenced by thousands of atoms. To compute these large systems with quantum mechanical models, I implemented ways to model the environment on a coarser level. This allows us to simulate larger systems at lower computational cost. To allow other researchers to use these techniques, I made the code available open source in the VOTCA-XTP library.

With the help of my coarse-grained environment quantum mechanics model, I investigated how excitons move around by jumping from molecule to molecule. I confirmed the experimental finding that small defects can trap an exciton on its way and severely limit its movement range. What these traps look like chemically is still not clear, but now researchers can test their ideas using this code. Eliminating the defects is critical, because the only reliable way to make an organic solar cell convert more than 1% of the incoming light is to introduce areas with electron-attracting molecules to pull the excitons apart. The understanding provided by my research can help create more advanced fabrication techniques to reduce the number of defects and enable the excitons to reach these areas.

Title of PhD thesis: Investigation of exciton properties in organic materials via many-body perturbation theory. Supervisors: Barry Koren, Björn Baumeier, both TU Eindhoven