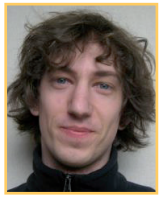
PHD GRANT



Non-equilibrium quantum modeling of nano-structure based solar cells

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The development of solar photovoltaic systems has been essentially related to inorganic semiconductors. However, solar cells based on organic materials have emerged, showing many advantages compared to their inorganic counterparts. One important difference is that light absorption does not lead instantaneously to free charge carriers but instead to an exciton (see Fig. 1) The efficiency of organic cells therefore relies on a good charge separation of the exciton at the donor-acceptor interface. Understanding the influence of the electron phonon interaction in this process is crucial because in organic systems it may lead to the formation of a polaron. In this project we study the influence of polaron formation on the electron transfer process as well as its effect on photocurrent efficiency. So far we have developed and benchmarked a new numerical method to take into account the role of polarons [1]. We apply now this new formalism to study charge injection at the donor-acceptor interface.

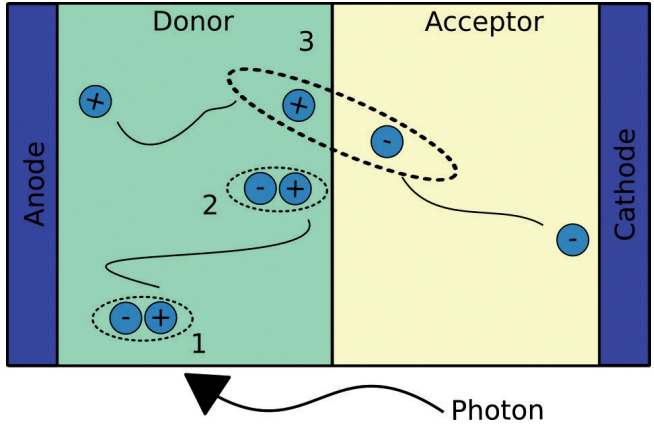

Fig. 1: Generation of a photocurrent in a bulk-heterojunction organic solar cell.

OUTCOMES

[1] Inhomogeneous Dynamical Mean Field Theory of the Small Polaron Problem. arXiv:1806.04543 (2018).

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