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Key electronic processes in organic solar cells: a theoretical perspective

VEACESLAV COROPCEANU, Center for Organic Photonics and Electronics and School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA 30332-0400, USA

In this contribution, we discuss state-of-the-art quantum-chemical approaches used to derive the microscopic parameters and model the key electronic processes in organic solar cells. We illustrate the application of recently developed computational methods by computing the electronic couplings and the rates of exciton dissociation and charge recombination in several model donor-acceptor complexes. The contributions of both intra-molecular and inter-molecular vibrations to the electron-vibrational interaction will be discussed in detail. The impact on the charge-transport characteristics of the interplay between electron-vibration coupling and electronic coupling is investigated in the framework of band, disorder, and semi-classical models.