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Organic Semiconductors: A Molecular Picture of the Charge-Transport and Energy-Transport Processes.

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Conjugated organic oligomer and polymer materials are being increasingly considered for their incorporation as the active semiconductor elements in devices such as photo-voltaic cells, light-emitting diodes, or field-effects transistors. In the operation of these devices, electron-transfer and energy-transfer processes play a key role, for instance in the form of charge transport (in the bulk or across interfaces), energy transport, charge separation, or charge recombination [1]. Here, we provide a theoretical description of electron-transfer phenomena based on electron-transfer theory, which allows us to provide a molecular, chemically-oriented understanding. In this presentation, we focus on the parameters that impact the mobility of charge carriers [2], that is the electronic coupling within chains and between adjacent chains and the reorganization energy of the chains upon ionization. Materials under study include conjugated oligomers such as oligoacenes, oligothiophene-acenes, oligothiophenes, and oligothienacenes.

[1] J.L. Brédas, D. Beljonne, V. Coropceanu, and J. Cornil, "Charge-Transfer and Energy-Transfer Processes in pi-Conjugated Oligomers and Polymers", Chemical Reviews, 104, 4971-5004 (2004).
[2] V. Coropceanu, J. Cornil, D.A. da Silva Filho, Y. Olivier, R. Silbey, and J.L. Brédas, "Charge Transport in Organic Semiconductors", Chemical Reviews, 107, xxx (2007).