Polarons in organic conjugated materials: interplay between electronic and vibrational properties

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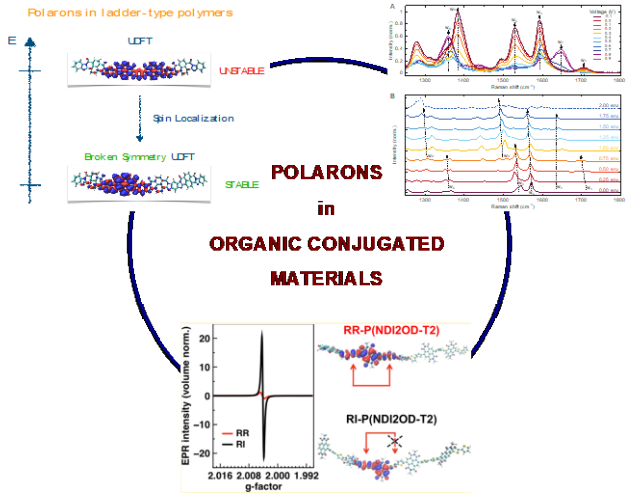
Abstract

Polarons (i.e., excess charges localized within the nuclear structure) play a crucial role in governing charge transfer, thermo-electric and redox mechanisms in organic functional materials.[1,2] Their accurate description at the quantum-chemical level is therefore essential to understand the fundamental relationships governing their structure-property functions.[3,4]

In this talk, I will briefly overview different approaches to model the electronic and vibrational properties of polarons in conjugated molecules and polymers, active materials for opto-electronic (e.g., OFET), energy-saving (e.g., battery) and biomimetic (e.g., bioneural device) applications. Possible structure-property correlations will be suggested to describe the charge transport and redox mechanisms occurring at the microscopic scale. Specific case studies will be discussed, encompassing low-band gap conjugated polymers, as characterized by various structural architectures and backbone flexibilities,[1-5] and small molecules, featuring neutral-to-zwitterionic ground state character.[6]



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