Structure-property relationships from modeling electronic and charge transport properties of n-type and p-type organic semiconductors

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In the perspective of an opto-electronic technology based on organic semiconductors, a major objective is to achieve a deep understanding of their behavior in terms of structure-property relationships. The interplay between intramolecular properties and intermolecular interactions governs, among others, charge conduction mechanisms, energy transfer, optical properties. Over the past few years we have modelled, with computational tools, structural, electronic, optical and charge transport properties of a number of core-extended conjugated molecules, paying increasing attention to the effects that condensed phase and structured environments can have on the properties of the molecular material. Although cooperative effects can have a relevant role, the performance and the properties of molecular-based materials can often be related to the structure and behavior of its constituting molecules. The electronic structure, optical and charge transport properties of organic semiconductors can be therefore tuned by molecular design. In recent years we have explored these properties for several n-type extended-core π systems that can be considered models for graphene nanoribbons and more recently for p-type sulfur-decorated organic semiconductors. I will summarize our recent simulation results by paying attention also to thermally induced dynamical effects that can modulate electronic intermolecular interactions in this class of molecular materials.