Séminaire de Chimie Théorique

Salle conférence, 3eme Est, bat. A12

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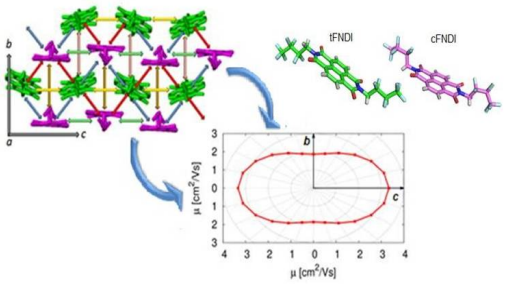
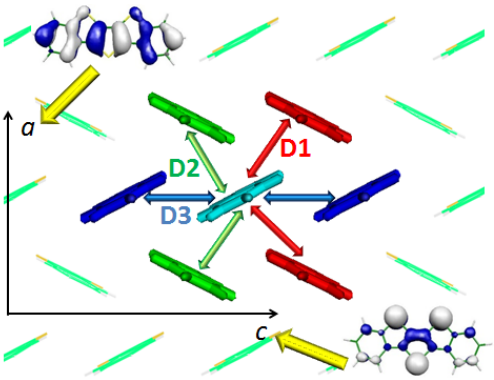
Unravelling structure-property relationships from modelling charge transport and exciton couplings in organic semiconductors

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. Measurements in single-crystal devices[1,2] offer a superior substrate for testing molecular models of charge transport. In recent years we have explored these properties for several n-type extended-core π systems[3-5] that can be considered models for graphene nanoribbons and more recently for p-type sulfur-decorated organic semiconductors.[6] I will summarize our recent simulation results on the topics above and on the prediction of the aggregate character and excited state nature, along with exciton interaction in perylene bisimide dyes (PBI) that are essential to design more efficient molecular architectures for exciton transport.

[1] A. Lv, Y. Li, W. Yue et al. Chem. Comm. 2012, 48, 5154-5156
[2] R.J. Li, L. Jiang, Q. Meng et al. Adv. Mater. 2009, 21,4492-4495
[3] E. Di Donato, R.P. Fornari, S. Di Motta, Y. Li, Z.H. Wang, F. Negri, J. Phys. Chem. B 2010, 114, 5327-5334
[4] S. Di Motta, M. Siracusa, F. Negri, J. Phys. Chem. C 2011, 115, 20754−20764
[5] S. Canola, F. Negri, Phys. Chem. Chem. Phys. 2014, 16, 21550-21558
[6] S. Canola, F. Negri, J. Phys. Chem. C 2015, 119, 11499-11505

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