Contribution ID: **44** Type: **Invited Speaker / Conférencier invité**

Modeling the structure, optoelectronic properties and charge transport of organic semiconducting conjugated polymers with DFT

Thursday, 19 June 2014 13:45 (30 minutes)

Conjugated organic polymers exhibit high electronic conductivity when doped and other optoectronic properties such as electroluminescence, electrochromism, and large non-linear optical responses. Many applications have been proposed for conjugated polymers and oligomers and some have already been commercially implemented. The most important applications involve the devices such as the organic light emitting diodes (OLEDs) and organic photovoltaic cells. Better performance of these devices is continually being sought. This effort requires better knowledge of their optoelectronic and transport properties. In addition, our computational investigations indicate that the structure plays a critical role in determining the charge transport in organic macromolecular systems such as those used, for example, in the bulk heterojunction solar cells. Our main theoretical/computational tool is the density functional theory (DFT). DFT based methods that we employ in our computations are: molecular DFT to obtain ground state structures of monomers and oligomers, time-dependent DFT (TD-DFT) to study the excited states and 1D and 3D solid-state DFT to determine the polymer crystalline structures. In recent years, the DFT approaches have been extended to include the long-range electron correlations (the dispersion forces) which allow scientists to more accurately describe the molecular configurations where the bindings are dominated by the dispersion forces. In this talk, I will give examples of using primarily DFT and DFT-based methods to investigate the optoelectronic properties, charge transport and the structure of fluorene and carbazole based organic conjugated polymers. I will discuss the effect of intermolecular distance and molecular orientation on optimizing the charge transfer rates in conjugated polymers used in bulk heterojuction solar cells. I will show how results of 1D band structure and molecular cluster calculations of conjugated polymers employed in hole- and electron-transport layers in a multilayered OLEDs can be used to generate a more balanced charge transport in these devices. Finally, I will discuss the effect of side-chain length on the solid-state structure and optolelectronic properties of fluorene-alt-benzothiadiazole based conjugated copolymers.

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Session Classification: (R2-4) Computational Materials Mini-symposium II - DCMMP-DMBP / Mini-symposium sur les matériaux numériques II - DPMCM-DPMB

Track Classification: Condensed Matter and Materials Physics / Physique de la matière condensée et matériaux (DCMMP-DPMCM)