

STRUCTURE OF ORGANIC MATERIALS FOR ORGANIC SOLAR CELLS: COMBINED DIFFRACTION AND MODELLING APPROACHES

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ABSTRACT

Among the electroactive materials for organic solar cells (OSC), poly(3-alkylthiophenes) (P3AT) and phenyl-C61-butyric acid methyl ester (PCBM) are still respectively the reference donor and acceptor materials. Although extensive structural and morphological studies of both P3AT's and PCBM and their blends have been accumulating over the years, only relatively few detailed atomistic models of the structural organization of these materials have been developed.

In efficient organic solar cells both the acceptor and the donor components are crystalline only in part and largely nanocrystalline: reliable structural information essential to clarify structure-properties relationships will have to rely substantially on effective atomistic modeling of amorphous components on the one hand and of crystalline materials on the other, not to speak of the interphases. Indeed the determination of P3AT's and substitutes fullerenes crystal structures and our ability to model them effectively accounting for the their photo-electronic properties represents a challenge which has been met only in part so far but represents a precondition for structural understanding of processes taking place in solar cells.

Our contribution to the understanding of both P3ATs polymorphism and properties and more recent studies devoted to the unravel the structural organization of both solventless and solvent containing PCBM, in amorphous phases and crystalline polymorphs, will be reviewed and discussed. Detailed modeling with ad-hoc developed force-fields able to mirror in reasonable detail much of the described polymorphic behavior and opening viable perspectives to the study of disordered states of organic electronic materials will also be discussed.

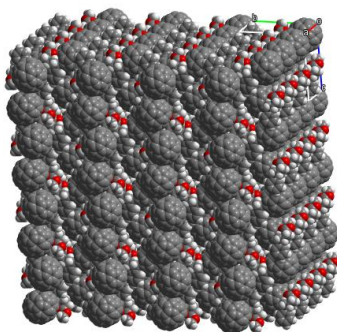


Fig. 1: A view of one of the crystalline solventless phases of PCBM

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