PÔSTER - RESUMO - MATERIAIS E BIOMATERIAIS

MODELING THE ELECTRONIC STRUCTURES OF CONJUGATED POLYMERS USING QUANTUM WELL STRUCTURES

Gustavo Moreno Mantuani Reis (gustavo.reis@unesp.br)

Florian Steffen Günther (florian.gunther@unesp.br)

Conjugated polymers form an important group of materials that find applications in the rapidly growing field of organic electronics. The ability of organic chemistry to connect different units has led to the development of a large number of new materials with significant potential for future applications. In particular, the class of donor-acceptor polymers [1], in which electron-deficient and electron-rich units are regularly connected, has driven the development of new polymeric semiconductors. However, synthetic strategies and thin-film fabrication processes can introduce structural defects or disorder into the system, which may lead to localization effects, for example, due to finite-size effects or homocoupling of identical units. In many cases, it remains unclear whether these localization effects are related to the specific chemical structure of the materials or whether they are linked to more fundamental quantum

mechanical phenomena. In our work, we model the electronic structure of conjugated polymers via sequences of quantum wells, which is the simplest form to represent the one-dimensional nature of polymers. For these cases transcendental equations can be formulated which represent the eigenvalue system of the associated Schrödinger Equation. Although formulating and numerical solving of these equations is possible, it becomes impractical for arbitrary combinations of quantum wells. We therefore approach the problem using the more efficient shooting method [2]. Furthermore, our implementation is versatile enough to incorporate periodic boundary conditions and infinite potential barriers, allowing for a broader range of structural simulations. In this contribution, we are presenting results from a case study modeling the homocoupling effect in copolymers made from dithiazolyldiketopyrrolopyrrole (TzDPPTz) and tetrafluorobenzene (F4) [1]. We observe that fundamental effects, such as localization at the homocoupling defect and contribution of individual sub-units, are well reproduced using quantum wells with lengths and depth associated with the size and energetic position of molecular orbitals of the respective polymer units.

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References

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Palavras-chave: conjugated polymers; organic electronics; donor-acceptor polymers; quantum wells; shooting method; homocoupling defects.