APRESENTAÇÃO ORAL - 1) ENERGY CONVERSION AND STORAGE

ASSISTED SOLVENT EVAPORATION: AN APPROACH TO MODEL NON-CRYSTALLINE ORGANIC SEMICONDUCTORS

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A continuous challenge for the organic electronics field is obtaining p-conjugated materials to achieve high charge carrier mobility. The arrangements of the molecules directly affect the optical and electronic performances of the device's active layers. Besides, the choice of solvent during the processing is crucial in determining the microstructure of non-crystalline organic semiconductors (NCOS) [1,2]. Molecular modeling techniques based on classical and quantum mechanics can complement experimental observations and provide in-depth physicochemical insights into the structure–processing-property relationships [3]. We have developed a solvent evaporation methodology to model the microstructure of this kind of material to address the interplays between NCOS and solvent-NCOS in the bulk of organic semiconductors. We have used molecular dynamics (MD) simulations to achieve this goal, employing OPLS-AA or GROMOS-53A6 forcefield implemented in the GROMACS package [4]. The NCOS and solvent molecules were randomly added in a cubic box, and the system was equilibrated to reach experimental data density. Afterward, the solvent was gradually removed until a dry film was obtained, considering the most energetic molecules [5,6]. We also performed solvent-free simulation to compare the morphologies from different procedures. The results showed that the solvent-free protocol produced more twisted chains than the others and an unfavorable profile for intermolecular

interactions, which is undesirable for organic semiconductor materials. Moreover, we observed that the nature of the solvent induced the molecular architecture of the material, leading to different entanglements. According to the results, MD simulation is a sensitive tool that provides a molecular understanding of bulk chains' structural conformations.

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Palavras-chave: molecular dynamics; organic semiconductors; material modelling.