PÔSTER - RESUMO - DISPOSITIVOS OPTOELETRÔNICOS

SOLVENT EFFECTS ON THE CONFORMATION OF A PHOSPHATE-FUNCTIONALIZED FULLERENE

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The selection of appropriate solvents remains a major challenge in the fabrication of high-quality organic thin films for applications ranging from hybrid solar cells to organic field-effect transistors. Solvent choice can significantly influence molecular organization and film morphology, thus impacting device performance [1]. Although fullerene derivatives are widely used in organic electronics, detailed molecular-level insights into how solvent-specific interactions influence their conformational behavior and aggregation - particularly for branched derivatives with polar functional groups - are still relatively scarce [2,3]. In this work, we investigated a branched phosphate-functionalized fullerene derivative using molecular dynamics simulations in three solvent environments: pure toluene, pure isopropyl alcohol, and a 1:1 v/v mixture. Our goal was to elucidate specific solute-solvent interactions and assess their influence on the side chain conformations of the fullerene derivative, as well as potential implications for thin film formation. The simulations revealed a marked interaction between the oxygen atoms of the phosphate group and isopropyl alcohol molecules, promoting more extended

side chain conformations. In contrast, toluene favored intermolecular aggregation, with side chains adopting more compact and coiled arrangements. These solvent-dependent behaviors suggest a competition between solvation and intermolecular interactions that governs the conformational equilibrium of the branched fullerene. Complementary electronic structure calculations performed on representative conformers indicated minor differences in frontier orbital energies, suggesting that the electronic properties are relatively insensitive to side chain conformation. This suggests that performance differences are primarily governed by intermolecular interactions and the degree of aggregation.

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