

Analysis of Structural Defect States in Thin Films of Small-Molecular Organic Semiconductors Using Complex Impedance Data and DFT

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Abstract. Defects in organic semiconductors can significantly affect the functionality of organic photonic devices. However, unlike inorganic materials, they are still little researched. This article investigates structural defect states in the bandgap of n-type small molecular semiconductor 2,2'-{[5,5'-(Naphthalene-2,6-diyl)bis(thiophene-5,2-diyl)]bis(2,2,2-trifluoroethan-1-yl-1-ylidene)}dimalononitrile (TNT-FEC). Using the energy-resolved electrochemical impedance spectroscopy (ER-EIS), we mapped the presence of defect states in this material, and by comparing measurements in the solution and the film, we identified the structural ones. Furthermore, we investigated the influence of the substrate on defect formation. Finally, using DFT and DFTB calculations, we analyzed the possibility of the conformers' presence, which can influence the structural properties of thin films. The combination of experimental and theoretical approaches in the analysis of defect states has been shown as suitable for studying structural defects' presence in the thin films of organic semiconductors.