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Oxygen-related defect in PPV MARILIA CALDAS, Inst. Physics, University of Sao Paulo, Sao Paulo, Brazil, ALICE RUINI, CNR Nat. Center nanoStructures and bioSystems at Surfaces (S3), Modena, Italy, ARRIGO CALZOLARI, CNR-INFM DEMOCRITOS National Simulation Center, Trieste, Italy — Pristine poly-para-phenylene vinylene (PPV) films are structured as crystalline grains immersed in amorphous regions. Inside the grain we must look at three-dimensional (3D) properties, while on-chain processes possibly dominate in the amorphous regions. Defect and impurities due to environmental contamination are usually present and the role of defects can be distinct in one-dimensional (1D) systems compared to its 3D counterparts. We investigated simple defects in PPV that can be introduced by exposure to water, the impact the electron transport properties of 1D chains [1], and on the electronic structure of the crystalline regions. We start from classical molecular dynamics, and proceed to ab initio Density Functional Theory calculations both for single chains and bulk systems through large-supercell defect simulations. For he special case of the C=O keto-defect we find a state with unexpected electron-hole separation, which suggests that the experimentally detected photoluminescence bleaching and photoconductivity enhancement could be due to exciton dissociation caused by the spatial characteristics of the defect. [1] L. Zoppi et al, Phys. Rev. B 78, 165204 (2008). We acknowledge support from CNR, Italy. MJC acknowledges support from FAPESP and CNPq, Brazil.

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