Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Modification of the electronic properties of rubrene crystals by extrinsic species LEONIDAS TSETSERIS, Vanderbilt University and University of Thessaloniki (Greece), SOKRATES PANTELIDES, Vanderbilt University and Oak Ridge National Laboratory — The chemical stability of organic semiconductors is one of the most important factors for the performance of related electronic devices. Here, we report the results of first- principles calculations on the effect of some of the most typical defect culprits in the prototype system of rubrene, the current record-holder organic semiconductor in terms of carrier mobilities. We identify the most stable water and oxygen- related impurity structures, with species in either substitutional or interstitial configurations, and we analyze their complex role in changing the shape and profile of rubrene energy bands. In certain cases the impurities either give rise or help annihilate carrier traps. We discuss the relevance of our findings for the optimization of rubrene-based electronic systems, and, in particular, the possibilities for effective defect engineering. This work was supported in part by DOE Grant DEFG0203ER46096.

Leonidas Tsetseris
Vanderbilt University and University of Thessaloniki (Greece)

Date submitted: 20 Nov 2008 Electronic form version 1.4