

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Impurities and carrier trap formation in rubrene LEONIDAS TSETSERIS, Aristotle University of Thessaloniki, Greece, and Vanderbilt University, SOKRATES PANTELIDES, Vanderbilt University and Oak Ridge National Laboratory — Rubrene has emerged recently as a very promising system for applications in organic electronics. In particular, measured carrier mobilities of rubrene films have been among the highest values reported for organic semiconductors. Here we present the results of first-principles calculations on impurities in rubrene crystals. We find that the most stable atomic H defect induces deep traps in the energy band gap of this prototype organic semiconductor, but we further show that the formation of a stable pair of vicinal H impurities eliminates these traps. We thus establish a dual role of hydrogen in carrier trap formation in rubrene devices. We also find that the incorporation of oxygen and water-related impurities is energetically favorable, and we address their possible role in the appearance of energy levels in the band gap of rubrene. Finally, we discuss the relevance of our findings for the development and operation of rubrene-based devices. This work was supported in part by DOE Grant DEFG0203ER46096.

Leonidas Tsetseris
Aristotle University of Thessaloniki, Greece, and Vanderbilt University

Date submitted: 26 Nov 2007

Electronic form version 1.4