

## **Theoretical modeling of organic electronic materials**

**Leonidas Tsetseris**

Department of Physics, Aristotle University of Thessaloniki, and  
Department of Physics and Astronomy, Vanderbilt University

The use of computational modeling has been an integral part in the study of organic materials and the optimization of corresponding electronic devices. Here, we first present an overview of several computational techniques of varying levels of sophistication and accuracy, from Monte-Carlo simulations to quantum-mechanical *ab initio* calculations, and we outline the capabilities and limitations of theoretical modeling to address the key physical mechanisms that control the electronic, optical, and transport properties of organic-based devices. We then detail with results based on first-principles calculations outstanding impurity effects in the prototype organic systems of oligo-acenes and rubrene, and we examine processes that may enable the growth of templates of acene thin films. The work has been performed in collaboration with Prof. S. T. Pantelides, and it has been supported by the McMinn Endowment at Vanderbilt University, and by DOE Grant No. DEFG0203ER46096.