

Abstract Submitted  
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**Charge Carrier Mobility in Conjugated Organic Polymers—  
A Multi-Step Computational Approach**<sup>1</sup> YAPING LI, JOLANTA B.  
LAGOWSKI, Memorial University of Newfoundland — In this work, we investigate charge transport characteristics of conjugated organic polymers (mostly fluorene and carbazole based) used in the construction of the organic solar cells using computational means. In particular we employ a multi-step approach that involves the use of the density functional theory (DFT), semiempirical (ZINDO), and Monte Carlo (MC) theoretical methods to determine their transfer integrals, reorganization energies, transfer rates and mobilities. We find that, in organic conjugated polymers, one dimensional (1D) approach to estimating trends in mobilities gives reasonable results, i.e. is in good agreement with experiment trends, provided their relative intermolecular distances can be obtained with some accuracy. However, greater understanding of the mobilities must take into account the three dimensional (3D) structure and/or the inherent disorder that is present in the organic thin films. We illustrate this requirement with some case studies. Another case study involving orientational disorder will also be presented. The proposed approach illustrates that theoretical computations/simulations based on chemical structure and known morphology of organic semiconductors is an important and reliable approach to studying charge mobility in organic materials used in devices such as solar cells.

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