

Abstract Submitted
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Charge Transport in Organic Conjugated Polymers Used in Solar Cells - A Computational Study¹ YAPING LI, JOLANTA LAGOWSKI, Memorial University of Newfoundland — Solar cells are one of the most important devices that can be used to solve the world energy and environmental needs. Recently, organic solar cells, because of their lightweight, low cost and processing flexibility, have attracted considerable attention in this field. To improve their efficiency, it is necessary to study their material properties. We investigate their charge transport characteristics using computational means. In particular we employ both the DFT and ZINDO theoretical approaches, to determine their transfer integrals, reorganization energies, transfer rates and mobilities. We find that polymers with large transfer integrals tend to have lower transfer rates if their reorganization energies are large. This suggests that in organic polymers, in addition to the transfer integral, the reorganization energy is also an important factor in determining charge transport rates. Trends in the transfer rates and mobilities for various organic polymers (in pristine and heterogeneous molecular environments) suitable for photovoltaic cell usage will be discussed. Our computational results will be compared with experimental values whenever possible.

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Yaping Li
Memorial University of Newfoundland

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