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Organic Solar Cell Efficiency Limitations and Pathways to Overcoming Them[1]

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Organic solar cell device efficiencies are often limited by a reduced external quantum efficiency, particularly for low band gap materials used in either single- or double-junction devices. This can be attributed to loss mechanisms occurring either at the device-physics scale, in the form of carrier recombination, or at the molecular donor-acceptor scale, in the form of incomplete photo-carrier generation and/or geminate recombination. Here mechanisms at both scales are addressed, utilizing drift-diffusion models of device operation and kinetic models of photo-carrier production. At the device-physics level, the negative impact of dark carriers, commonly derived from defect states in the organic semiconductor, is demonstrated. For dark carrier densities above a typical threshold of 10^{16} cm^{-3}, depletion at one of the electrodes leads to a field-free region of the device and substantial carrier recombination. At the molecular level, the fundamental impact of the molecular reorganization energy λ on device efficiency is considered through use of a Marcus Theory-based kinetic model. It is shown that substantial gains in efficiency, to values approaching 20%, are possible for hypothetical materials in which λ has been reduced to approximately 0.3 eV. Finally, measurements of molecular alignment at interfaces are presented, and implications on the above two mechanisms are explored.

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