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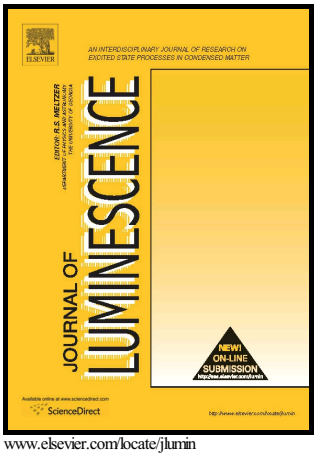

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Electron transfer and charge transport of photolectric material in external electric field

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Abstract

In this work, detailed theoretical analysis of Marcus-Levich-Jortner electron transfer rates upon photoexcitation of the *N*,*N*′-3,4,9,10-perylenediimide:[6,6]-phenyl C_{70}-butyric acid methyl ester (PDIB:$PC_{70}BM$)blend in an external electric field was performed. The external electric field controlled electronic coupling and charge transport carrier mobility were quantitatively characterized with first-principles quantum mechanics combined with Marcus-Hush theory. The calculated orders of magnitude agreed well with the experimental values, and the electron mobility was found to be sensitive to the external electric field, while hole mobility revealed opposite result. When combining the rates of exciton dissociation and charge recombination in the electron transfer process with charge carrier mobility, vibrational relaxation and external electric field influences must be considered to obtain an accurate simulation of the charge transport process in solar cell photoactive materials.

Graphical abstract