Influence of acceptor on charge mobility in stacked π-conjugated polymers

Abstract:
We present a quantum molecular model to calculate mobility of π-stacked P3HT polymer layers with electron acceptor dopants coupled next to side groups in random position with respect to the linear chain. The hole density, the acceptor LUMO energy and the hybridization transfer integral between the acceptor and polymer were found to be very critical factors to the final hole mobility. For a dopant LUMO energy close and high above the top of the polymer valence band we have found a significant mobility increase with the hole concentration and with the dopant LUMO energy approaching the top of the polymer valence band. Higher mobility was achieved for small values of hybridization transfer integral between polymer and the acceptor, corresponding to the case of weakly bound acceptor. Strong couplings between the polymer and the acceptor with Coulomb repulsion interactions induced from the electron localizations was found to suppress the hole mobility.

Stichworte:
Hole mobility; Conductive polymers; P3HT; Electron acceptor

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