



**IMPACT:** The optimization of organic solar cells requires a fine balancing act. It involves finding the optimal compromise among a combination of material characteristics that sometimes happen to work in opposite directions. As an example the local donor/acceptor (D/A) interface geometry or morphology can have a positive impact on both exciton dissociation (which produces the photocurrent and needs to be maximized) and the recombination of charge-transfer states formed after exciton dissociation (which decreases the photocurrent and needs to be minimized), as well as on the magnitude of the reverse saturation current in the dark (which needs to be minimized to increase the open-circuit voltage). Theoretical characterization of the exciton-dissociation and charge-recombination processes at the D/A interfaces can provide an insight into the optimization of organic solar cells.

**DISCUSSION:** From the calculations based on their recently developed quantum-mechanical approach, CMDITR researchers found that, irrespective of the actual pentacene-fullerene orientation, both pentacene-based and C<sub>60</sub>-based excitons are able to dissociate efficiently. Importantly, in the case of parallel configurations of the molecules at the pentacene/C<sub>60</sub> interface, the decay of the lowest charge-transfer state to the ground state is calculated to be very fast; as a result, it can compete with the dissociation process into mobile charge carriers. Since parallel configurations are expected to be found more frequently in bulk heterojunctions than in bilayer heterojunctions, the performance of pentacene/C<sub>60</sub> bulk-heterojunction solar cells is likely to be more affected by charge recombination than that of bilayer devices.

More details can be found in: Y. Yi et al. *J. Am. Chem. Soc.* **131**, 15777–15783 (2009)

**KEY PERSONNEL:**

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