Self-Assembling Tripodal Small-Molecule Donors for Bulk Heterojunction Solar Cells

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Photovoltaic performance of bulk heterojunction (BHJ) organic solar cells (OSCs) could benefit from improved morphology through supramolecular self-assembly of redesigned small-molecule donor compounds. Herein we report on the synthesis of two tripodal 'star-shaped' small-molecule donor compounds based on diketopyrrolopyrrole (DPP) side chain for solution-processed BHJ OSCs. We demonstrate that the compound with linear side chains self-assembles into nanowires while its branched counterpart does not form a crystalline domain in solution. Our simulations explain the morphology difference by showing the linear compound to have a tighter π-π stacking distance, less geometric sterics and a stronger π-π interaction energy. The linear compound shows a 50% increase in power conversion efficiency relative to the branched compound, owing to a significant gain in fill factor.

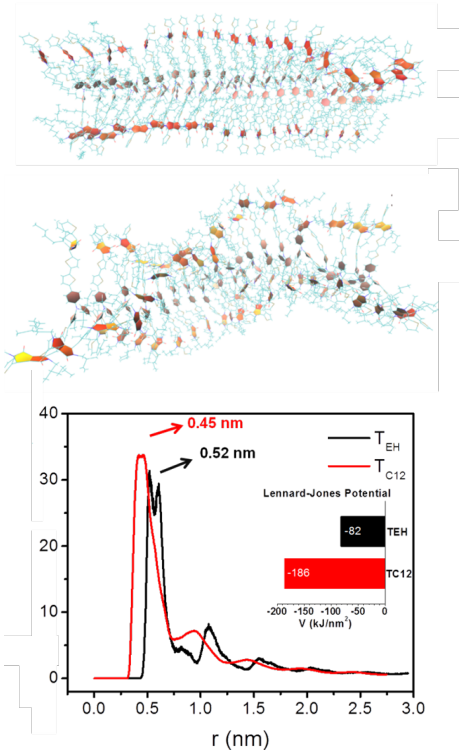

Figure: Snapshots of simulated self-assembled nanostructures from two DPP molecules. The radial distribution function and Lennard Jones energy demonstrate the improved π-π stacking of the linear compound.

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