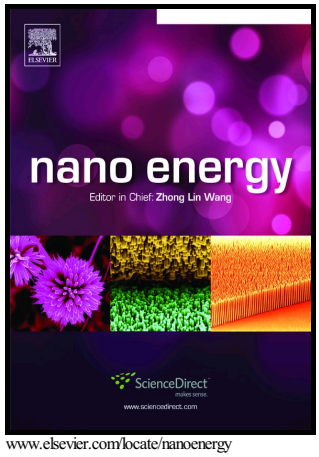

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Synergistic Effect of Halogenation on Molecular Energy Level and Photovoltaic Performance Modulations of Highly Efficient Small Molecular Materials

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Abstract

A series of small molecular donor materials with different halogenated and/or sulfuretted benzodithiophene (BDT) as the central units, **BDTTS-F-R**, **BDTTS-Cl-R** and **BDTTS-Br-R**, were synthesized successfully for efficient small molecular solar cells (SM-OSCs). The tiny structural variation by just changing the type of halogen atom would largely affect the absorption, crystallinity and charge transport of these small molecules (SMs). **BDTTS-F-R** showed a higher crystallinity due to the non-covalent effect caused by fluorine atoms, which resulted in a strong aggregation and inferior phase separation in device processing. This issue could be circumvented gradually by using the chlorine and bromine atoms instead of fluorine atom. On the other hand, the unoccupied *d* orbital of chlorine and bromine could accept the delocalized π-electrons, leading to more lower-lying highest occupied molecular orbital (HOMO) levels without obvious influence on the bandgaps. Finally,

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