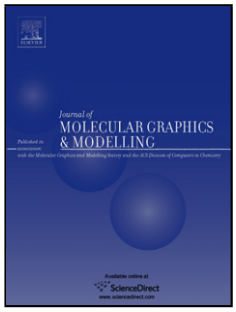

Title: A theoretical exploration of the effect of fluorine and cyano substitutions in diketopyrrolopyrrole-based polymer donor for organic solar cells

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PII: S1093-3263(17)30465-5
DOI: http://dx.doi.org/doi:10.1016/j.jmgm.2017.07.027
Reference: JMG 6986

To appear in: *Journal of Molecular Graphics and Modelling*

Received date: 19-6-2017
Revised date: 24-7-2017
Accepted date: 25-7-2017

Please cite this article as: Zhi-Wen Zhao, Qing-Qing Pan, Shuang-Bao Li, Yu-Ai Duan, Yun Geng, Min Zhang, Zhong-Min Su, A theoretical exploration of the effect of fluorine and cyano substitutions in diketopyrrolopyrrole-based polymer donor for organic solar cells, Journal of Molecular Graphics and Modellinghttp://dx.doi.org/10.1016/j.jmgm.2017.07.027

A Theoretical Exploration of the Effect of Fluorine and Cyano Substitutions in Diketopyrrolopyrrole-based Polymer Donor for Organic Solar Cells

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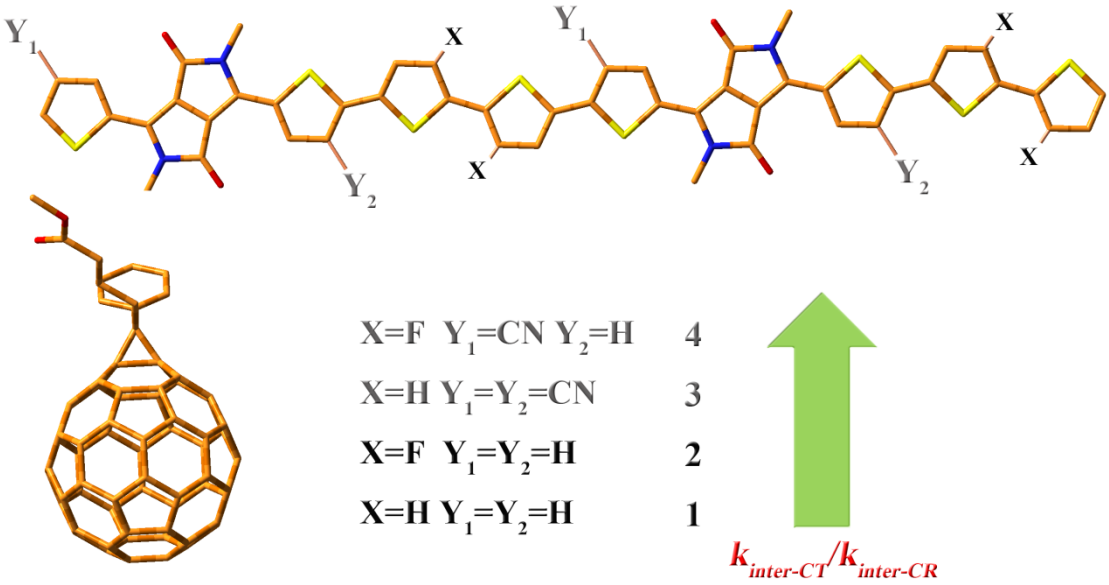
Graphical abstract



Highlights:

- Explaining the effect of fluorine and cyano substitution in polymer donor materials from a theoretical perspective.
- The substituent of asymmetric-cyano-groups and fluorine in polymer **3** and **4** performs better balance between large open-circuit voltage (V_{oc}) and high short-circuit current (J_{sc}) in OSCs.
- The designed molecules **3** and **4** with higher ratios of intermolecular charge transfer and recombination rates ($k_{inter\text{-}CT}/k_{inter\text{-}CR}$) are promising donor materials.

Abstract: A series of polymer donor materials **1-5** based on diketopyrrolopyrrole and thiophene unit which have been widely used in organic solar cells (OSCs) were investigated based on quantum chemical calculations. The effect of fluorine and cyano substitutions in polymer donor materials was focused on. Based on the investigation on electronic structures and optical properties of the reported molecules **1** and **2** and the analysis on some parameters relevant to charge dissociation ability at