Review of: "Completely non-fused electron acceptor with 3D-interpenetrated crystalline structure enables efficient and stable organic solar cell"

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Fullerene materials have played a very important role in OPV cells. Many studies have performed on designing new systems and improving its PCEs efficiency. However, just as the authors state that, non-fullerene acceptors also have more potential to realize low-cost OPV cells. In this paper, they designed a new bithiophene-based non-fused core, based on which a three-dimensional interpenetrating network can be formed. Importantly, a high PCE of 15.2% is achieved based on PBDB-TF:A4T-16, also the device retains ~84% of its initial PCE after 1300 h under the simulated AM 1.5 G illumination. Generally speaking, this work is interesting, it could be accepted for publication after minor revise.

1. In the theoretical simulation section, the author optimized molecular structure and calculated the relaxed potential surface energy et al., using DFT at the B3LYP/6-31 G (d, p) level. The simulating result give some supporting for material design. So I want to know the validity and accuracy of calculation method, whether the authors have tried another methods?

2. From the single crystal structure information, it seem that the experimental and theoretical results are not in good agreement, such as the dihedral angle et al., Why?

3. The authors state that, the twisted backbone of A4T-21 that suppressed the ICT effect, does the conclusion have direct more direct evidence?

4. PBDB-T, J52-2F, PTO2 and PBDB-TCl was selected as donors, and the photovoltaic parameters of the polymers: A4T-16-based cells were analyzed. What is the basis for selection? What are its structural advantages of PBDB-TF?