

Computational Strategies for Designing Stable and High-Performance Non-Fullerene Acceptors in Organic Solar Cells

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The design and development of several new high-performing non-fullerene acceptors (NFAs) improved the power of conversion efficiency of organic solar cells. However, the photovoltaic performance is still lower than the commercial inorganic solar cells. In this presentation, we show how the current architecture of NFA limits the performance of organic solar cells. Our results indicate design and choosing the right combination of functional units in NFAs would be an effective way further to improve the power conversion efficiencies of organic solar cells.

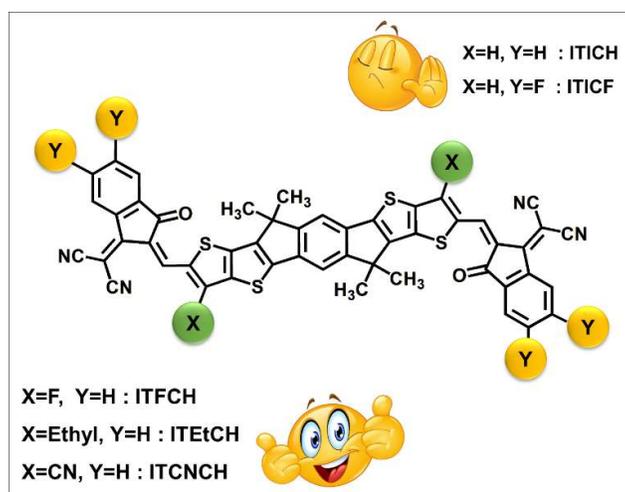


Fig. 1 Chemical structures of ITICH and its derivatives ITICF, ITFCH, ITEtCH, and ITCNCH.

References

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