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UNDERSTANDING THE STRUCTURE-PROPERTY CORRELATIONS OF N-TYPE ORGANIC SEMICONDUCTORS IN OFFTS

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ABSTRACT

In the organic electronic research field, the development of high-performance unipolar n-type semiconductors is still challenging. Here we present an in-depth study of a series of ladder-type semiconductors, which due to their all-acceptor backbones, exhibit unipolar n-type transport in OTFTs.

It is well know that the performance of organic semiconductors is governed not only by their molecular structures but also by their intermolecular assembly in the solid state. Thus, highly planar backbones are beneficial for a good molecular packing and film ordering leading to good charge transport characteristics. In this contribution, we study a series of BTI small molecules and polymers, both from a molecular and from a supramolecular point of view, in order to establish useful structure-property relationships that may guide the rational synthesis of new and improved materials.

To carry out this study, we make use of different spectroscopic techniques, supported by quantum theoretical calculations at the DFT level.

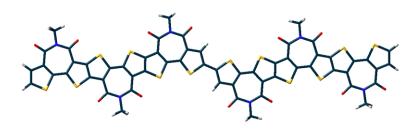


Figure 1. Optimized minimum-energy geometry (B3LYP/6-31G**) for one of the studied BTI-based semiconductors.

REFERENCES

[1] Y. Yang, H. Guo, S. Ling, I. Arrechea-Marcos, Y. Wang, J. T. López Navarrete, R. Ponce Ortiz, X. Guo, *Angew. Chem. Int. Ed.* 2017, 56, 9924-9929.

[2] Y. Wang, H. Guo, A. Harbuzaru, M. A. Uddin, I. Arrechea-Marcos, S. Ling, J. Yu, Y. Tang, H. Sun, J. T. López Navarrete, R. Ponce Ortiz, H. Y. Woo, X. Guo, *J. Am. Chem. Soc.* 2018, 140, 6095-6108.

[3] J. Mei, Y. Diao, A. L. Appleton, L. Fang, Z. Bao, JACS 2013, 135 (18), 6724-6746.