UNTANGLING THE ELECTRONIC PROPERTIES OF TRIINDOLE-BASED SEMICONDUCTORS

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Organic semiconductors have emerged as an important class of materials that offer interesting prospects for high throughput, low-cost and flexible electronic circuits. In this sense, triindole-based systems have demonstrated great potential as p-type semiconductors in organic field-effect transistors (OFETs).[1] Recently, we have performed a combined experimental and theoretical study of three new crystalline N-trimethyltriindoles endowed with different functionalities at 3, 8 and 13 positions, either unsubstituted or with three methoxy or acetyl groups (Figure 1a), with the main goal of exploring the correlation between the electronic nature of the substituents and their solid-state organization, electronic properties and semiconductor behavior.[2] On the other hand, the design and synthesis of covalent organic framework materials (constructed from the union of different covalently linked conjugated platforms) are being deeply investigated in organic electronics.[3] In line with this , we have also investigated how the structural and the electronic properties of 2D triindole-based polymers (Figure 1b) can be modulated by the (i) modification of the linkage position from para (T_2) to meta (T_3), (ii) by the insertion of different π-bridges between the cores and (iii) by the increment of the number of π-bridges from 3 to 6 units ($T_{2,3}$).[4] Overall, the results of this work open the door to the control of the degree of the π-conjugation for their subsequent synthesis and real application in organic electronic devices.

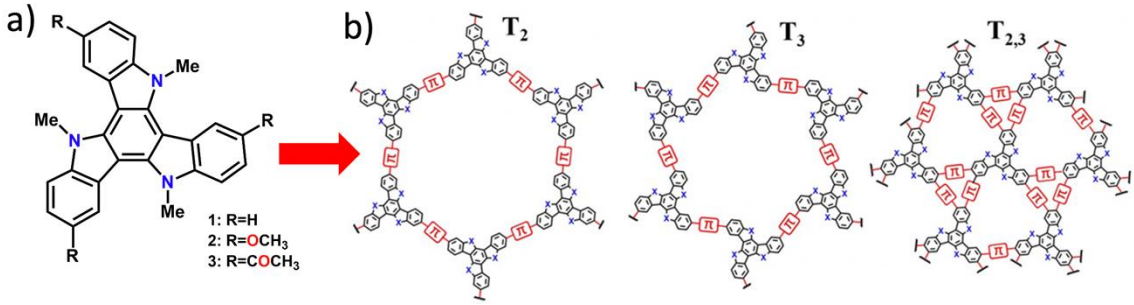

Figure 1. Chemical structures of triindoles (a) and their corresponding 2D polymers (b).

References

[1] M. Reig, G. Bagdziunas, A. Ramanavicius, J. Puigdollers and D. Velasco. Phys. Chem. Chem. Phys, **2018**, 20, 17889–17898.

[2] S. Gámez-Valenzuela, A. Benito-Hernández, M. Echeverri, E. Gutierrez-Puebla, R. P. Ortiz, M.C Ruiz Delgado and B. Gómez-Lor. Molecules, **2022**, 27, 1121-1135.

[3] C. Li, Y. Wang, Y. Zou, X. Zhang, H. Dong and W. Hu. Angew. Chem. Int. Ed. **2020**, 59, 9403–9407.

[4] S. Gámez-Valenzuela, M. Echeverri, B. Gómez-Lor, J. I. Martínez, and M.C Ruiz Delgado. J.Mater. Chem. C, **2020**, 8, 15416-15425.