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Untangling the electronic and charge transport properties of new Naphthalene and Perylene Diimides based-semiconductors.

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Abstract:

Organic semiconductors have emerged as an important class of materials that offer interesting prospects for high throughput, low-cost and flexible electronic circuits. Nevertheless, high-performance electron-transporting (n-type) semiconductors are still rare compared to their high efficiency hole-transporting (p-type) counterparts. In this sense, the development of high-mobility and environmentally stable n-type materials for thin-film transistors has experienced a tremendous impetus in the last decade. Naphthalene-diimides (NDIs), perylene-diimides (PDIs) and their derivatives have demonstrated great potential as n-type semiconductors in Organic Field-Effect Transistors (OFETs).[1-3] In this project, a mixed experimental and theoretical study of four new semiconductors (Figure 1) has been carried out with the aim to explore the impact of the following effects on the electronic and charge-transport properties: (i) the extension of the conjugated platform, going from a shorter conjugated core in naphthalene-diimides to a larger conjugated core in perylene-diimides, (ii) the different donor units attached to the cores. For that, IR, UV-Vis absorption spectroscopy, and spectroelectrochemical measurements have been used in combination with theoretical calculations based on the Density Functional Theory (DFT). In addition, the four studied compounds have been implemented in OFETs , to assess their potential as active materials in organic electronics.

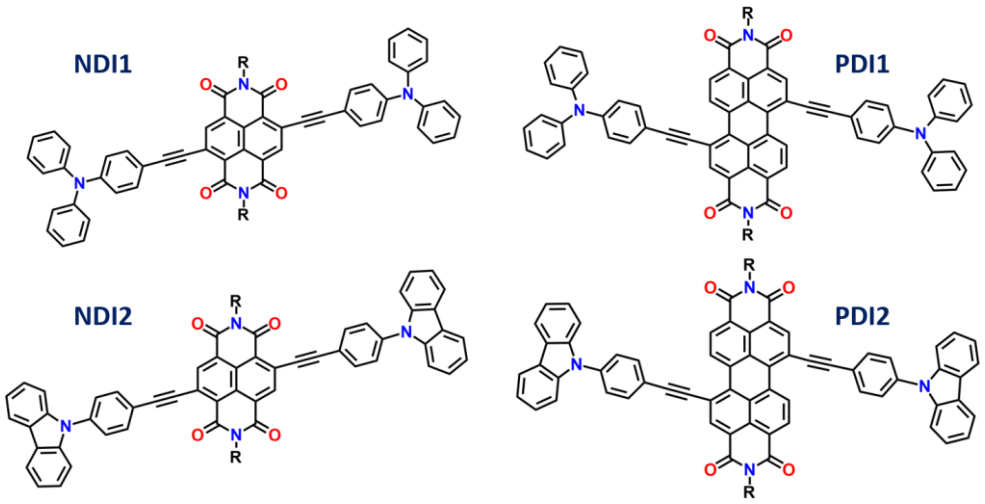

Figure 1. Chemical structures of NDI and PDI compounds under study.

References:

(1) Würthner, F.; Stolte, M. *ChemComm* **2011**, *47*, 5109.

(2) Hartnett, P. E.; Timalsina, A.; Matte, H. S. S. R.; Zhou, N.; Guo, X.; Zhao, W.; Facchetti, A.; Chang, R. P. H.; Hersam, M. C.; Wasielewski, M. R.; Marks, T. J. *J. Am. Chem. Soc.* **2014**, *136*, 16345.

(3) Zhao, Z.; Zhang, F.; Hu, Y.; Wang, Z.; Leng, B.; Gao, X.; Di, C.-a.; Zhu, D. *ACS Macro Lett.* **2014**, *3*, 1174.