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Controlling the structural flexibility of NDI-based organic semiconductors using $C_6H_6N_2$ constitutional isomers

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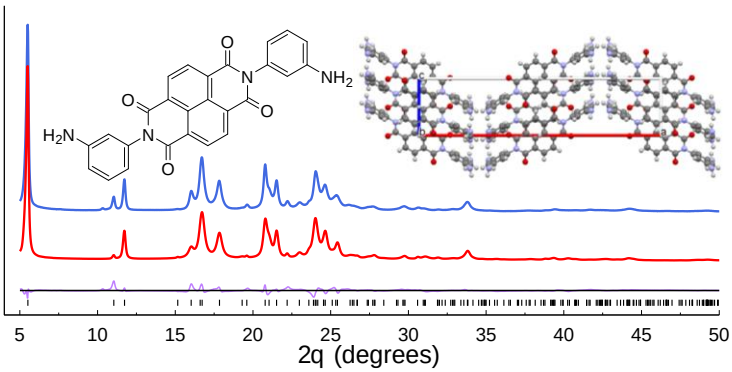

PXRD pattern of the NmpDI compound.
Inset: molecular sketch (left) and crystal packing (right) of NmpDI.

Organic thin films based on naphtalenediimides (NDIs) have attracted the attention of the researching community thanks to their interesting properties, such as excellent flexibility, easy chemical functionalization and rapid and simple processability from solution. Consequently, NDIs derivatives have emerged as promising candidates for application in photovoltaics (OLEDs, solar cells, sensors and thermoelectrics). [1] Among them, NDIs based on alkyl chain substituents have been widely studied. However, due to extended poly-morphism, they exhibit a notable structural flexibility, [2] detrimental for their implementation in devices. Hence, more rigid aryl analogues containing $C_6H_6N_2$ constitutional isomers were considered as possible alternatives. The rationale behind their syntheses, their structural diversity (crystals exhibit parallel stacking of the NDI cores) and their extreme thermal stability (with decomposition temperatures as high as 500 °C, depending on the stereochemistry of the integrated branching amino-aryls) will be discussed, together with spectroscopic, structural, electronic and optical properties and thin-film characterization. [3] Funding by MIUR, Project PRIN 2017L8WW48.

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[2] S. Milita, F. Liscio, L. Cowen, M. Cavallini, B.A. Drain, T. Degousée, S. Luong, O. Fenwick, A. Guagliardi, B.C. Schroeder, N. Masciocchi, *Polymorphism in N,N'-diaklyl-naphthalenediimides*, J. Mater. Chem. C (2020), 8, 3097-3112.
[3] V.M. Abbinante, G. García-Espejo, G. Calabrese, S. Milita, L. Barba, D. Marini, C. Pipitone, A. Guagliardi, N. Masciocchi, *Conformationally rigid molecular and polymeric naphthalene-diimides containing $C_6H_6N_2$ constitutional isomers*, 2021, under review.

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