Cholesteric Aggregation at the Quinoidal-to-Diradical Border Enabled Stable n-Doped Conductor

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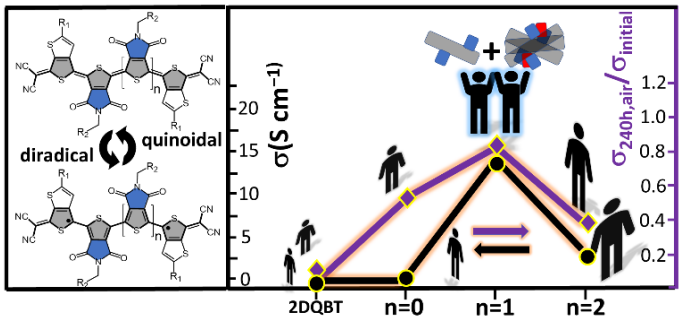
Semiconductor materials constitute the heart of solar cells since they are responsible of the photovoltaic effect. For this reason, the search of new materials to improve the efficiency and stability of these devices is on the focus of the organic electronics. These semiconductors are typically formed by p-doped materials. Despite the relative high abundance of molecules suitable for photovoltaic purposes, that is, able of absorbing light and allowing the transport of the new created charges through them, n-doped organic semiconductors are not plentiful due to their well-known ambient instability.

In this project, a series of thienoquinoidal oligothiophenes from a dimer to a pentamer and substituted with odd and even number of pyrrolo-dione groups has been proved to be n-dopable materials showing outstanding ambient stability, excellent electrical and thermoelectric behaviour. Along the series of the four compounds, a progressive change of the diradical character and of the aggregation mode converge into the tetramer to show a small-to-medium diradical character that allows favourable intermolecular contacts with π-π multi-bonding features, whereas the presence of the two dione groups promotes a particular helicoidal π-stacking piling of aggregated molecules. Both features synergistically contribute to form an excellent material with the up-to-date best ambient stability for a N-doped material with very high electrical conductivities and excellent thermoelectrical figures of merit among the known organic materials.[1]



Referencias

[1] Yuan, D., Huang, D., Medina Rivero, S., Carreras, A., Zhang, C., Zou, Y., Jiao, X., McNeill, C. R., Zhu, X., Di, C., Zhu, D., Casanova, D., and Casado, J., *Chem (accepted)*, **2019**.