

Total landscape of hydrogen-bonding in organic electronics

Gabriel Martinez¹, Amparo Ruiz-Carretero¹

¹University of Strasbourg, Institut Charles Sadron, CNRS, UPR22, 23 Rue du Loess, 67034, Strasbourg Cedex 2, France.

ABSTRACT: The presence of noncovalent interactions in organic semiconductors has been demonstrated to be beneficial in several applications, resulting in the enhancement of charge transport and device efficiency.¹ Particularly, the incorporation of H-bonding in organic semiconductors has been proven to increase solar cell efficiency by 50%.² Nevertheless, the race for achieving efficiency records has hampered research focused on solving other fundamental issues. Regarding H-bonding, no comparative studies have been performed, finding scattered examples in the literature.³ Our group works on demonstrating the power of H-bonds in organic electronics by performing comparative and systematic studies using DPP as a model ⁴, varying multiple parameters and expanding the results to state of the art derivatives. In this work, we explore two hydrogen-bonded thiophene-capped diketopyrrolopyrrole (DPP) derivatives containing amides with different topology (C- or N-centered), and compare them to a control analogue without hydrogen

bonds. We demonstrate the differences in the optoelectronic and self-assembly properties of the two amide-containing DPP derivatives, as well as in their charge carrier lifetimes. We prove the superior properties of the hydrogen-bonded derivatives in comparison to the control molecule without hydrogen bonds, and show that our molecular design strategy results in supramolecular structures with particularly long charge carrier lifetime compared to other amide-containing semiconductors reported in literature.⁵

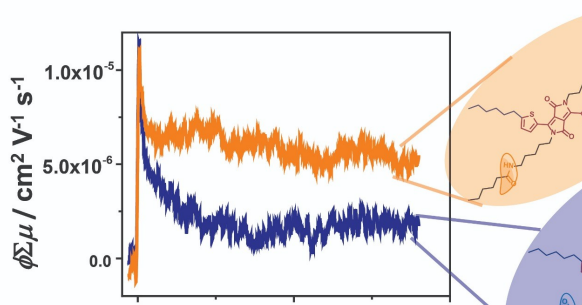


Figure: Kinetic traces of photoconductivity transients of HDPPBA-C (blue) and HDPPBA-N (orange).

KEY WORDS: organic electronics, semiconductors, H bonding, supramolecular aggregation, diketopyrrolopyrrole

References

1. T. Aida, E. W. Meijer, S. I. Stupp, *Science* **2012**, 335, 813–817
2. T. Aytun, L. Barreda, A. Ruiz-Carretero, J. A. Lehrman, S. I. Stupp, *Chem. Mater.* **2015**, 27, 1201–1209
3. T. Ghosh, J. Panicker, V. Nair, *Polymers* **2017**, 9, 112
4. A. Ruiz-Carretero, N.R. Á. Roveló, S. Militzer, P. J. Mésini, *J. Mater. Chem. A* **2019**, 7, 16777–16784
5. N.R. Á. Roveló, G. Martinez, A. Ruiz-Carretero, *et al.* *J. Phys. Chem. C* **2022**, 126, 26, 10932–10939