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funded under the Excellence Initiative program

Control of π-interactions in conjugated (macro)molecular systems for organic electronics

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ABSTRACT:

Molecular organization is a parameter of primarily importance as it affects the properties of the materials. The control of the molecular organization of π-conjugated systems can be achieved through a reasoned functionalization by flexible chains (usually aliphatic chains). The natural molecular segregation between these chains and the conjugated moieties may lead to the formation of mesomorphic organizations whose structural features can be tailored using geometric molecular parameters, in particular.

In this communication will be described the original functionalization by short siloxane chains. Compared to aliphatics, siloxane chains present a greater flexibility and a greater segregating power which allows a finer control of the organizations and the intermolecular interactions. Through some selected examples, we will illustrate the impact of siloxane chain functionalization to stabilize a complex donor-acceptor molecular system into a smectic liquid crystal organization,[1,2] or else to stabilize conjugated polymers with enhanced π-stacking interactions, ultimately leading to enhanced charge transport properties (see figure).[3]

Through other examples, we will show how functionalization with siloxane chains led to the preparation of π-conjugated molecular liquids.[4,5], e.g. compounds that are in a stable liquid state (without solvent) at room temperature. The structural characterization by X-Ray scattering shows that short-range π-molecular interactions are preserved in the liquid state, allowing us to explain the significant electronic conduction measured in these liquid molecular systems.[4]
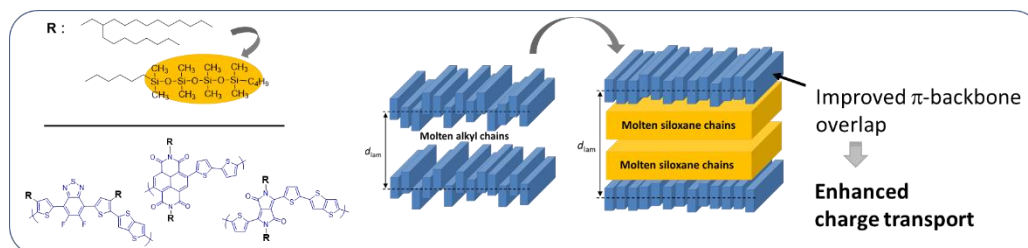
Figure. Illustration of the enhanced polymer π-stacking overlap by aliphatic-to siloxane substitution, ultimately leading to a significant improvement of charge transport properties

References
1- T. Roland, J. Léonard, G. Hernandez Ramirez, S. Méry, O. Yurchenko, S. Ludwigs, S. Haacke *PCCP*.14, 273-279, (2012)
2- M. Polkehn, H. Tamura, P. Eisenbrandt, S. Haacke, S. Méry, I. Burghardt, *J. Phys. Chem. Letters* 7, 1327 (2016)
3- N. Kamatham, O. A. Ibraikulov, P. Durand, J. Wang, O. Boyron, B. Heinrich, T. Heiser, P. Lévêque, N. Leclerc, S. Méry *Adv. Funct. Mater.* 2007734 (2020)
4- J.C. Ribierre, L. Zhao, M. Inoue, P.O. Schwartz, J.H. Kim, K. Yoshida, A.S.D. Sandannayaka, H. Nakanotani, L. Mager, S. Méry, C. Adachi, *Chem. Commun.* 52, 3103 (2016)5- J. Shaya, G. Correia, B. Heinrich, J.-C. Ribierre, K. Polychronopoulou, L. Mager, S. Méry, *Molecules* 27, 89, (2022)