NanoSaclay
Laboratoire d'Excellence en Nanosciences et Nanotechnologies

Séminaire Labex NanoSaclay

Le 30 Octobre à l'ISMO, à 11h dans l'amphi du bât. 520, au 3ème étage

Cooperation and competition mechanism of halogen and hydrogen bonding in 2D self-assembled polymorph by STM

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Abstract:

Hydrogen bond and halogen bond are two kinds of key intermolecular interactions because of their strength, directionality, and high selectivity, although the former has been more extensively studied. The competition mechanism between the formation of hydrogen bond and halogen bond in molecular self-assembly still remains obscure and predicting structures involving both hydrogen bond and halogen bond is still challenging.[1-2] Scanning tunneling microscopy (STM) allows the atomic scale characterization of two-dimensional (2D) molecular packing at room temperature and at the solid/liquid interface, which is essential to assess the intermolecular interactions. We have designed and synthesized several series of organic molecules with halogen atoms and other groups (such as C=O, –COO–, –COOH, S) systematically. Combing STM with density functional theory (DFT), we found that the competition and cooperation of halogen bond and hydrogen bond could induce the controllable polymorphic nanostructures by adjusting the solvent and solution concentration at the liquid-solid interface.[3-6] In this talk, I will show the effects of the solvent and concentration on halogen-and hydrogen-bonded nanostructures for the phenanthrene, thienophenanthrene, and fluorenone derivatives. I will also show the fabrication of chiral patterns by halogen bonding. These results will provide new insights to fabricate complex polymorphic halogen-bonded nanostructures and understand the cooperation and competition mechanism of halogen and hydrogen bonds.

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2. Arri, P. et al. Halogen bonding versus hydrogen bonding in driving self-assembly and performance of light-responsive supramolecular polymers. *Adv. Funct. Mater.* **2012**, 22, 2572–2579.

3. Hu, X. Y. et al. Effects of the position and number of bromine substituents on the concentration-mediated 2D self-assembly of phenanthrene derivatives. *Phys. Chem. Chem. Phys.* **2016**, **18,** 7208–7215.

4. Li, J. X. et al. Geometry symmetry of conjugated cores along C–Br bond effect on the 2D self-assembly by intermolecular H⋯ Br and Br⋯ Br bonds. *J. Phys. Chem. C*, **2018**, 122, 15338–15343.

5. Zha, B. et al. Controllable orientation of ester-group-induced intermolecular halogen bonding in a 2D self-assembly. *J. Phys. Chem. Lett.* **2016**, 7, 3164–3170.

6. Miao, X. R. et al. Concentration-dependent multiple chirality transition in halogen-bond-driven 2D self-assembly process. *Appl. Surf. Sci.* **2018**, 433, 1075–1082.