Chemical structures and mechanical properties of molecules studied

by high-resolution force microscopy

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Since the first direct observation of the chemical structure of pentacene, atomic force microscopy (AFM) became a powerful tool for surface chemistry.[1] The low reactivity and the tilting effect of a carbon monoxide tip, prepared at low temperature, allows us to image inner structures of molecules. Such direct observation is quite beneficial to identify the conformation of molecules on the surface, such as position, bend, tilt, and rotation. Further, via such observed molecular conformation, the angle and gap of intermolecular bonds can also be identified. Figure 1 shows an AFM image of supramolecular structure of partially fluoro-substituted phenyleneethynylene.[2] The different extents of the pi-electron induces the different diameters of non- and fluoro-substituted benzene rings (smaller: fluorobenzene).[3] We found that the molecules are aligned alternatively. The assembly is established by a weak C-F…C-H hydrogen bonding but the adoption on the corrugated substrate of $Au(110)-1\times 2$ induces the bending of molecule and consequently the length and angle of the hydrogen bond vary.

In the presentation, recent AFM studies on the C-F \cdots F-C halogen bonding (Fig.2),[4] mechanical properties of conjugated polymers [5] and on-surface chemical reaction will be present.

References:

- [1] L. Gross et al., Science **325**, 1110 (2009)
- [2] S. Kawai et al., ACS Nano 7, 9098 (2013).
- [3] N. Moll et al., Nano Letters ASAP, (2014) DOI: 10.1021/nl502113z.
- [4] S Kawai et al., (submitted).

[5] S. Kawai et al., Proc. Natl. Acad. Sci. USA 111 3968-3972 (2014).

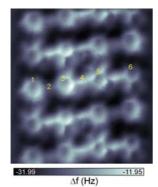


Fig. 1. AFM image of fluoro-substituted phenyleneethynylene assembly

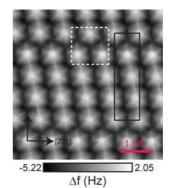


Fig. 2. AFM image of fully fluoro-substituted phenyleneethynylene assembly