Large thermal expansion of a 2D supra-molecular network in UHV

Scherb S.[1], *Hinaut A.*[1], *Vilhena J. G.*[1], *Pawlak R.*[1], *Müllen K.*[2], *Glatzel T.*[1], *Narita A.*[2], *Meyer E.*[1]

[1]Department of Physics, University of Basel, Basel, Switzerland
[2]Max Planck Institute for Polymer Research, Mainz, Germany

Thermal expansion plays an important role in the usability of materials and especially polymers in variable environments. Due to expansion or compression stress can hinder or even damage the use of materials, but also be used for specific purposes, like adjustable materials. This holds true for nanoscale applications, where functional systems can be built up by self-assembly.

In this study we report the experimental and theoretical investigation of the thermal expansion of a molecular assembly on Au(111). A shape persistent polyphenylene Spoked Wheel molecule (Fig. a,f) [1] was deposited onto Au(111) surfaces in UHV by electrospray deposition [2]. The assembly formation studied at room temperature by ncAFM and at low temperature by STM/AFM shows a large positive thermal expansion coefficient from 4.7 K to 300 K (Fig. b,c). High resolution studies of single molecules and small assemblies with submolecular resolution (Fig. f) and comparison with molecular dynamics simulations (Fig. d,e) allow us to propose an explanation of the mechanism of expansion due to alkyl chain mobility in combination with increased molecular diffusion.

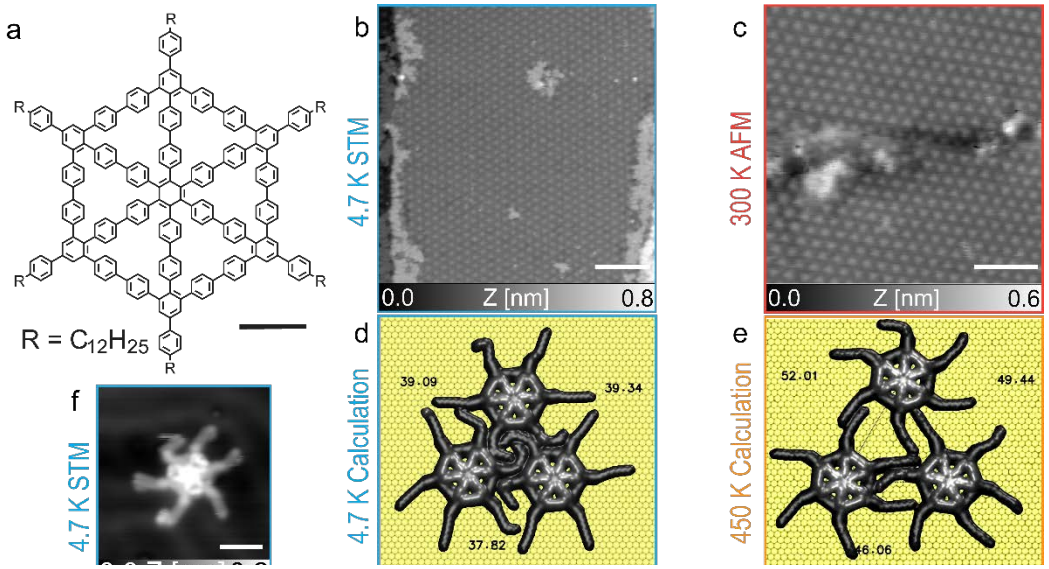

Figure 1: a: Chemical structure of graphylene-1. b,c: Scanning probe imaes at RT and LT. d,e: Calculations at LT and RT. f: Single molecule with submolecular resolution.

[1] Liu, Y. *et al.*, *J. Am. Chem. Soc.*, **138,** (2016), 15539.
[2] Hinaut *et al.*, *Nanoscale*, **10**, (2018), 1337.