

Large thermal expansion of a 2D supramolecular assembly

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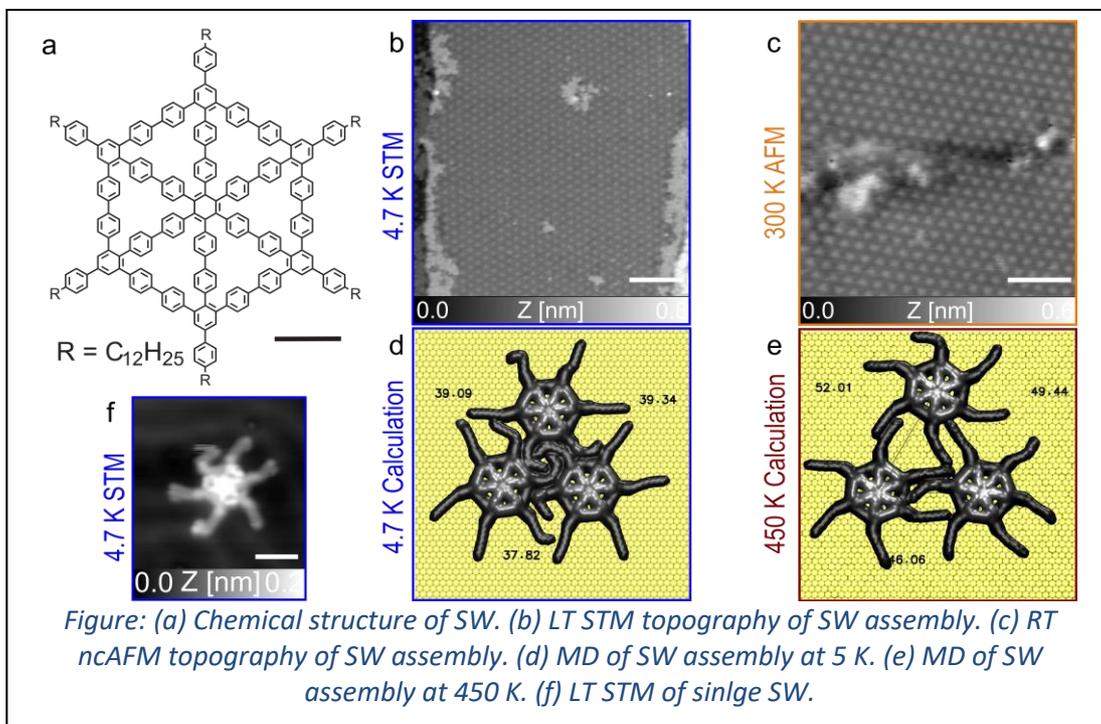
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Supramolecular chemistry allows us new avenues in understanding how single molecules, when assembled together can give rise to collective phenomena not present on single molecular level [1]. Possible uses range from sensors to molecular electronics and even to pharmaceutical sciences. Such assemblies are built up by self assembly mechanisms due to molecular recognition and result in non covalent bonded networks. For two-dimensional supramolecular chemistry not only molecule-molecule recognition, but also interactions at interfaces must be considered for the creation and tuning of the material properties.

Thermal expansion is an important aspect in the study of applicable materials, especially for mechanical uses. Fundamental studies are useful for material knowledge allowing the reduction of material aging and the elaboration of materials with thermomechanic behavior.

Here we present the study of an electro spray [2,3] deposited self assembly of shape persistent polyphenylene molecules [4] (Fig. a, f) in UHV at 5 K (Fig. b) and 300 K (Fig. c) using LT STM/AFM and RT ncAFM, respectively. Complimenting with state-of-the-art, micro-second long all atom molecular dynamics simulations of the formed molecular assemblies (Fig. d, e), we find that alkyl chain functionalizing molecular cores promotes large thermal expansion of the molecular network when heated as a result of entropic effects enhanced by large fluctuations experienced by the alkyl chains.



References:

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