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Large thermal expansion of a self-assembling monolayer in UHV — ●SEBASTIAN SCHERB¹, ANTOINE HINAUT¹, GUILHERME VILHENA¹, RÉMY PAWLAK¹, AKIMITSU NARITA², THILO GLATZEL¹, and ERNST MEYER¹ — ¹Department of Physics, University of Basel, Basel, Switzerland — ²Max Planck Institute for Polymer Research, Mainz, Germany

Self-assemblies of structurally complex molecules in UHV provide interesting prospects for applications in optoelectronics, nanomechanical devices and molecular electronics. To investigate their viability for specific applications, high-resolution studies of their behavior under a variety of conditions are required.

In this study we report the experimental and theoretical study of the adsorption behavior of a molecular assembly on Au(111) under different thermal conditions. A shape persistent polyphenylene Spoked Wheel molecule [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 LT to RT. Comparing with molecular dynamics simulations we propose an explanation of the mechanism of expansion due to alkyl chain mobility in combination with increased molecular diffusion.

[1] Liu, Y. et al., J. Am. Chem. Soc., 138, 15539-15542 (2016). [2] Hinaut et al., Nanoscale, 10, 1337-1344 (2018).

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Topic: Organic molecules on inorganic substrates:
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