

Force-Induced Inversion of Bowl-Shaped Molecule Sumanene

K. Iwata,^{1, #} R. Kuno,² I. Hamada,² H. Sakurai,³ and Y. Sugimoto¹

¹*Department of Advanced Materials Science, University of Tokyo, Kashiwa, 277-8561, Japan*

¹*Department of Precision Engineering, Osaka University, Suita, 565-0871, Japan*

¹*Division of Applied Chemistry, Osaka University, Suita, 565-0871, Japan*

Presenting author's e-mail: kiwata@g.ecc.u-tokyo.ac.jp

Mechanical stimuli, such as compression, tensile, or shear stress, applied on solid sometimes induces chemical reaction. Such mechanically induced reaction is known as the “mechanochemistry” and attract great interest. In recent decade, thanks to the high spatial resolution of the scanning tunneling microscope (STM) and atomic force microscope (AFM), many chemical reactions have been studied in the single molecule scale. However, in general, studies on mechanochemistry have been performed on a macroscopic scale. So far, only a few experiments reported the structural changes of single organic molecule induced by the mechanical stimuli from the tip of scanning probe microscope [1-3].

In this study, we demonstrate the structural change of single molecule induced by the mechanical stimuli from an AFM tip. We investigated bowl-shaped molecule, sumanene, shown in Fig. (a). Inversion of a bowl is expected by simply applying the force by the AFM tip. Experiments were carried out using a qPlus based AFM/STM system operated in ultra-high vacuum at 5 K. Figure (b) shows a high-resolution AFM image of sumanene layer on an Au(111) substrate. Sumanene layer consists of bowl-up and -down sumanenes and form a 6×6 periodicity. This structure is different from the previously reported sumanene layer on Au(111) [3] but is rather similar to that on Ag(111) [4]. This is because we successfully prepared a sumanene layer with a monolayer thickness. We performed force curve measurement above sumanene in the bowl-down structure. A sudden jump of force curve was observed in repulsive regime. Subsequent imaging confirmed successful structural inversion from bowl-down to bowl-up. With the support of theoretical calculations, the mechanism of inversion will be discussed in detail.

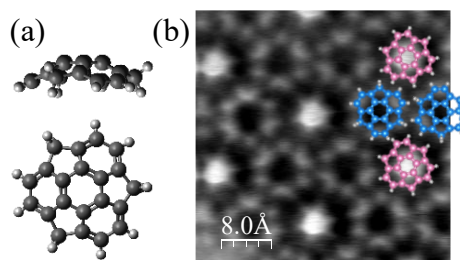


Figure (a) Side and top views of sumanene. Black and white spheres represent C and H atoms. (b) High resolution AFM image of the sumanene layer. Positions of bowl-up (blue) and -down (pink) sumanenes determined based on the AFM image are partially overlaid.

References

- [1] R. Pawlack et al., ACS Nano **6**, 6318 (2012).
- [2] J. N. Ladenthin et al., Nat. Chem. **8**, 935 (2016).
- [3] A. Ishii et al., Chem. Sci. **12**, 13301 (2021).
- [4] S. Fujii et al., J. Am. Chem. Soc. **138**, 12142 (2016).
- [5] R. Jaafar et al., J. Am. Chem. Soc. **136**, 13666 (2014).