Characterization and Single-Molecule Reactions of Trioxosumanene /Au(111)

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Recently, attempts to induce chemical reactions using mechanical stimuli such as compression, tension, or shear stress have been attracting interest [1]. However, experimental measurements of macroscopic systems, which consist of a number of molecules on the order of Avogadro's constant, inherently provide only ensemble-averaged information. Research at the single-molecule level does exist, but it is limited [2,3]. Consequently, insights into the microscopic mechanisms of such mechanochemical processes remain poor.

The purpose of this study is to investigate mechanochemical reactions at the single-molecule level. To achieve this goal, we characterized the structural and electronic properties of trioxosumanene (TOSUM) [Fig. 1(a)] on Au(111) by scanning tunneling microscopy (STM) and atomic force microscopy (AFM). During the STM measurement, we found that TOSUM/Au(111) react via tunneling electrons, as shown in Fig. 1(b). The formation of two distinct product types was observed to be dependent on the bias voltage. Their identification of these products was performed through scanning tunneling spectroscopy and high-resolution AFM imaging. Additionally, a force-induced single-molecule structural change by the localized force from AFM tip will be discussed.

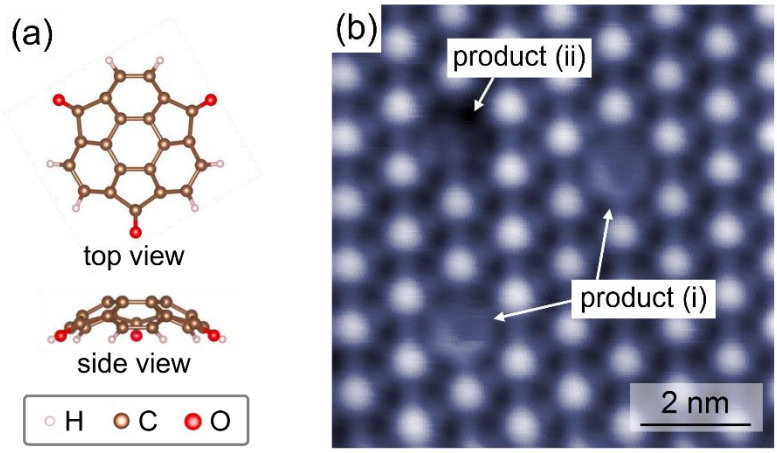

Figure 1. (a) Ball-and-Stick model of TOSUM (b) STM image of TOSUM layer on Au(111). Two product types of current-induced reactions can be distinguished. Imaging condition: Constant current mode. V = 2.0 V, I = 50 pA, T = 77 K.

Reference

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[3] A. Ishii et al., Chem. Sci. **12**, 13301 (2021).