Manipulating the dynamic motion of confined trimethylphosphine molecules in self-assembled pyrrole molecular fences

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Introduction - Devices with various electronic functions using single molecules can be tailored, based on their inherent properties. Our group has confined trimethylphosphine (TMP) molecules in pyrrole molecular fences and this can be used as a molecular switch or memory device in quantum computers if the motion of the TMPs can be controlled [1]. In this study, we have attempted to manipulate the dynamic motion of TMP by changing bias conditions and tunneling current conditions of scanning tunneling microscopic (STM) measurements.

Experimental - The STM measurements were carried out under ultra-high vacuum (1×10^{-8} Pa) conditions using a chemically etched tungsten tip. As the substrate, small pieces (1 mm × 7 mm) of n-type Si (111) was used. The Si sample was cleaned by flash heating under UHV conditions and highly ordered Si(111)-(7×7) structure was obtained. Cleaned Si surface was directly exposed to 1.5 L (Langmuir, 1L = 1×10^{-6} Torr s) of purified pyrrole gas. Then, the sample was exposed to 0.5 L of TMP gas. Dosing process and STM measurements were carried out at room temperature. Finally, the dynamic motion of TMP molecules imaged under different conditions.

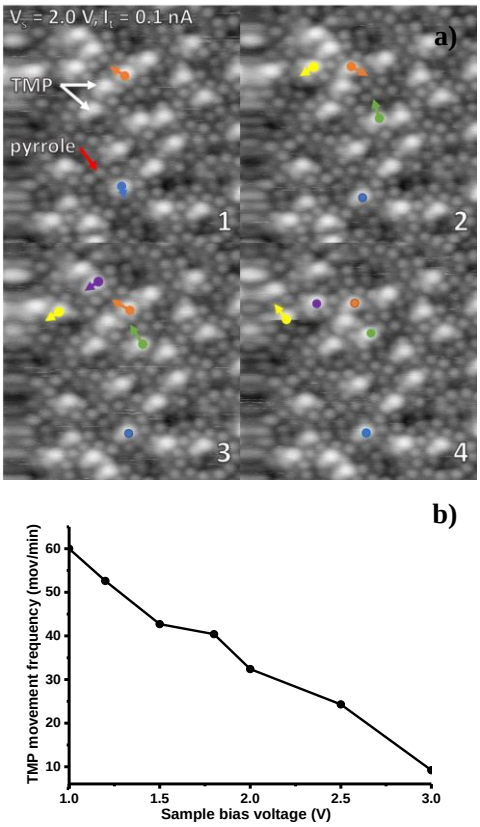

***Fig 1**. a) Continuous STM images showing TMP movement in pyrrole molecular fence and b) TMP movement dependency at different sample bias*

Results and discussion - Bright spots marked with white arrows in the first STM image of Fig 1.(a) show the TMP molecules confined in pyrrole molecular fence, marked with red arrow. We observed that TMP movement would occur more often if the positive sample bias was decreased. The relationship between the TMP movement and the positive sample bias is shown in Fig 1.(b). Also, we observed that changing tunneling current would not affect the movement of TMP molecules significantly. Therefore, we can suggest that TMP movement may be affected due to the shallow electronic states present in TMP adsorbates. At lower bias conditions, Si-TMP antibonding orbital get stimulated efficiently by incoming tunneling electrons from the tip, weakening the bond and forcing TMP molecules to move more frequently.

Conclusion – The movement of TMP molecules inside the pyrrole molecular fence can be manipulated by changing the sample bias. Tunneling current does not have a significant effect regarding this.

References - [1] M. Shimomura, A. Iwanabe, and T. Kiyose, The Journal of Physical Chemistry C **118**, 27465 (2014).