

### 分子が電子に逢ったとき

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The study of single molecules provides new insights into quantum mechanics and the nature of chemical bonding that forms the critical bases for controlling the properties and functions of nanometer-scale materials. The scanning tunneling microscope (STM) is a versatile and powerful tool for investigating individual molecules on the surface. One of the most striking characteristics of the STM is that its operation involves tunneling electrons. The coupling of tunneling electrons to the electronic and vibrational states of the target molecule allows us to image, manipulate, spectroscopically characterize the single molecule.

In this talk, I will address three main issues with a concerted experimental and theoretical effort. The first part is assigned to the novel method for detecting vibrational signals of molecules showing motions induced by injecting tunneling electrons [1-6]. In the second part, I discuss how the spatial distribution of MOs of an adsorbate at resonant states can affect electron-vibration coupling and thereby affect the resulting molecular motions and reactions, based on the experimental findings and density functional theory (DFT) calculations [3,5]. This provides a deeper understanding of the electron interaction with individual molecules in the STM junction and of molecular dynamics controlling reactions on surfaces at a single-molecule level. Finally, I will introduce state-controlled reaction of a water molecule at the surface of a ultrathin insulating film, where the lifetime of excited states are greatly elongated [6].

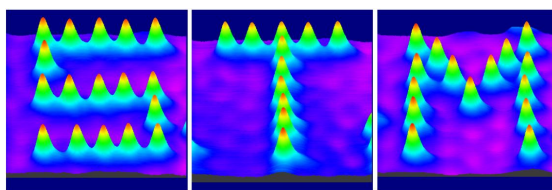


Figure: Three-dimensional images of the letters, S, T, and M with  $\text{CH}_3\text{S}$  molecules of  $\text{Cu}(1,1,1)$ .

#### References

1. Y. Kim, T. Komeda, M. Kawai: Phys. Rev. Lett. 89 (2002) 126104.
2. T. Komeda, Y. Kim, M. Kawai, B.N.J. Persson, H. Ueba: Science 295 (2002) 2055.
3. Y. Sainoo, Y. Kim, T. Okawa, T. Komeda, H. Shigekawa, M. Kawai: Phys. Rev. Lett. 95 (2005) 246102.
4. S. Katano, Y. Kim, M. Hori, M. Trenary, and Maki Kawai: Science 129 (2007) 1883.
5. M. Ohara, Y. Kim, M. Kawai: Phys. Rev. Lett. 100 (2008) 136104.
6. H-J. Shin, J. Jung, K. Motobayashi, H. Yanagisawa, H. Morikawa, Y. Kim, M. Kawai: Nature Materials (2010) in press.

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