Role of a tip apex in AFM/STM for manipulation and vibrational spectroscopy of a CO molecule

Norio Okabayashi
Graduate School of Natural Science and Technology, Kanazawa University

The role of a tip apex in scanning probe microscopy (SPM) is very important in the manipulation and vibrational spectroscopy of a molecule adsorbed on a metal surface. The apex of a metallic tip in SPM has a dipole moment due to the Smoluchowski effect (Fig. 1(a)) [1]. When the tip whose apex consists of a single atom is located on a CO molecule which also has the dipole moment, however, its direction is opposite to that of CO molecule (Fig. 1(a)), the attractive force acts between the tip and the CO molecule. Owing to this attractive force, when the tip is scanned over the CO molecule, we see the dip in the constant-height frequency shift image. Recently it was reported that the number of the dip in the frequency shift image corresponds to the number of the atoms at the tip apex, which is in contrast to the case of the tunneling current showing always dip regardless of the tip-apex atom number (Fig. 1(b)-(e)) [2].

In this presentation, I will talk on the manipulation of a CO molecule on a Cu(111) surface which takes place only by the force between the tip and molecule, i.e., the vibrational excitation is not essential in the present case. We have found that not only the lateral force bending the CO molecule but also the vertical force changing the conformation of the CO molecule synergistically contribute to the manipulation [3]. In order to investigate the conformation change of a CO molecule during the manipulation, inelastic electron tunneling spectroscopy (IETS) is effective. Toward that purpose, firstly the role of a tip apex to yield a higher-intense IET signal is investigated. We have found that the tip whose apex consists of a single atom provides the four times larger IETS signal over the tip whose tip apex consists of three atoms (Fig. 1(f)) [4]. This finding was interpreted in terms of (1) the ratio of the current through the molecule to the total current and (2) efficiency of the inelastic process for the tunneling involving the CO molecule. With relevance to the main topic, I will also talk on (i) the IETS on alkanethiol self-assembled monolayers [5-7] and (ii) fluorine ions desorption from a F/Si(100) surface by the irradiation of highly charged ions [8].

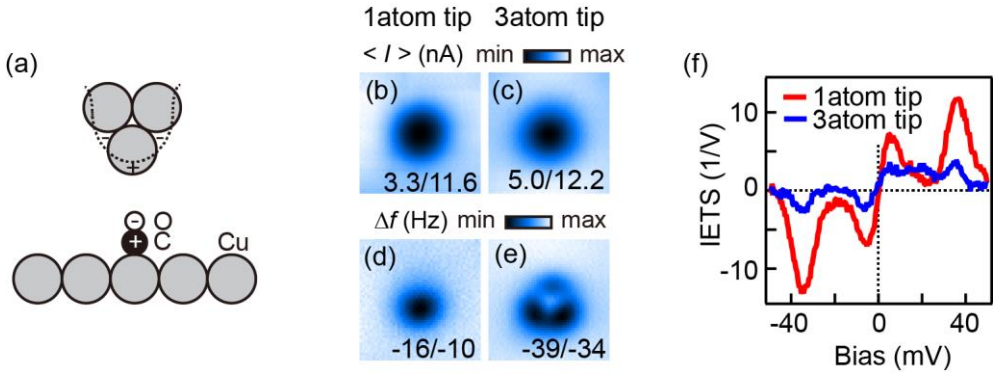

Fig.1 (a) Schematic image of dipole moments at the apex of the tip and the CO molecule. Constant-height, (b)[(c)] current and (d)[(e)] frequency shift images for a CO molecule on Cu(111) by a single-atom tip [three-atom tip]. (f) Normalized IETS for a CO molecule with a single-atom tip [three-atom tip].

[1] M. Schneiderbauer, F. J. Giessibl et al., Phys. Rev. Lett. **112**, 166102 (2014).
[2] M. Emmrich, F. J. Giessibl et al., Science **348**, 308 (2015).
[3] M. Emmrich, M. Schneiderbauer, F. Huber, A. J. Weymouth, N. Okabayashi, and F. J. Giessibl, Phys. Rev. Lett. **114**, 146101 (2015).
[4] N. Okabayashi, A. Gustafsson, A. Peronio, M. Paulsson, T. Arai, and F. J. Giessibl, arXiv:1504.04790
[5] N. Okabayashi, Y. Konda and T. Komeda, Phys. Rev. Lett. **100**, 217801 (2008).
[6] N. Okabayashi, M. Paulsson, H. Ueba, Y. Konda, and T. Komeda, Phys. Rev. Lett. **104**, 077801 (2010).
[7] N. Okabayashi, M. Paulsson, H. Ueba, Y. Konda, and T. Komeda, Nano Letters **10**, 2950 (2010).
[8] N. Okabayashi, K. Komaki, and Y. Yamazaki, Phys. Rev. Lett. **107**, 113201 (2011)