Dipole induced repulsive manipulation of single molecules
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Carbon monoxide (CO) is one of the simplest molecules has a strong impact on the conductance of atomic-size metal contacts. In related to this, AFM/STM single metal and molecular manipulation has been widely done to understand this phenomenon. Single metal and molecular manipulation has been done by utilizing a few interactions in scanning probe microscopy i.e.; (i) the metal-metal interactions, (ii) metal-molecule interaction, (iii) the electron transfer from the tip which excites the CO horizontal stretching mode and causes energy transfer to the in-plane vibration and lead to lateral hopping of molecules, (iv) tip-induced reduction of the activation energy barrier between adjacent nanospaces, allowing diffused atoms to jump into the desired nanospace, accompanied by atom trapping below the tip.

In this research, we demonstrate the lateral hopping of CO molecule on Cu (111) substrate due to the electronic dipole induced repulsive force from CO-terminated tip, which is different from molecular manipulation done so far. This would bring new insights on the CO molecular dynamics. One of the advantage from this method is that even without excitation, with the use of low current mode, there are possibility that molecular manipulation on insulator could be applied. In other words, molecules which exhibits similar dipoles interaction could expand the variation on the same system.

Here, interactions between (i) CO monomer and CO monomer, as well as (ii) CO monomer and CO dimer were studied by means of our home-built UHV-STM set up working at 5 K with combinations of CO-tip and CO single molecules adsorbed on an atomically-flat Cu (111) substrate, together with theoretical DFT calculations. From experimental result, we could observe a big difference in the I-z curve with bare-tip or CO-tip. Theoretical calculations show that with bare-tip, attractive force dominates, whereas with CO-tip, repulsive force dominates. During the approaching process between two CO monomers, both molecules have been considered to tilt due to repulsive interactions. We could deduce that the hopping during the use of CO-tip was due to the repulsive dipole moment induced by the adsorbed CO molecule on the substrate. This new mechanism differs from reported lateral hopping system up till now. The effect of the repulsive dipole moment was also checked by the difference in the I-z curve of CO-dimer and CO-monomer. The drop in the conduction value also supports the different repulsive potential distributions that occur between the monomer (~60 nA: 0.0015 G₀ -> 30 nA) occurs at z~160 pm and dimer (~80 nA: 0.0020 G₀ -> 40 nA) occurs at z~130 pm. The CO-dimer produces larger electrostatic potential compared to the CO-monomer, pointing that the system has a stronger dipole than the CO monomer, where during hopping, the tip position is farther compared to the monomer system.