Dissipative Dynamics in Single-Molecule Manipulation

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The manipulation of single molecules using a scanning tunneling microscope (STM) or atomic force microscope (AFM) probe has been widely studied as a model system for exploring friction. Previous work has mainly focused on the forces that induce manipulation [1], while dynamics and energy dissipation have received little attention. Here, we investigate these aspects using a system of a carbon monoxide (CO) molecule adsorbed on a copper surface under ultra-high vacuum and low-temperature conditions. Our approach combines STM, AFM, lateral force microscopy (LFM), inelastic electron tunneling spectroscopy (IETS), and density functional theory (DFT) calculations.

Our model is based on DFT results shown in Fig. 1, where preferred CO adsorption sites on Cu(110) are mapped by varying the probe position laterally and vertically [2][3]. The probe scans along the $[\bar{1}10]$ atomic row, with d representing the Cu atom spacing; x/d = 0 and 1 correspond to top sites, and 0.5 to a bridge site. The light gray, blue, and red regions indicate CO adsorbed at top, adjacent top, and bridge sites. When the probe reaches the height marked by the green dashed line, manipulation from top to adjacent top begins. Further approach induces transitions from top to bridge and then to the adjacent top.

Experiments support this model. Site changes between top and bridge along the red line are confirmed by IETS [3]. When using conventional AFM (tip oscillating perpendicular to the surface), energy dissipation is observed only along the red line, consistent with theory [2][3]. This agreement supports our model, though the dissipation is not directly attributable to manipulation-induced energy loss. In contrast, with LFM, dissipation appears not only along the red line but also the blue, clearly linked to manipulation [4]. Additionally, current fluctuations from switching between two adsorption states are measured at fixed tip positions as functions of lateral and vertical displacement, reinforcing this interpretation [4]. These findings enable quantitative evaluation of the work required to sustain molecular manipulation.

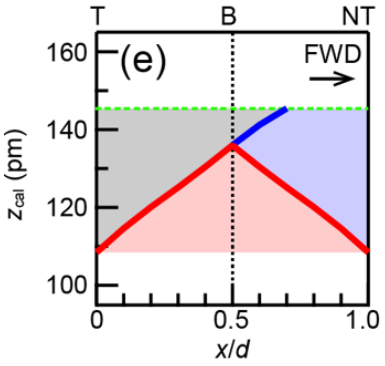

Fig.1. Calculated configurations of a CO molecule as a function of tip height and lateral position.

References

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