INVITED ORAL PRESENTATION

Non-contact atomic force microscopy as a tool for catalysis research

Eric I. Altman
Department of Chemical and Environmental Engineering, Yale University, New Haven, CT 06520 USA

The ability to image surfaces with atomic resolution has been a boon to catalysis research over the last 40 years. One atomic resolution imaging method that has received less attention is non-contact atomic force microscopy (NC-AFM), despite its ability to quantify the interactions that govern catalysis at the individual surface atom level. In this talk I will provide an overview of the method and the steps we have taken to simplify it through the development of tuned-oscillator AFM and to obtain quantitative force and energy data with 0.01 Å spatial resolution through three dimensional atomic force microscopy(3D-AFM). I will then discuss our recent applications of these methods to problems in catalysis. It will be shown how NC-AFM in conjunction with 3DAFM can be used to extract surface diffusion barriers and how they are affected by the surrounding environment. The focus is on the diffusion of benzene and phenyl radicals on Cu(100). For benzene, the results indicate that the molecules were either pushed, pulled, jumped to the tip or did not move, depending on both the chemical surroundings on the surface as well as the chemical identity of the tip. Comparison with theory suggests that the tip lowers the energy barrier the benzene must overcome to translate on the surface, which evolves with the chemical identity of the tip. Meanwhile, the missing H of the phenyl radical opens up additional motions including rotation and flipping of the molecule around the C-Cu bond. Different jump distances and barriers were seen that may be associated with these motions. Next, I will discuss how we are using functionalized tips to image the structure and characterize key interactions in immobilized molecular CO_2 reduction catalysts. By functionalizing the AFM tip with Co it was possible to not only image the structure of a promising Co phthalocyanine (CoPc) that efficiently converts CO_2 to methanol but also generate force and potential energy interaction maps between the tethered CO and the CoPC catalyst. From this data, maps of catalytically important equilibrium distances and bonding energies could be generated.