Tuning Dihydrogen Adsorption at Metal Centers of Surface-supported Supramolecular Networks

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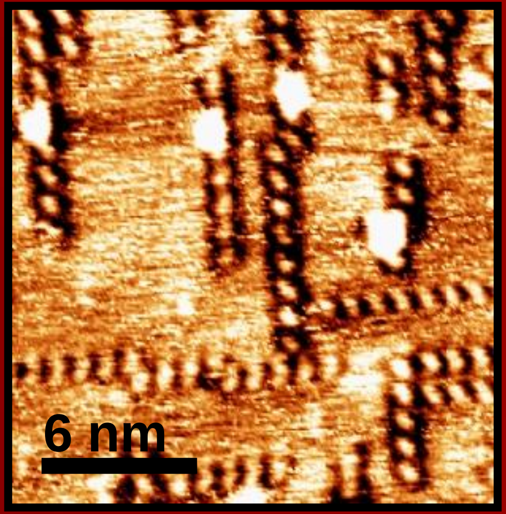
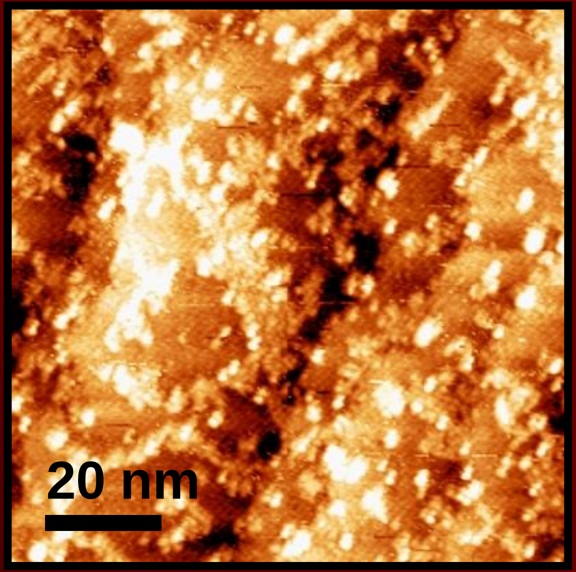
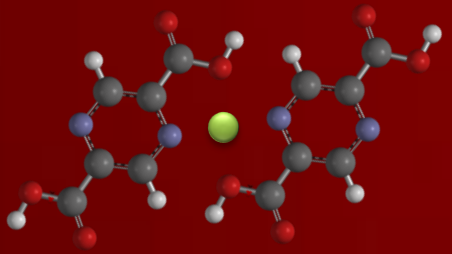
The goal of this project is to utilize coordinatively-unsaturated metal centers in **metal—organic frameworks at surfaces** to study the tuning of these metal sites for dihydrogen adsorption. The delicate challenge of binding the intact dihydrogen molecule requires stable adsorption at the metal site through donation of σ electrons from H_2 to unoccupied *d* orbitals of the metal, while avoiding excessive back donation to the H_2 anti-bonding orbital. We are studying a new type of binding site, a metal-organic complex at a solid surface. We have obtained molecular resolution images of self-assembled 2,5-pyrazine dicarboxylic acid (PDA) nanostructures on the Cu(100) surface, as well as results of the complexation of that molecule with Cr.

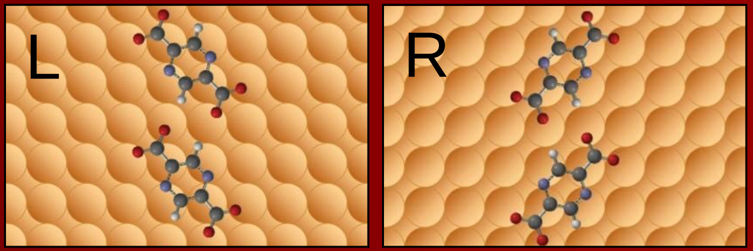


One-dimensional, self-assembled chains of PDA on Cu(100) at room temperature.
Image size 20 nm x 20 nm.





Surface complexes of
PDA + Cr on Cu(100) by STM.
Image size 100 nm x 100 nm.



Upon adsorption, PDA molecules adopt one of two adsorption chiralities and assemble into enantiopure chains.