

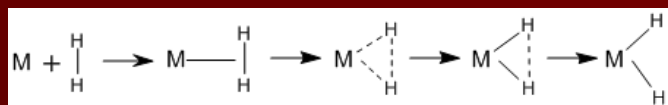
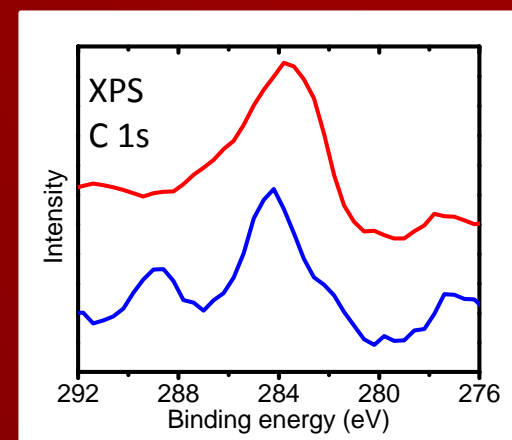


Tuning Dihydrogen Adsorption at Metal Centers of Surface-supported Supramolecular Networks

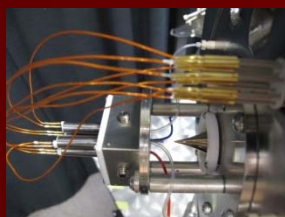
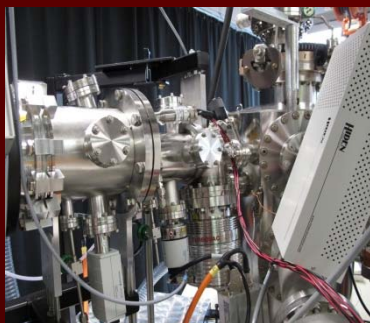
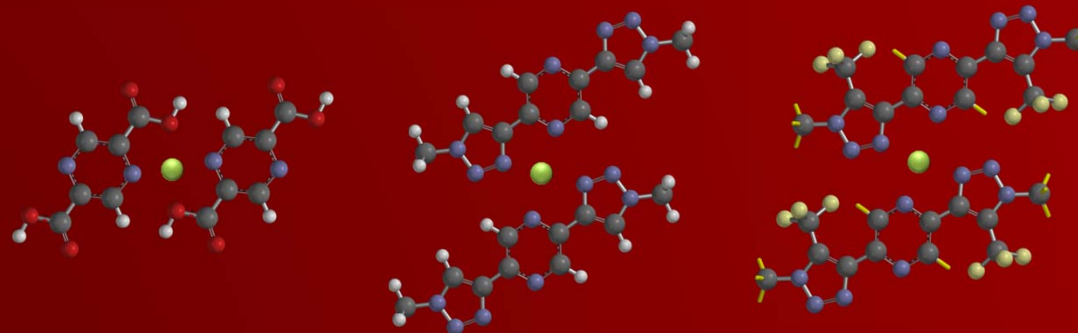
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We utilize coordinatively-unsaturated metal centers in **metal—organic frameworks at surfaces** to study the tuning of these metal sites for dihydrogen adsorption. The delicate challenge of binding the intact dihydrogen molecule requires stable adsorption at the metal site through donation of σ electrons from H_2 to unoccupied d orbitals of the metal, while avoiding excessive back donation (BD) to the H_2 anti-bonding orbital. This balance determines the difference between molecular H_2 adsorption vs. $H-H$ scission and hydride formation (see scheme below). Tuning is accomplished by substituting electron donating or withdrawing groups on the ligands.



Metal – dihydrogen interaction at varying strengths. For weak BD (left) the H_2 molecule is weakly attached and remains intact. With increasing BD (to the right), hydride formation occurs.



Organic and metal components are vapor deposited to a surface and characterization by photoelectron spectroscopy (see figure) and scanning tunneling microscopy. We characterize chemical function and binding strengths using a new pulsed supersonic molecular beam (photos) and mass spectrometer.