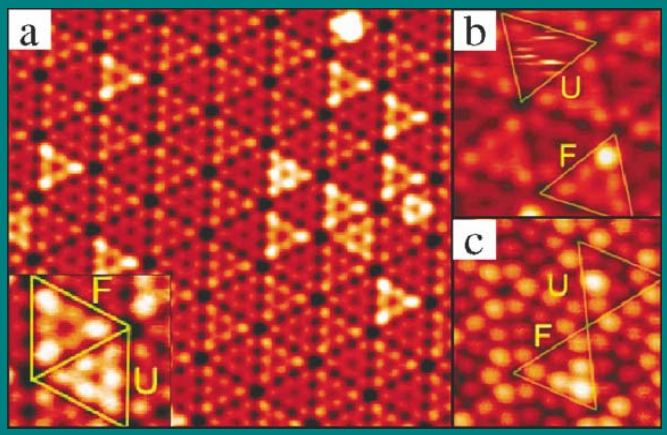
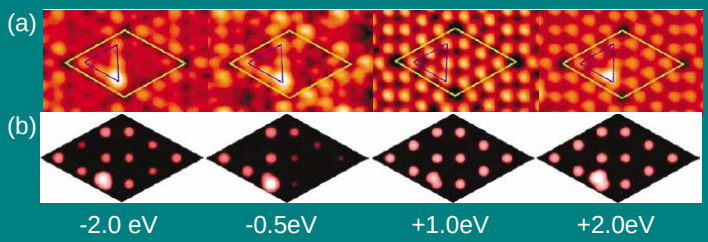
Experimental and Theoretical Investigation of Single Cu, Ag, and Au Atoms Adsorbed on Si(111)-7×7

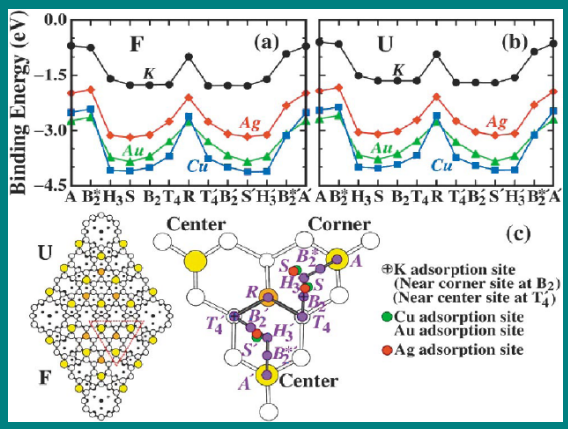
Phys. Rev. Lett. **94**, 176104(2005), Chun Zhang, Gang Chen, Kedong Wang, Hongwei Yang, Tao Su, C.T. Chan, M. M. T. Loy, Xudong Xiao



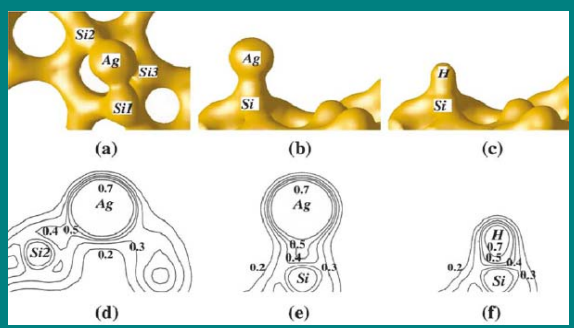
Topographic STM images of Ag on Si(111)-7×7 at (a) 298, (b) 78, (c) 5 K. The tunneling current and sample bias are set 50 pA and -2 V, respectively. The fuzzy image in UHUC at 78 K is due to the nonfrozen motion of Ag. The insert in (a) gives typical images of single Ag in FHUC and UHUC, respectively, showing brightness contrast between the corner and center spots.



(upper) STM images of a single Ag atom in the faulted Si(111)-7×7 half unit cell at 77 K for a number of sample biases.
(lower) the simulated STM images, with the charge density calculated at 3 Å above the Ag adatom.



The binding energy obtained from the first principle calculations for K, Cu, Ag and Au at selected sites in (a) FHUC and (b) UHUC. (c) The DAS model and the basin on which the selected sites are labeled.



The isosurfaces of charge density at 0.3e/Å^3 plotted for (a) Ag at S site (top view), (b) Ag, and (c) H at corner Si adatom site (side view) in FHUC. (d)-(f) are the corresponding charge density contours in the cross section of the bonds (e/Å^3).

Using STM and density functional calculations, we systematically identified the adsorption sites of single Cu, Ag, and Au atoms on the Si(111)-7×7 surface. Despite their monovalence, the atoms were found to adsorb at high coordinate sites to saturate the maximum number of dangling bonds. This is in contrast with the conventional idea that monovalent atoms on Si surfaces saturate the dangling bonds by forming a covalent bond.