Charge Measurement of Atoms and Atomic Resolution of Molecules with Noncontact AFM
LEO GROSS, IBM Research - Zurich

Individual gold and silver adatoms [1] and pentacene molecules [2] on ultrathin NaCl films on Cu(111) were investigated using a qPlus tuning fork atomic force microscope (AFM) operated at 5 Kelvin with oscillation amplitudes in the sub-Ångstrom regime. Charging a gold adatom by one electron charge increased the force on the AFM tip by a few piconewtons. Employing Kelvin probe force microscopy (KPFM) we also measured the local contact potential difference (LCPD). We observed that the LCPD is shifted depending on the sign of the charge and allows the discrimination of positively charged, neutral, and negatively charged atoms. To image pentacene molecules we modified AFM tips by means of vertical manipulation techniques, i.e. deliberately picking up known atoms and molecules, such as Au, Ag, Cl, CO, and pentacene. Using a CO terminated tip we resolved all individual atoms and bonds within a pentacene molecule. Three dimensional force maps showing the site specific distance dependence above the molecule were extracted. We compared our experimental results with density functional theory (DFT) calculations to gain insight on the physical origin of AFM contrast formation. We found that atomic resolution is only obtained due to repulsive force contributions originating from the Pauli exclusion principle.