AFM on a Hydrogenated Si 7x7 Surface: Exploring Different Interaction Regimes

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The non-contact atomic force microscope (nc-AFM) allows us to probe forces acting between the apex of the AFM probe and the surface of the sample on the atomic scale. Especially when the imaging mode is combined with an on-site force spectroscopy [1], valuable information on the character of inter-atomic forces can be obtained [2,3]. However, the detected forces and the mechanism by which they arise may differ markedly depending on the structure and reactivity of the AFM-tip termination. Here we have explored the interaction between an AFM probe and the Si (111)-7x7 surface exposed to a low-coverage of atomic hydrogen at RT, both experimentally and theoretically. We have identified two profoundly different types of tip termination, distinguished by the image contrast as well as the interaction forces measured over the hydrogen-passivated and non-passivated Si adatoms. The statistics of the tip-dependence of the measured forces, which are obtained using various tip states with different cantilevers, reveals the typical values of the force and their distribution in the two characteristic interaction modes. Our experimental results were corroborated by density functional theory (DFT) calculations performed for different atomic models of tips in order to interpret the observed force curves (see Fig. 1).
In this contribution, we will point out the role of the chemical reactivity and the van der Waals forces in terms of chemical composition of the tip-apex termination. Finally, we will also discuss the mechanisms of interaction forces by combining the projected density of states (PDOS) calculations with the maps of electron density redistribution at the tip-sample interface.

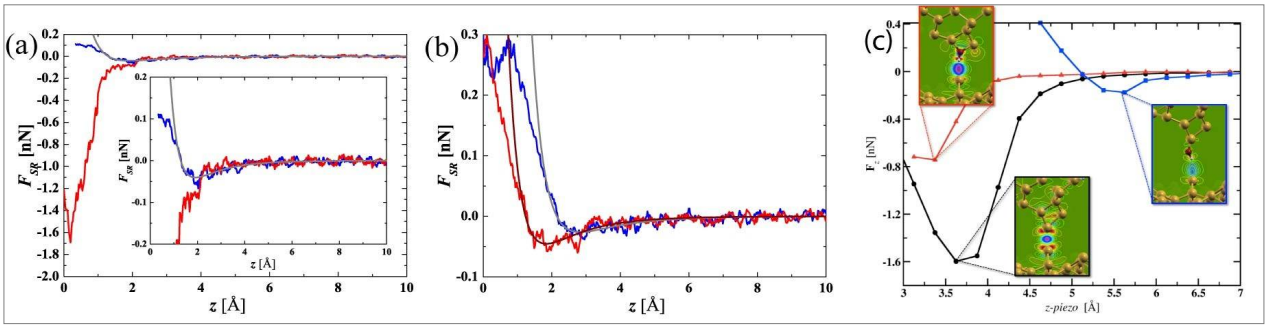

Fig. 1: Short-range interaction forces over Si (red) and hydrogen-passivated Si (blue) adatoms recorded using a reactive tip **(a)** and a non-reactive tip **(b)**. **(c)** Calculated short-range force curves for three different tip models on Si adatom. Inset: the charge density difference maps between tip and a surface silicon adatom at a distance close to the maximum attractive short-range force.

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[3] L. Gross et al. Science 325, 1110–1114 (2009).