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Atomic Force Microscopy Characterization of Hydrogen Terminated Silicon (100) 2x1 Reconstruction

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Hydrogen terminated silicon (100) 2×1 (H:Si(100)) is examined using a novel non-contact atomic force microscopy (NC-AFM) approach. NC-AFM gives access to unique information on the surface such as unperturbed surface charge distributions, chemical bonding, and surface forces.

H:Si(100) is an attractive surface for examination due to its potential for nano-electronics. Dangling bonds on the surface act as atomic silicon quantum dots and have application in quantum dot cellular automata-based nano-computing, which through geometrical arrangement can be used to create ultra-fast, ultra-low-power wires and logic gates. It also provides a promising platform for AFM examination of electronically decoupled adsorbed atoms, physisorbed molecules, and chemisorbed molecular structures.
As part of this AFM analysis of H:Si(100), images were taken in the as yet unexplored constant height scanning mode. By incrementing the tip-sample distance above the surface, different force regimes were accessed. Attractive van der Waals forces were observed in the long range, and repulsive interactions indicative of Pauli-repulsive forces were seen at close range. An evolution of surface topography from attractive to repulsive surface forces is demonstrated, with the repulsive regime showing the first direct observation of the chemical bond structure of H:Si(100).

Furthermore, site-specific force spectroscopy on key surface lattice points reveals unique force contributions. These location-specific profiles are compared to Density Functional Theory modeling for the surface, with catalogued site-specific differences having application in subtraction of background forces for the aforementioned deposited molecule or atom examination. NC-AFM contributes strongly to our understanding of forces at play in the surface structure of H:Si(100), opening the way for many future experiments.

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