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# Seeing the Unseen:Decoding Atomic Adsorption, Nucleation, and Electronic Structure with Functionalized Scanning Probe Microscopy

**ABSTRACT**

Recent improvements in scanning tunneling microscopy (STM) and non-contact atomic force microscopy (NC-AFM) allow us to study surface structures, molecule adsorption, and electronic stateswith exceptional clarity.This study combinesexperiments and theoryusing CO-functionalized AFM tips on qPlus sensors to investigate key processes that affect molecular adsorption, ice nucleation, and electronic structure on metal surfaces.

We first reveal that CO adsorption on Cu(111) saturates at ~26%, well below the 33% expected for the √3×√3R30° structure, independent of dosing and deposition temperature, indicating an intrinsic thermodynamic constraint. Statistical analysisand first-principles calculations show that nanometer-scale, substrate-mediated interactions (~5.3 nm), arising from surface-state electron confinement and elastic strain,suppress higher coverageand enforce a self-limiting adsorbate density.

Next, we demonstrated that CO-tip AFM can distinguish individual transition-metal atoms in molecular structures. Fe and Co atoms in metal phthalocyanines show different imaging contrasts and force signatures, indicating variations in orbital occupation above them.

Third, we demonstrate the presence of a commonwater cluster on both hydrophilic Pt(111) and hydrophobic Cu(111) surfaces, thereby observing the onset of ice nucleation. We identified a critical nucleus of 15 water molecules, with growth patterns that depend on surface properties.

In summary, these findings highlight how CO-functionalized scanning probe microscopy can reveal important interactions, structural details, and electronic properties that influence surface chemistry and phase changes at the atomic level.

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**BIOGRAPHY**

Prof. Nan Yao is Professor of the Practice at the Princeton Materials Institute, Princeton University, USA, and the founding Director of Princeton's Imaging and Analysis Center. He is an internationally recognized expert in materials characterization, advanced microscopy, nanomaterials, and complex materials. His research integrates advanced imaging, diffraction, spectroscopy, in-situ techniques, and computational modeling to investigate materials at the atomic and nanoscale levels. Prof. Yao has authored more than 340 scientific publications and two books, and has contributed to landmark discoveries including the first natural quasicrystal. He is a Fellow of the AAAS, Materials Research Society, Microscopy Society of America, and Royal Microscopical Society.