Decoding Atomic Landscapes: Integrating Electronic Structure Theory and High-Resolution Atomic Force Microscopy

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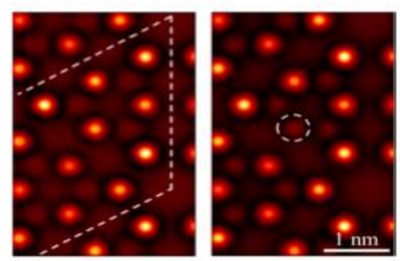
Atomic force microscopy (AFM) is a transformative tool for probing matter at the atomic scale. Recent advances in high-resolution AFM (HR-AFM), especially with CO-functionalized tips, have enabled direct visualization of individual bonds and orbital features within single molecules, offering new insights into molecular structure and reactivity. These capabilities are crucial for investigating complex organic and inorganic species and surfaces.

HR-AFM leverages frequency-modulation techniques and hybrid approaches with scanning tunneling microscopy (STM) to achieve submolecular resolution. Tip functionalization enhances image contrast and sensitivity to electronic states, while theoretical frameworks—such as virtual tip models, density functional theory, frozen density embedding, and tip tilting corrections—enable quantitative interpretation of tip–sample interactions.



Simulated AFM images of pure (left) and B-doped (right) Si(111) 7x7 surface

Our work with HR-AFM has enabled identification of bond orders, functional groups, heteroatoms, and orbital fingerprints in single molecules, as well as characterization of hydrocarbons and complex materials. Notably, we have visualized the reconstructed Si(111)-(7×7) surface, revealing atomic-scale features (see Fig.) and validating theoretical models of surface symmetry disruption [1]. These studies underscore the power of HR-AFM for resolving electronic and structural properties at the atomic level.

[1] D. Fan, Y. Sakai, J.R. Chelikowsky, D. Meuer, A.J. Weymouth and F.J. Giessibl, Phys. Rev. Research 7, L012046 (2025).