"Seeing" the covalent bond: Simulating Atomic Force Microscopy Images

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Advances in atomic force microscopy (AFM) have made it possible to achieve unprecedented images of covalent bonds, in some cases even to resolve the bond order in polycyclic aromatics. However, fundamental questions remain about interpreting the images and modeling the AFM tip. For example, the bright spots in non-contact AFM images can have a close correspondence to the atomic structure of a given specimen, but there can be contrast changes with tip height that cannot be interpreted directly by atomic positions. While the nature of the tip can be crucial in understanding the details of the image, the atomic structure of the tip is often unknown. This situation is compounded by the difficulty in simulating AFM images. In order to perform computational studies of AFM, one must determine the interatomic forces as a function of the tip height on a fine grid above the specimen.

We propose new high performance algorithms to solve for the quantum forces between the tip and the specimen. This approach coupled with a simple theory that avoids an explicit model of the AFM tip, allows us to replicate accurately AFM images and resolve outstanding issues in their interpretation.

References: T.-L. Chan, C.Z. Wang, K.M. Ho, J.R. Chelikowsky:"Efficient first-principles simulation of noncontact atomic force microscopy for structural analysis," Phys. Rev. Lett. 102, 176101 (2009) and M. Kim and J.R. Chelikowsky: "Simulated non-contact atomic force microscopy for GaAs surfaces based on real-space pseudopotentials," Appl. Surf. Sci. 303,163 (2014).