Quantitative Analysis of Electronic Properties Of Carbon Nanotubes By Scanning Probe Microscopy

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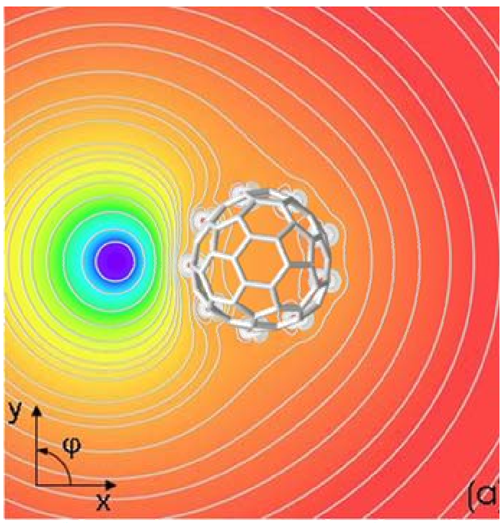
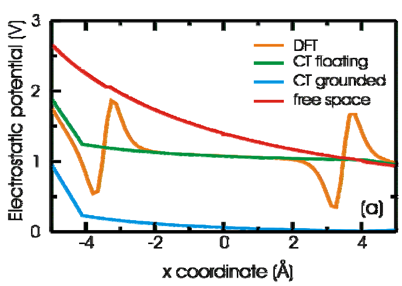
Large scale first-principles modeling of the interactions between a point charge and a carbon nanotube is combined with continuum theory to encompass effects ranging from atomic to mesoscopic length scales that affect the image formation in modern SPM experiments.



Local transport imaging techniques such as Scanning Gate Microscopy (SGM) and Scanning Impedance Microscopy (SIM) have great power for understanding the transport properties of 1D systems such as carbon nanotubes and semiconductor nanowires. SGM images the change in the local resistance due to the presence of a field generated by a probe, while SIM measures the local potential amplitude in an operational nanocircuit. Despite outstanding progress, SGM and SIM have largely remained qualitative techniques since the complexity of the electrostatic probe-sample interactions and geometry of the system has precluded any rigorous interpretation of SPM data in terms of atomic-scale properties.



A new multiscale analysis for the interaction between a probe and a one-dimensional system on a substrate can lead to a straightforward numerical interpretation of the SPM data in terms of relevant electronic properties of the nanotubes. The combination of first-principles and continuum modeling constitutes a solid framework for the quantitative analysis of localized electronic phenomena in reduced-dimensionality systems. The quantum nature of the system is described by one parameter, the inverse screening length, which is numerically determined from accurate first principles calculations. The potential on the nanotube is only a fraction of the applied tip bias. Thus, the application of 10 V to the SPM tip shifts the Fermi level on the nanotube by tens of a meV, comparable with estimated energy levels of defects. It has long been realized that the shift of the Fermi level of the nanotube is significantly smaller than the tip bias but any previous attempts to model this effects were phenomenological and could not explicitly address the electrostatics of tip, tube, and substrate interactions as developed here.

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