Computational Modeling of Scanning Microscopy

Currently, there is a heightened interest in developing materials with unique electronic, chemical, and mechanical properties. In this project, we are using computer simulation to understand and design atomic force microscopy (AFM) and scanning gate microscopy (SGM) experiments, which are important for characterizing new materials. The initial aim of this research was to determine which ab initio methods best modeled the interaction of the microscope tip with a carbon nanotube. The modeled substrates, benzene and coronene, were analyzed with SCF, DFT, and MP2 methods using NWChem. The investigation was carried out in two phases. First, the tip of the AFM, represented by a point charge above the plane of the molecule, was brought down to the plane from a distance of 10-0Å. The SCF and DFT interaction energies were compared to the more accurate MP2 values. It was found, somewhat surprisingly, that the DFT/LDA calculations compared very well to the MP2 calculations. Second, an electron density plot was created for the molecule with a point charge with a distance of 5-0Å to determine how the electrons redistribute in the presence of the microscope tip. We are now in the process of larger computations involving actual nanotubes with over 100 atoms. In the future, the interaction energies and charge redistributions will be used to parameterize a semi-empirical model that can be used in much larger simulations.

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