Scanning Tunneling Microscopy Simulation of Nanoscale Materials

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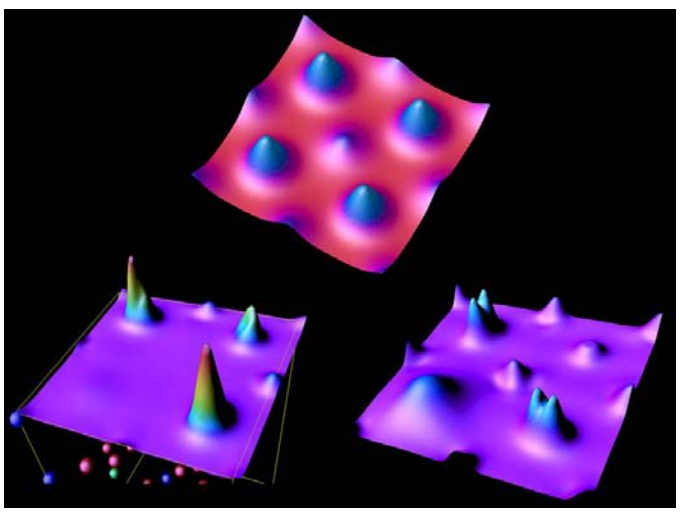
Local probe techniques constitute an important class of experimental techniques for investigating the local electronic and transport properties on the dimension ranging from the mesoscale to the nanoscale. To make use of the full capabilities of scanning probes require accurate models of the interaction of the probes with the specimen, and in turn of the electronic and mechanical processes governing to image formation. The key challenges for utilizing the full capabilities of these probes for use in nanoscale chemistry, nanobiology, and nanoelectronics are threefold: They consist in the intimate knowledge of the geometric and electronic states of the sample under investigation, the understanding of the interaction of the probe with the specimen and the substrate, and the interpretation and prediction of actual measurements.

Transport Model of the SPM. The successful theoretical approach must include a precise description of the electronic properties of the sample, an unambiguous depiction of the transmission of electrons in the sample and/or the tip, and the more challenging understanding of the tip-sample coupling strength in the various contact modes discussed above. The ultimate goal is to develop an efficient multi-functional package accounting for the versatility of possible tip-sample configurations encountered in actual experiments. The transport properties of the probe-sample system will be evaluated within the Buttiker/Landauer formalism that is used for calculating the electronic transmission probability in multi-terminal systems, using a non-equilibrium (Keldysh) Green's functions approach. The actual calculation of the electron transmission in the multi-terminal devices (*i.e.* the probe *coupled* to the sample) will require the implementation of the generalized Landauer/Buttiker formalism. However, a crucial aspect of this proposal is in the development of a suitable model for interface between the electronic transport module and the module representing the interaction between the probe and the sample. Thus, the role of the probe (*i.e.* the nature of the contact and its invasiveness in the electronic process) will be understood in a realistic manner, and its consequences on the computed SPM image unequivocally determined. One of the major application areas driving our development effort is anticipated to be the understanding and prediction of chemical and electronic properties at the nanoscale. While some of the necessary techniques are special purpose, *e.g.*, non-equilibrium Green functions, most of the required methods cut across all other domains calling for quantitative simulation of large systems. The required methods include high-order quantum methods for quantitative calculations on large systems such as multi-grid DFT methods with localized orbital basis sets.



Funding:
[<here I would put the transport project but I do not know how to phrase it…>]