Simulating Scanning Probe Microscopy

Adam S. Foster

COMP, Department of Applied Physics, Aalto University, Helsinki, Finland

Email: adam.foster@aalto.fi

As surface science has increasingly moved to the nanoscale over the past decade, it has entered a realm that is also accessible to highly accurate computational approaches. Simulations have become a key partner in many studies, with the interplay between theory and experiment being the critical element in real understanding. This is especially true in Scanning Probe Microscopy (SPM), where joint experimental and theoretical studies are common [1,2].

In this lecture, I will try to introduce the most popular tools used in computational surface science, along with examples highlighting their interaction with experiment. I will also show examples where common methods fail, and point out the consequences of some "short-cuts" often hidden in the technical details. From this, I will walk through the stages of building a simulation of SPM, with the details mostly relevant to modelling of noncontact Atomic Force Microscopy (AFM) in UHV. We will also touch on some the issues involved in modelling of more complex systems, such as dissipation [3], kelvin probe microscopy [4] and AFM in liquids [5].

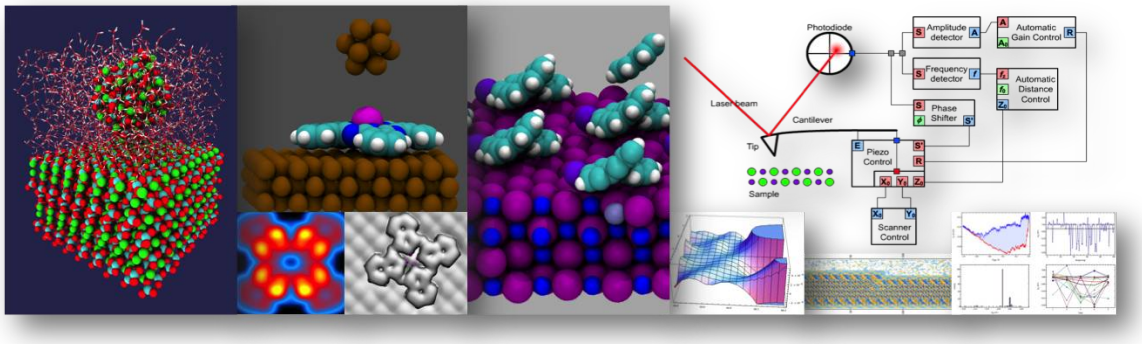

Figure 1: Examples from a variety of SPM simulations.

References

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