Theoretical Approaches and Simulators for the Scanning Tunneling Microscopy

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Scanning probe microscopy (SPM) is a family of powerful experimental methods used to observe atomic-scale structures and properties of nano-materials. SPM, which is composed of a variety of methods such as scanning tunneling microscopy (STM), atomic force microscopy (AFM), Kelvin probe force microscopy(KPFM) and many others, can observe not only geometrical structures of materials, but also their electronic structures, local charge distribution with their responces to the probe, as well as other miscellaneous materials properties. In spite of remarkable progress of experimental techniques, “what and how does SPM see the sample?” is not trivial, and supports from theory and theoretical simulations are necessary.

So far we have been involved in the development of basic theories and simulators for SPM in general[1]. In this talk, various remarkable topics revealed by recent theory of SPM will be introduced. They include the effect of the atomic/electronic structures of the tip, rapid simulation methods and nano-mechanics for bio-materials, dynamic AFM in liquids, mechanism of the local contact potential difference in KPFM and others.

[1]M.Tsukada, Analytical Sciences, 27, 121 (2011)