The non-contact atomic force / Kelvin probe force microscope simulator: a tool to address atomistic processes influencing imaging

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The non-contact atomic force / Kelvin probe force microscope (nc-AFM/KPFM) simulator is a realistic numerical implementation of the electronics of a nc-AFM setup including KPFM operational modes [1,2]. The simulator has been demonstrated to be able to reproduce the dynamical performances of the instrument upon the operating conditions and the used probe (cantilever or tuning fork) [3]. The code may either receive a pre-computed ab initio interaction force field, or computes it at run time by means of analytical expressions or semi-empirical potentials. Thus, the simulator is able to perform virtual experiments such as images at constant Δf or constant height, or spectroscopic measurements: Δf vs. z or bias voltage. In the near past, the simulator has been used to unravel the origin of the atomic-scale contrast in KPFM images on a bulk KBr(001) single crystal [2]. Thus, the influence of the polarizability of both, the foremost tip atom and surface atoms has been pointed out. Recently, following the results from the IBM Zurich group [5,6], the code has been upgraded and targeted at the calculation of images of molecules on surfaces and molecular systems on surfaces with stiff sensors such as tuning forks [3,4]. In this talk, the numerical scheme of the simulator will be presented along with a set of results illustrating the potential of such a tool to address the atomistic processes influencing imaging and spectroscopic measurements in nc-AFM and KPFM.

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