Large-scale Simulations using the LOTF Embedding Method for the Imaging and Mechanical Manipulation of Single Atoms on the Si(111)-(7x7) Surface by NCAFM

Gabor Csanyi*, Pavel Jelinek and Rubén Pérez
Departamento de Física Teórica de la Materia Condensada
Universidad Autónoma de Madrid, E-28049 Madrid, Spain
* Theory of Condensed Matter, Cavendish Laboratory
University of Cambridge, Cambridge CB3 OHE, UK

N. Oyabu[1], O. Custance[2], M. Abe[1] and S. Morita[1,2]
[1] Department of Electric Engineering, Graduate School of Engineering, Osaka University, 2-1 Yamadaoka, Suita, Osaka 565-0871, Japan
[2] Handai Frontier Research Center, 2-1 Yamadaoka, Suita, Osaka 565-0871, Japan

A detailed knowledge of the short-range tip-sample interactions is the key ingredient for the understanding of the experimental topographical and damping images obtained with the Noncontact Atomic Force Microscope. An accurate determination of these forces as a function of the tip-sample distance requires the use of quantum mechanical ab initio simulations, that are very time consuming in the case of large reconstructions of semiconductor surfaces like the Si(111)-7x7. Moreover, understanding the recent mechanical manipulation experiments on this same surface [1] demands a dynamical study of those interactions that can only be done by long molecular dynamics simulations at the same ab initio level. Hybrid methods, that combine quantum mechanical modeling on the relevant small area with a classical force-field description of the rest of the system are a natural tool to tackle these problems: The area where quantum accuracy is needed corresponds to the tip apex and the corresponding contact area in the surface, while the elastic response of the rest of the tip and sample can be properly modeled at the classical level. Our simulations employ the recently developed Learning-On-The-Fly (LOTF) scheme [2], where ab initio forces are used to continuously update the empirical potentials assigned to the atoms in the critical regions. Using these approach we perform different lateral scans and approach curves on different positions of the Si(111)-7x7 unit cell in order to understand (1) the contrast between different adatoms observed in the topographical and damping images and (2) The atomistic mechanism behind the vertical manipulation of adatoms with the NCAFM.

[1] N. Oyabu *et al.*, Phys. Rev. Lett., **90**, 176102 (2003)

[2] G. Csanyi *et al.*, in preparation (2004); G. Trimarchi et al, Proc. of the 10th CIMTEC Conference (Florence, Italy, July 14 19, 2002, Editor P. Vincenzini) in press.