Simulation of Lateral Manipulation of Atoms on Ge(111)-c(2x8) Surface

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Near Contact atomic Force Microscopy (NC AFM) was recently used to laterally manipulate Sn adatoms on the Ge(111)-c(2x8) surface [1]. The tip plays a key role in the process, acting as a catalyst which significantly lowers the energy barriers involved in the process. While the procedure is reproducible and supposed to consist of pair-wise hops of Sn and Ge adatoms, the atomistic picture is still missing. In particular, on energetic grounds it is not clear how two adatoms can move simultaneously, and how the tip affects the potential energy surface (PES) and lowers the barrier. To this end we have performed simulations of the NC AFM lateral manipulation. The PES was described using density functional calculations with transition states located with the nudged elastic band method [2]. The simulation results shed light on the atomistic details of the manipulation and complement the experimental findings.

[1] N. Oyabu, Y. Sugimoto, M. Abe, Ó. Custance, and S. Morita, Nanotechnology **16**, S112 (2005).
[2] G. Mills and H. Jonsson, Phys. Rev. Lett. **72**, 1124 (1994).