# Unveiling the atomic processes during the manipulation of single atoms at semiconductor surfaces using the FM-AFM in the repulsive regime.

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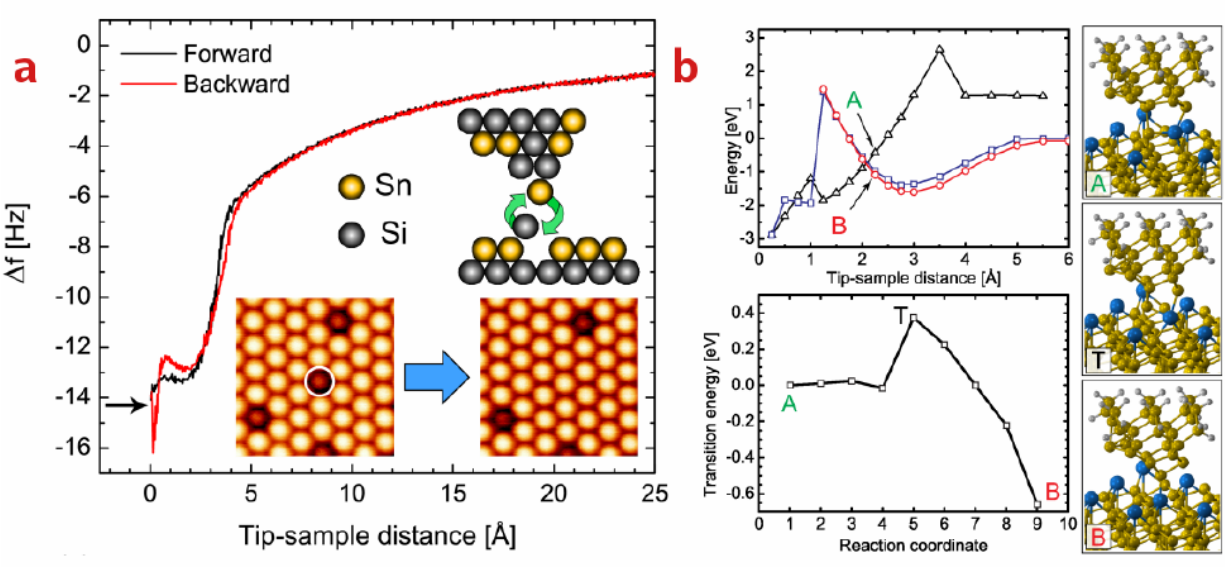
**Resumen**

The artificial assembling of complex atomic patterns by the reproducible vertical interchange of atoms between the tip apex of an atomic force microscope and a semiconductor surface has been achieved using the FM-AFM at room temperature and in a very favorable time scale [1]. At variance with previous methods [2], these novel manipulations are produced by the gentle exploration of the repulsive part of the short-range chemical interaction between the closest tip-surface atoms. While imaging and manipulation in the attractive regime involve mainly the bonding interaction between the closest tip-surface atoms [3], in the so far unexplored repulsive regime a larger contact including several atoms is expected, leading to a very complex energy landscape. The structure of the contact at closest approach determines the most likely output among the different competing processes -atom interchange, atom transfer to the tip, deposition of tip atoms, or recovery of the original structure- when the tip is pulled out from the surface. In this work, using first-principles calculations, we cast some light on the complex mechanisms driving these vertical atomic interchanges; we characterize the key atomic processes involved and the magnitude of the energy barriers between the relevant atomic configurations leading to vertical manipulation. Furthermore, the energy landscape associated with these vertical atomic interchange processes provides an explanation for both the dissipation signal and the intriguing features exhibited by the experimental short-range force curves at close tip-surfaces distances.

**Referencias:**

[1] Y. Sugimoto, P. Pou, O. Custance, P. Jelínek, M. Abe, R. Pérez, S. Morita, 2008 submitted
[2] Y. Sugimoto et al., Nature Materials 4, 156 (2005).
[3] Y. Sugimoto et al., Phys. Rev. Lett. 98, 106104 (2007).

**Figuras:**


a
Forward
Backward
Sn
Si
Δf [Hz]
Tip-sample distance [Å]
b
Energy [eV]
A
B
Tip-sample distance [Å]
Transition energy [eV]
T
A
B
Reaction coordinate
A
T
B