Spin locking at the apex of nano-scale platinum tips

Richard Korytár, Ferdinand Evers

PII: S0039-6028(13)00262-8
DOI: doi: 10.1016/j.susc.2013.09.008
Reference: SUSC 20042

To appear in: *Surface Science*

Received date: 6 June 2013
Accepted date: 5 September 2013

Please cite this article as: Richard Korytár, Ferdinand Evers, Spin locking at the apex of nano-scale platinum tips, *Surface Science* (2013), doi: 10.1016/j.susc.2013.09.008

Spin locking at the apex of nano-scale platinum tips

Richard Korytár[1,*] and Ferdinand Evers[2,3,4]

[1] *Institut für Nanotechnologie, Karlsruhe Institute of Technology (KIT), D-76344 Eggenstein-Leopoldshafen, Germany, phone: +49 721 608 28127*

[2] *Institut für Nanotechnologie, Karlsruhe Institute of Technology (KIT), D-76344 Eggenstein-Leopoldshafen, Germany, phone: +49 721 608 26444*

[3] *Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology (KIT), D-76128 Karlsruhe, Germany*

[4] *DFG-Center for Functional Nanostructures, Karlsruhe Institute of Technology (KIT), D-76131 Karlsruhe, Germany*

Abstract

Nanostructures based on platinum, such as small clusters or STM-tips, often exhibit an atomistic structure that relies upon one or very few strongly under-coordinated platinum atoms. Here, we analyze a paradigmatic example, an apex atom on a pyramidal platinum cluster employing the density functional theory. We show that such a pristine platinum tip exhibits a spin polarization of the apex atom with a remarkable robustness. Due to a depletion of the projected density of states at the apex position, the apex-magnetization is efficiently locked to about $0.6\mu_{\mathrm{B}}$.

PACS numbers: 31.15.A-,81.07.-b,75.75.-c

Keywords: Molecular electronics, nano-magnetism, platinum electrode, first-principles calculations

*richard.korytar@kit.edu, to whom correspondence should be addressed