AFM imaging of the $Au/CeO_2(111)$ system: DFT study

Krzysztof Kośmider[1], Maria Verónica Ganduglia-Pirovano[2], Rubén Pérez[1]
[1]Departamento de Física Teórica de la Materia Condensada, UAM, Madrid, 28049, Spain
[2]Instituto de Catálisis y Petroleoquímica, CSIC, 28049 Madrid, Spain
krzysztof.kosmider@uam.es

Ceria-supported gold has recently attracted significant interest [1] as a potential catalyst for the industrially very important water-gas shift (WGS) reaction. However, despite the significant amount of research performed in this topic, there is still a lack of fundamental understanding of the Au-Ceria interaction and the mechanism controlling adsorption at the atomic scale. Theoretical investigations [2] show that charge transfer in this system depends on the Au adsorption site and may even change sign in the presence of vacancies. Furthermore, different exchange-correlation functionals and calculation details seem to provide conflicting results for this charge transfer. Non-contact atomic force microscopy (NC-AFM), which proved to be capable to distinguish between different charge states of Au on NaCl/Cu [3], is a promising method to experimentally determine the Au charge states.

Here, we present a systematic DFT+U study of the NC-AFM imaging of the $Au/CeO_2(111)$ sample. We exploit the different charge states for Au adsorbed on the clean or reduced surface to address the possible AFM visualization of oppositely charged Au atoms. We simulate AFM force spectroscopy with different tips, including O- and OH-terminated tips [4] and analyze the influence of the tip apex on the contrast. We provide guidelines for prospect AFM measurements.

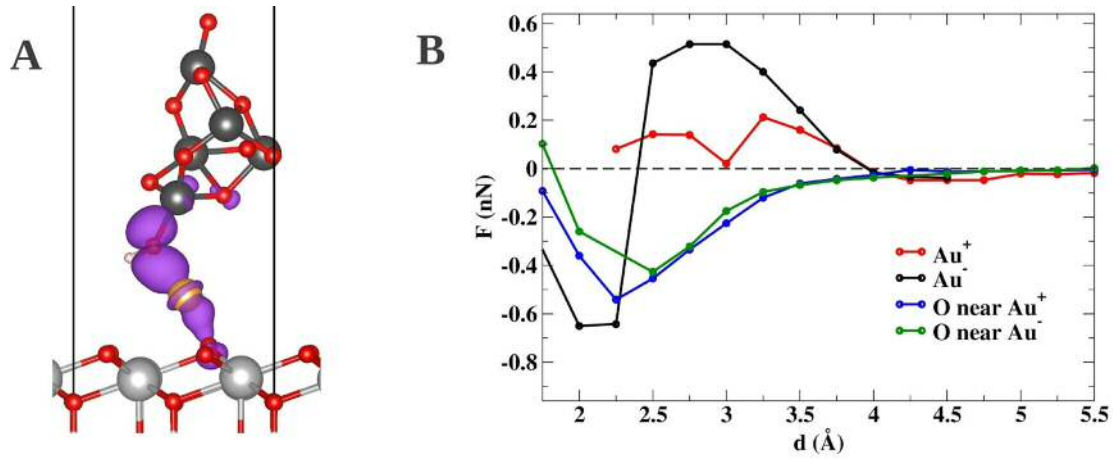

Figure 1. A) Structure for an OH-terminated TiO_2 AFM tip making contact with the $Au/CeO_2(111)$ sample, B) Computed tip-sample forces between this tip and positively /negatively charged Au and nearby O surface atoms.

[1] J. A. Rodriguez et al., Science, **318**, 1757, (2007).
[2] C. Zhang, A. Michaelides and S.J. Jenkins, Phys. Chem. Chem. Phys. **13**, 22, (2010).
[3] L. Gross et al., Science **324**, 1428, (2009).
[4] A. Yurtsever et al., Phys. Rev. B **85**, 125416, (2012).