Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Role of residual hydrogen on the XPS of organic molecules on surfaces ARAN GARCIA-LEKUE, Donostia International Physics Center (DIPC); Ikerbasque, ANE SARASOLA, University of the Basque Country UPV/EHU, Spain, MIKEL ABADIA, Materials Physics Center (CFM), Spain, GIACOMO LOVAT, Columbia University, USA, LUCA FLOREANO, CNR-IOM, Italy, CELIA ROGERO, Materials Physics Center (CFM), Spain — It is a well-known experimental issue that residual H is abundant in a seemingly ideal UHV environment, which might have a significant effect on STM and XPS measurements. For example, additional XPS peaks are often observed when evaporating organic molecules on a surface.[1,2] In this work, a set of DFT based tools is employed to elucidate the influence of chemical and surface-induced changes on the core-level shifts (CLSs) of XPS experiments. The capabilities of our tools are demonstrated by unraveling the origin of an unpredicted component in the N 1s XPS spectra of metal phthalocyanine molecules on a metal surface. On one hand, we prove that surface effects, such as LUMO splitting and surface screening, cannot account for the huge experimental CLSs. On the other hand, we show that, when adsorbed at low temperatures, these molecules capture residual H atoms from the surface, giving rise to hydrogenated molecular species without demetalation of the molecule and, thus, to an extra component in the molecular CLS spectra.[3] [1] A. Garcia-Lekue et al., J. Phys. Chem C 116, 15378 (2012). [2] G. Lovat et al., Phys. Chem. Chem. Phys. 17, 30119 (2015). [3] A. Sarasola et al. (submitted)

Aran Garcia-Lekue
Donostia International Physics Center (DIPC); Ikerbasque

Date submitted: 07 Nov 2016

Electronic form version 1.4