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View Abstract

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TITLE: Tuning the Magnetic Moment of high density FePc/Ag(110) phases by oxygen dosing

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ABSTRACT BODY:

Abstract Body: Molecular overlayers on substrates have a broad field of application in catalysis, sensing, molecular electronics, light-to-energy conversion, etc. In particular, iron-phtalocyanines (FePc) are being investigated as viable substitutes for precious metals in catalysis of the Oxygen Reduction. Recent studies of FePc on Ag(110) have shown that sub-monolayer phases are catalitically active [1]; remarkably, in oxygen-dosed phases O2 intercalates between the molecules and the surface, thereby substantially changing the Fe magnetic moment. Reversible switching of the Fe magnetic moment in some low-density (LD-R1/R2) FePc phases upon an oxygenation-annealing cycle has been demonstrated [2]. In this contribution, we report on the oxygenation capabilities and associated magneto-structural changes of higher-density FePc/Ag(110) phases, the oblique (OB) and square (SQ)/quasi-squared (R3) high-density phases, investigated by combining high-resolution Scanning Tunneling Microscopy (STM), Scanning Tunneling Spectroscopy (STS), Density Functional Theory (DFT) simulations and x-ray magnetic circular dichroism (XMCD) at the Fe L2,3, edge. The STM images reveal the steric impediments of high-density phases to allocate O2 between the FePc and the substrate, which result in less efficient oxygenation / deoxydation processes compared to previously reported LD phases. In the SQ/R3 squared phases, only a fraction of the molecules are able to oxygenate, rotating and suffering a displacement. For the OB oblique phase, the oxygenation efficiency is smaller; and among the oxygenated molecules, only a minor fraction do rotate, while the majority allocate O2 without rotation. The XMCD spectra of the oxygenated phases reflect the different distribution of non- oxygenated, oxygenated-rotated and non-rotated species in the samples (Fig. 1).

References: [1] F. Sedona et al., Nat. Mater. 2012, 11, 970.
[2] J. Bartolome et al., J. Phys. Chem. C 2015, 119, 12488.

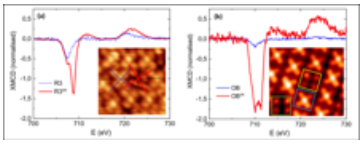

Fig. 1 XMCD of as deposited and oxygenated (a) R3 and (b) OB phases, and STM images of the O2 dosed samples.

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