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Quantitative investigation of the "surface trans-effect" in an adsorbed metal-organic complex by means of X-ray Standing Waves

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On-surface coordination chemistry is an emerging field that holds promise for applications in, e.g., nanotechnology, molecular spintronics and heterogeneous catalysis. Previous work provided evidence for a "surface trans-effect", where the interaction [1] and even the magnetic coupling [2] between the metal ion of adsorbed metal-organic species and the underlying substrate can be affected by ligation of an adduct in trans position. Corresponding changes in the height of the metal center with respect to the substrate were theoretically predicted [3], although they appeared strongly overestimated. Here we present a quantitative analysis of this effect using synchrotron-based normal incidence X-ray standing waves. In particular, for iron phthalocyanine on Ag(111) we determine quantitatively the increase in the height of the Fe ion upon ligation of NH3 and H2O [4]. New dispersion-corrected DFT calculations accurately model this structural effect, and the predicted charge redistribution suggests that the Ag(111) surface acts in a similar manner as a molecular ligand.

[1] W. Hieringer et al., J. Am. Chem. Soc. 133 (2011), 6206.
[2] Ch. Wäckerlin et al., Nat. Commun. 1 (2010), 61.
[3] C. Isvoranu et al., J. Chem. Phys. 134 (2011), 114710.
[4] P. S. Deimel et al., Chem. Sci. 7 (2016), 5647.

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