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Exploring Kondo Phenomena in Physisorbed Nitric Oxide RYAN REQUIST, SISSA, Trieste, Italy, ALEXANDER SMOGUNOV, CEA Saclay, France, PIERPAOLO BARUSELLI, MICHELE FABRIZIO, ERIO TOSATTI, SISSA, Trieste, Italy — The NO molecule is a S=1/2 system that can be physisorbed on gold surfaces. As there are presently no data indicating whether or not physisorbed NO retains its spin and displays an observable Kondo effect, we investigate that question by means of our ab-initio based DFT+NRG approach [1]. DFT calculations for NO/Au(111) confirm that at low coverage the on-top adsorption site is the most stable, with the NO molecule forming an angle of approximately 60 degrees with the surface normal. Spin-polarized DFT calculations reveal that the molecule retains one unpaired electron in an antibonding π orbital that hybridizes, albeit moderately, with the surface. Based on these ingredients, we discuss the possibility of observing a zero-bias Kondo anomaly in scanning tunneling spectroscopy above NO/Au(111). The influence of gold surface states and rovibronic motion of the molecule are also investigated. [1] P. Lucignano et al., Nature Mat. 8, 563 (2009).

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