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Single oxygen and CO molecules on Au(110): what can we learn?[1]

YANNING ZHANG, YING JIANG, WILSON HO, RUQIAN WU, University of California, Irvine — Studies of O_2 and CO molecules on the reconstructed Au (110) surface are crucial for the understanding of unusually high activity of Au nanostructures that are useful in heterogeneous catalysis. Moreover, the O_2/Au system is ideal to probe the Kondo effect using surface science techniques, due to the persisting magnetization of triplet O_2 in physisorption systems. In this work, scanning tunneling microscope (STM) measurements and density functional calculations were performed to investigate the adsorption geometries and physical properties of single O_2 and CO molecules on Au(110). The calculated atomic structures and vibration frequencies are comparable favorably with our STM experimental results at low temperature, allowing efficient establishment of structural models. Interestingly, the O_2 molecule takes a defect site over the Au row, with a tilted geometry. The magnetic moment of O_2 is still as large as 1.9 μ_B, which furthermore induces a pronounced Kondo resonance in a large spatial region. The cloud of Kondo enhancement was found to closely follow the distribution of the calculated spin density at the fermi level, a correlation which is important for the understanding of Kondo effect in molecular systems.

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