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Why CO + $\frac{1}{2}$O2 $\rightarrow$ CO2 is so Active under One and a Third Gold Layer on Titania Mo(112) SHIZHONG YANG, JAMES PHILLIPS, LIZHI OUYANG, Physics Department, University of Missouri-Kansas City — Carbon monoxide oxidization on two types of substrates, one layer and one and a third layer gold, gold fully wetted surface supported with titania Mo(112) system[1] was studied using first-principles density-functional theory method. The geometry feature of active adsorption sites, adsorption energy and electronic properties were calculated. The active CO oxidation mechanism based on the energetic diagram and electronic properties was discussed. **References**: [1]. M. S. Chen and D. W. Goodman, *Science*, **306**, 252 (2004).

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