

Abstract Submitted
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Modeling the effects of the oxide substrate on O₂ dissociative adsorption on Au nanostructures¹ SERGEY STOLBOV, TALAT S. RAHMAN, University of Central Florida — In this work we apply the density functional theory calculations to explore the mechanism of high reactivity of Au nanoparticles on oxide substrates. We test the idea that the substrate – nanoparticle interaction makes the O₂ dissociative adsorption favorable on this system, in contrast to bulk Au, and then the O atoms, so adsorbed, are consumed by reactants for further oxidation. We exploit the observation that the 2-layer Au film on TiO_x displays an exceptionally high reactivity as compared to a monolayer Au film, as well as those with 3 or more layers [1]. We calculate the energy E_{da} of dissociative adsorption of O₂ on the surfaces 1, 2, 3, and 5 Au(111) layer structures in two environments: 1) free standing layers, 2) on TiO fragments (modeling a substrate). We find E_{da} to be negative for the 2- and 3-layer Au films on the “substrate” while it is positive for all other systems under consideration. This result along with the experimental finding [1] point to the O₂ dissociative adsorption as being the main mechanism for the observed reactivity of Au nanostructures. Calculated local densities of electronic states and local charges in the system will be presented for further insights into the nature of the effect. [1] M. S. Chen, D. W. Goodman, Science **306**, 234 (2004).

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