Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

The unsuspected origin of gold's nobleness[1] MARISOL ALCANTARA ORTIGOZA, SERGEY STOLBOV, University of Central Florida — Understanding the "inertness" of Au toward oxidizing agents - appreciated since long before the beginning of recorded history – has remained a challenge. Its nobleness has long been attached to its weak interaction with adsorbates, which contrasts with the fact that Au forms stable alloys and can be made reactive. Density-functional-theory (DFT) calculations of the binding energy (BE) of O on (111) surfaces, in fact, have shown that Au stands out for rendering the weakest BE. Here, we reveal the origin of gold's unique inertness by revising the adsorption of this prototype oxidizing agent on several (111) metal surfaces. We show via DFT that, judging by BE of O on Au(111) and Ag(111), e.g., *both* the d-band-center argument *and* analysis of the electronic density of states fail to describe the relatively low reactivity of Au. Nevertheless, we establish that, rather than failure of the above paradigms, a key element to understand BE of adsorbates has been left behind so far. Namely, we demonstrate that, although BE of O is higher on Ag(111) than on Au(111), (1) The local Au-O bonds are *indeed stronger* than the Ag-O ones; (2) the low BE of O on Au is, paradoxically, caused by an unusually large perturbation on Au-Au bonds upon O adsorption.

[1]This work was supported by NSF under Grant CBET-1249134.

Marisol Alcantara Ortigoza
University of Central Florida

Date submitted: 12 Dec 2012 Electronic form version 1.4