Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Theoretical Studies of the Stability and Electronic Properties of Pd_n, and Pd_nO_2 ($1 \leq n \leq 13$) Clusters[1] DEBESH R. ROY, J. ULISES REVELES, SHIV N. KHANNA, Department of Physics, Virginia Commonwealth University, Richmond, VA 23284, USA, ANDREAS M. KOSTER, Departamento de Quimica, Cinvestav, Avenida Instituto Politecnico Nacional 2508, A.P. 14-740, Mexico D.F. 07000, Mexico — First principles electronic structure studies on the ground state geometry, electronic structure and magnetic moment of $Pd_n (1 \leq n \leq 13)$ clusters have been carried out using a gradient corrected density functional approach. The clusters are found to be magnetic with a moment per atom that varies with cluster size. In particular, Pd_{13} is shown to have a two layers structure that can be looked upon as a fragment of the bulk and has a spin magnetic moment of 6 Bohr magnetons. The calculated magnetic moments are compared with available data from Stern Gerlach experiments. We also study the effect of adding an O_2 molecule on the electronic and magnetic properties by carrying out corresponding studies on Pd_nO_2 ($1 \leq n \leq 13$) clusters. Our findings on the strength of binding of oxygen will be compared with recent experiments on the oxidation of palladium clusters by oxygen.

[1]We gratefully acknowledge support from the Air Force Office of Scientific Research through a MURI Grant (FA9550-08-1-0400).

Shiv N. Khanna
Department of Physics, Virginia Commonwealth University,
Richmond, VA 23284, USA

Date submitted: 18 Nov 2009 Electronic form version 1.4