Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Electronic structure of palladium and gold-palladium nano clusters, both free and supported on MgO(100)[1] CARLOS QUINTANAR, REYNA CABALLERO, RAUL ESPEJEL, ELIZABETH CHAVIRA, Universidad Nacional Autónoma de México, MAGALI UGALDE, FRANCISCO ESPINOZA, Centro de Investigación en Materiales Avanzados, SAMUEL TRICKEY, University of Florida — Ideal (or model) metal nano-clusters, both free and supported on MgO(100), have been the subject of numerous experimental studies. This work probes the characteristics of non-ideal systems. For that, palladium nano clusters first were synthesized using a sol-gel-microwave method. A mono-phase of metallic Pd was obtained as corroborated by thermo gravimetric analysis, x-ray powder diffraction, scanning electron microscopy, and high resolution transmission electron microscopy studies (HRTEM). Among the HRTEM micro-graphs we found an almost planar nano-surface (facet) with only forty six atoms (Pd_{46}). From that micro-graph we obtained the coordinates of the atoms in the Pd_{46} nano-surface. With those coordinates, we did a DFT study of the Pd_{46} nano-surface electronic structure. From the Pd_{46}nano surface, nine and eighteen Pd atoms were chosen to build A_8Pd_9 and A_8Pd_{18} clusters respectively. Starting from a near-planar Au8 cluster, the Au_8 geometry was optimized over the fixed Pd_9 and Pd_{18} nano-surfaces, charge transfer was determined with charge density difference analysis (CDDA) and Fukui analysis was done and. The Au_8Pd_9 cluster was positioned on an MgO(100) surface with an O vacancy and charge transfer was determined with CDDA

[1]Acknowledgment: financial support PAPIIT-UNAM IN116912 project.

Carlos Quintanar
Universidad Nacional Autónoma de México

Date submitted: 10 Nov 2014 Electronic form version 1.4