Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Computational Studies on the Energy Landscape of Pt-Pd nanoparticles ALVARO POSADA-AMARILLAS, Dept. de Inv. en Física, Unison, RAFAEL PACHECO-CONTRERAS, Dept. de Química, Cinvestav, DORA J. BORBÓN-GONZÁLEZ, LAURO OLIVER PAZ-BORBÓN, Fritz Haber Institut, ROY L. JOHNSTON, School of Chemistry, University of Birmingham, J. CHRISTIAN SCHÖN, Max Planck Institute for Solid State Research — Bimetallic nanoparticles such as Pt-Pd are currently the subject of intense research mainly due to their important catalytic properties. Clusters structure, composition and degree of mixing or segregation all play important roles in determining their chemical activity. It is presented here an exhaustive study of the structure of Pt-Pd nanoparticles, obtained by a Genetic Algorithm (GA) which incorporates the Gupta potential to mimic interaction for bimetallic atoms. This procedure provided an icosahedral structure as the lowest in energy. The threshold method (TM) is used to analyze the energy landscape of 13-atom Pt@Pd_{12} nanoparticle, as well as the transition probabilities for those structures with pentagonal symmetry found by the TM. Disconnectivity graphs are obtained for both a vast exploration of the potential energy surface (PES) and the exploration around the lowest energy structure. We found low interconversion transition rates for the putative global minimum provided by the GA code, which was confirmed by the TM algorithm.

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Date submitted: 07 Dec 2010 Electronic form version 1.4