## Abstract Submitted for the MAR07 Meeting of The American Physical Society

Structural and Energetic Study of PtxPd98-x Nanoparticles¹ ALVARO POSADA-AMARILLAS, Dept. de Investigación en Física, UNISON, DORA JULIA BORBÓN-GONZÁLEZ, Dept. de Matemáticas, UNISON, LAURO OLIVER PAZ-BORBÓN, ROY L. JOHNSTON, School of Chemistry, U. of Birmingham — Cluster structure, composition and degree of mixing or segregation all play important roles in determining the physical and chemical properties of bimetallic nanoparticles such as PtPd, which are currently the subject of intense research mainly due to their important catalytic properties. In this work we present an exhaustive study of the structure and energetic of PtxPd98-x nanoparticles, obtained by a Genetic Algorithm which incorporates the Gupta potential for bimetallic atoms. Excess energy and stability function indicate that the most stable configurations correspond to those compositions approximately with 50 % Pd and 50% Pt atoms. Segregation is observed for the lowest energy structures meanwhile mixing is predominant for disordered higher energy nanoparticles.

<sup>1</sup>LOPB and APA acknowledge CONACyT-México for financial support.

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Date submitted: 04 Jan 2007 Electronic form version 1.4