

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

H₂O Nucleation Around Noble Metal Cations PATRIZIA CALAMINICI, PAVEL OROPEZA ALFARO, MARTIN JUAREZ FLORES, ANDREAS KÖSTER, CINVESTAV, Departamento de Química, MARCELA BELTRAN, UNAM, J. ULISES REVELES, SHIV N. KHANNA, VCU, Physics Department, CINVESTAV COLLABORATION, UNAM COLLABORATION, VCU COLLABORATION — First principle electronic structure calculations have been carried out to investigate the ground state geometry, electronic structure and binding energy of noble metal cations (H₂O)_n⁺ clusters containing up to 10 H₂O molecules. The calculations are performed with the density functional theory code deMon2k [1]. Due to the very flat potential energy surface of these systems special care to the numerical stability of energy and gradient calculation must be taken. Comparison of the results obtained with Cu⁺, Ag⁺ and Au⁺ will be shown. This investigation provides insight into the structural arrangement of the water molecules around these metals and a microscopic understanding of the observed incremental binding energy in the case of the gold cation based on collision induced dissociation experiments.
[1] A.M. Köster, P. Calaminici, M.E. Casida, R. Flores-Moreno, G. Geudtner, A. Goursot, T. Heine, A. Ipatov, F. Janetzko, J. Martin del Campo, S. Patchkovski, J.U. Reveles, A. Vela and D.R. Salahub, deMon2k, The deMon Developers, Cinvestav, 2006

Patrizia Calaminici
CINVESTAV, Departamento de Química

Date submitted: 11 Feb 2008

Electronic form version 1.4