Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Density-Functional Study of Au_n^- ($n = 16 - 24$): Atomic and Electronic Structures and Interaction with O_2 BOKWON YOON, UZI LANDMAN, Georgia Institute of Technology, PEKKA KOSKINEN, MICHAEL MOSELER, Fraunhofer Institute for Mechanics of Materials, HANNU HAKKINEN, University of Jyvaskyla — Anionic gold clusters with 16 to 24 atoms are studied using the Born-Oppenheimer local-spin-density molecular dynamics method. The structures of the ground-state clusters and energetically lowest-lying isomers are 3-dimensional, while the ground-state structures of smaller Au_n^- with up to 14 atoms were reported to be planar (Häkkinen, et al., J. Chem. Phys. 117, 6982 (2002)). The calculated vertical electron detachment energies (vDE) are in good agreement with the experimental results (Taylor, et al., J. Chem. Phys. 98, 3319 (1992)); vDE's are smaller for even n's and larger for odd n's, with the exception of $n = 16$. Compared to the other even-numbered clusters, Au_{16}^- exhibits relatively large vDE, $vDE(Au_{16}^-)$=4.03 eV. The smallest vDE is measured for $n = 20$, $vDE(Au_{20}^-)$=2.71 eV, The adsorption of O_2 to Au_n^- is also sensitive to the cluster size; the O_2 adsorption is relatively strong for the even-numbered clusters with the exeption of Au_{16}^-. The O_2 binding energy, the intramolecular bond-length of O_2, and the excess charge on O_2 correlate strongly with the vertical electron detachment energy of Au_n^-.

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Date submitted: 02 Dec 2005 Electronic form version 1.4