Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Structural and electronic properties of sodium nanoclusters[1] LUIS A. PEREZ, Instituto de Fisica, UNAM, JUAN A. REYES-NAVA, IPICYT, IGNACIO L. GARZON, Instituto de Fisica, UNAM — Recent advances on mass selection of sodium nanoclusters and their characterization by photoemission electron spectroscopy [1] have given useful data for a variety of clusters sizes. These data may lead to assignments of the relevant structures by comparing the measured photoelectron spectra (PES) with the electronic density of states (DOS) obtained from DFT calculations. In this work, the lowest energy structures modeled by the many-body Gupta potential, are obtained by using molecular dynamics simulations for Na_n (n= 178, 204, 271, 298-300, 309). DFT calculations were then performed for neutral, positively- and negatively-charged Na_n clusters. A comparison between the DOS of clusters of the same size but different charge will be presented, as well as between the available experimental PES and the theoretical obtained DOS.

[1] H. Haberland, T. Hippler, J. Donges, O. Kostko, M. Schmidt, B. von Issendorff, Phys. Rev. Lett. 94, 035701 (2005).

[1]This work was supported by CONACyT No. 43414-F.

Luis A. Perez

Date submitted: 04 Dec 2005 Electronic form version 1.4