Structural and electronic properties of sodium nanoclusters\textsuperscript{1} LUIS A. PEREZ, Instituto de Física, UNAM, JUAN A. REYES-NAVA, IPICYT, IGNACIO L. GARZON, Instituto de Física, UNAM — Recent advances on mass selection of sodium nanoclusters and their characterization by photoemission electron spectroscopy \cite{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\textsubscript{n} (n= 178, 204, 271, 298-300, 309). DFT calculations were then performed for neutral, positively- and negatively-charged Na\textsubscript{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.


\textsuperscript{1}This work was supported by CONACyT No. 43414-F.

Luis A. Perez

Date submitted: 04 Dec 2005