Density-Functional Study of $\text{Au}_n^-$ $(n = 16 - 24)$: Atomic and Electronic Structures and Interaction with $\text{O}_2$ 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 $\text{Au}_n^-$ 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 ($v\text{DE}$) are in good agreement with the experimental results (Taylor, et al., J. Chem. Phys. 98, 3319 (1992)); $v\text{DE}$’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, $\text{Au}_{16}^-$ exhibits relatively large $v\text{DE}$, $v\text{DE}(\text{Au}_{16}^-)$=4.03 eV. The smallest $v\text{DE}$ is measured for $n = 20$, $v\text{DE}(\text{Au}_{20}^-)$=2.71 eV, The adsorption of $\text{O}_2$ to $\text{Au}_n^-$ is also sensitive to the cluster size; the $\text{O}_2$ adsorption is relatively strong for the even-numbered clusters with the exception of $\text{Au}_{16}^-$. The $\text{O}_2$ binding energy, the intramolecular bond-length of $\text{O}_2$, and the excess charge on $\text{O}_2$ correlate strongly with the vertical electron detachment energy of $\text{Au}_n^-$. 

Bokwon Yoon
Georgia Institute of Technology

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