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 exception 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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