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Interaction of O_2 with Silver Cluster Cations SEUNG BUM SUH, BOKWON YOON, UZI LANDMAN, School of Physics Georgia Institute of Technology, Atlanta, GA 30332-0430 — The interaction of oxygen molecules with silver cluster cations, Ag_n^+ for n=8-11, is investigated using the first- principles calculations based on the density functional theory with generalized gradient correction. The binding energy of single O_2, either molecularly or dissociatively adsorbed on Ag_n^+, exhibits an even-odd alternation as a function of n, where O_2 binds more strongly for even n. When two oxygen molecules are adsorbed, the dissociative adsorption of the first molecule favors the molecular adsorption of the second one. Analyses of the local density of states (LDOS) and the spatial distribution of the highest occupied molecular orbital (HOMO) are presented to explain our observations.

Seung Bum Suh
School of Physics Georgia Institute of Technology, Atlanta, GA 30332-0430

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