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Interactions of water and oxygen molecules with gold clusters SEUNG BUM SUH, BOKWON YOON, MINDE SUN, UZI LANDMAN, School of Physics. Georgia Institute of Technology, Atlanta, GA 30332-0430 — The interaction of water and oxygen molecules with neutral gold clusters, Au_n for n=2-8, is investigated using the first- principles calculations based on the density functional theory with generalized gradient correction. The O_2 binding energy, the intramolecular bond-length of O_2, and the excess charge on the adsorbed O_2 show even-odd alternations as a function of the number of gold atoms, correlating with the vertical electron detachment energy of Au_n. The influence of pre-adsorbed H_2O on the O_2 adsorption is pronounced when the O_2 is adsorbed with an Au-O bond with the gold cluster and an O-H bond with pre- adsorbed H_2O, while the influence is relatively small for O_2 adsorbed with double Au-O bonds. Compared to the O_2 adsorption in the absence of H_2O, the binding energy of O_2 are increased by 0.4 eV, and the intramolecular bond- length are stretched by up to 0.03 Å.

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