Bi-metallic particles Au-X, (X=Ir, Al) interacting with O_2 and CO on MgO(100)

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The structural and electronic properties of Au, Al, Ir, Au_2, Au-Al, Au-Ir, Ir-Au-O-O-C-O and Al-Au-O-O-C-O adsorbed on the neutral F_s color center (oxygen vacancy containing two electrons), and on the charged F_s^+ color center (oxygen vacancy containing one electron) of the MgO(100) surface, have been investigated using a density functional theory and a cluster embedding approach. Our studies also examine the effect of relaxation of the substrate. We report the geometry, adsorption, and dimerization energies of the lowest energy and low energy isomers at each adsorption site, and charge transfers from the MgO surface to the adsorbed atoms or particles. We observed that nearly one electron is transferred from the surface to the metal particle (Au2, Au-Ir, Al-Au), but for Ir-Au with Ir at the surface the electron goes to the gold atom. There is a noteworthy distortion of structure of contact and large charge transfer from the surface to the particle. The supported Ir-Au-O-O-C-O particle splits in CO_2 and Ir-Au-O, suggesting the oxidation of CO to CO_2.

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