Chemical properties of Au nanoparticles on oxides\footnote{Supported by the DOE} RUQIAN WU, University of California, Irvine — Using the density functional DMol, VASP and FLAPW approaches, we studied the electronic and chemical properties of Au nanoparticles on oxide substrates with O vacancies. Au clusters of more than 5 atoms are found to be unstable on MgO(001). Many configurations are explored for Au clusters on TiO$_2$(110) and SiO$_2$(0001). We found interesting size and shape dependence of their chemical properties, characterized by the density of states, HUMO/LUMO features and core level shifts. For substrates, we found that even SiO$_2$ monolayer displays a sizable gap on Mo(110).

\footnote{Supported by the DOE}