Abstract Submitted
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**Chemical properties of Au nanoparticles on oxides**[1] 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).

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