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Study on adsorption of submicrometer gold on kaolinite by quantum chemistry calculations

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ABSTRACT

The electronic structure and energies of Au atoms adsorbed on an atomic cluster of kaolinite were calculated using the self-consistent-field Discrete Variational (DV) method. A hexagonal ring of SiO_4 tetrahedra and three $AlO_2(OH)_4$ octahedra, comprising 38 atoms, was used to model the kaolinite crystal flake. An Au atom was used to model the submicrometer Au. Calculations were performed with Au atoms adsorbed at different sites. The systems with lower total energy are those with Au adsorbed on the edge surfaces. The adsorption of Au atoms on the edges is more stable than Au atoms adsorbed on the basal plane. Bond order calculations suggest that significant shifting of atomic charge and overlap of electron clouds between Au and the surface atoms of kaolinite takes place in the systems with Au adsorbed on the edges, especially at sites near Al octahedra.