Atomic and molecular adsorption on Au(111)

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Atomic and molecular adsorption on Au(111)

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Periodic self-consistent density functional theory (DFT-GGA) calculations were used to study the adsorption of several atomic species, molecular species and molecular fragments on the Au(111) surface with a coverage of 1/4 monolayer (ML). Binding geometries, binding energies, and diffusion barriers were calculated for 27 species. Furthermore, we calculated the surface deformation energy associated with the binding events. The binding strength for all the analyzed species can be ordered as follows: NH_3 < NO < CO < CH_3 < HCO < NH_2 < COOH < OH < HCOO < CNH_2 < H < N < NH < NOH < COH < Cl < HCO_3 < CH_2 < CN < HNO < O < F < S < C < CH. Although the atomic species preferred to bind at the three-fold fcc site, no tendencywas observed in site preference for the molecular species and fragments. The intramolecular and adsorbate-surface vibrational frequencies were calculated for all the adsorbates on their most energetically stable adsorption

site. Most of the theoretical binding energies and frequencies agreed with experimental values reported in the literature. In general, the values obtained with the PW91 functional are more accurate than RPBE in reproducing these experimental binding energies. The energies of the adsorbed species were used to calculate the thermochemical potential energy surfaces for decomposition of CO, NO, N_2, NH_3 and CH_4, oxidation of CO, and hydrogenation of CO, CO_2 and NO, giving insight into the thermochemistry of these reactions on gold nanoparticles. These potential energy surfaces demonstrated that: the decomposition of species is not energetically favorable on Au(111); the desorption of NH_3, NO and CO are more favorable than their decomposition; the oxidation of CO and hydrogenation of CO and NO on Au(111) to form HCO and HNO, respectively, are also thermodynamically favorable.

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