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Quantum Theoretical Study of Palladium and Silver Clusters
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— We continue our interest on the chemisorption of different atomic and molecular species on small clusters of metallic elements, by examining the interactions of H, O and F atoms with Pd_n and Ag_n clusters (n = 2 thru 12). Transition-metal clusters can be useful for the study of quantum size effects and for formation of metallic states, and are ideal candidates for catalytic processes. Hybrid ab initio methods of quantum chemistry (particularly the DFT-B3LYP model) are used to derive optimal geometries for the clusters of interest. We compare calculated binding energies, bond-lengths, ionization potentials, electron affinities and HOMO-LUMO gaps for the clusters of the two different metals. Of particular interest are the comparisons of binding strengths at the three important types of sites: edge (E) sites, hollow sites (H) site and on-top (T) sites. Effects of crystal symmetries corresponding to the bulk structures for the two metals will also be investigated. The implications for the molecular dissociation of the H_2 and O_2 species will be considered.

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