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Quantum Mechanics of Chemisorption on Palladium Clusters. CHLOE ROBINSON, AJIT HIRA, JOSE PACHECO, RUBEN RIVERA, Northern New Mexico College — In view of our interest in the chemisorption of different atomic and molecular species on small clusters of metallic elements, we present theoretical results on the interactions of H, H_2, O and CO adsorbates with Pd_n clusters (n = 2 thru 60). Transition-metal clusters are specially suited 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, including the influence of Jahn-Teller effects. We compare calculated binding energies, bond-lengths, ionization potentials, electron affinities and HOMO-LUMO gaps for the clusters. Of particular interest are the comparisons of binding strengths at the five important types of sites: edge (E), on-top (T), threefold sites, fourfold sites, and hexagonal sites. Effects of crystal symmetries corresponding to the bulk structures are investigated. Implications for the existing experimental results on icosahedral structures and cubic structures will be examined. The capacity of Pd clusters to adsorb H atoms will be compared to the capacity of other metallic clusters..

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