

Abstract Submitted
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Theoretical Study of Chemisorption on Nickel and Palladium Clusters AJIT HIRA, JOSE PACHECO, DANELLE JARAMILLO, FRANK NARANJO, Northern New Mexico College — We continue our interest in 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 Ni_n clusters (n = 2 thru 20). 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. 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), hollow (H), on-top (T), threefold sites and fourfold sites. Effects of crystal symmetries corresponding to the bulk structures for the two metals are investigated. The implications for the molecular dissociation of the H₂ and O₂ species will be considered.

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