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Dynamics and Interactions of Adsorbates on Palladium and Nickel Clusters AJIT HIRA, JOSE PACHECO, JUSTIN SALAZAR, CLIFTON BROWNRIGG, Northern New Mexico College — We continue our interest on the interactions of different atomic and molecular species with small clusters of metallic elements, by examining the interactions of H, O and F atoms with Pd_n and Ni_n clusters (n = 6 thru 12). The 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. Our theoretical results will be compared with the experimental studies where they are available. We will also study the dynamics of the atomic species, and the dynamics and dissociation of the molecular species on the clusters.

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