World Academy of Science, Engineering and Technology
International Journal of Chemical and Materials Engineering
Vol:12, No:06, 2018

Catalytic Thermodynamics of Nanocluster Adsorbates from Informational Statistical Mechanics

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Abstract : We use an informational statistical mechanics approach to study the catalytic thermodynamics of platinum and palladium cuboctahedral nanoclusters. Nanoclusters and their adatoms are viewed as chemical graphs with a nearest neighbor adjacency matrix. We use the Morse potential to determine bond energies between cluster atoms in a coordination type calculation. We use adsorbate energies calculated from density functional theory (DFT) to study the adatom effects on the thermodynamic quantities, which are derived from a Hamiltonian. Oxygen radical and molecular adsorbates are studied on platinum clusters and hydrogen on palladium clusters. We calculate the entropy, free energy, and total energy as the coverage of adsorbates increases from bridge and hollow sites on the surface. Thermodynamic behavior versus adatom coverage is related to the structural distribution of adatoms on the nanocluster surfaces. The thermodynamic functions are characterized using a simple adsorption model, with linear trends as the coverage of adatoms increases. The data exhibits size effects for the measured thermodynamic properties with cluster diameters between 2 and 5 nm. Entropy and enthalpy calculations of Pt-O2 compare well with previous theoretical data for Pt(111)-O2, and our Pd-H results show similar trends as experimental measurements for Pd-H2 nanoclusters. Our methods are general and may be applied to wide variety of nanocluster adsorbate systems.

Keywords : catalytic thermodynamics, palladium nanocluster absorbates, platinum nanocluster absorbates, statistical mechanics
Conference Title : ICMCN 2018 : International Conference on Metal Clusters and Nanoalloys
Conference Location : San Francisco, United States
Conference Dates : June 06-07, 2018