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Sub-nanometer Transition Metal Clusters for Dehydrogenation Catalysis: Is the d-band Model Valid? STAN ZYGMUNT, HAIYING HE, STEPHEN PLACE, MICHAEL ROEBACK, Dept. of Physics and Astronomy, Valparaiso University — The d-band model of Hammer and Nørskov successfully rationalizes the catalytic properties of transition metal (TM) surfaces and nanoparticles. The model predicts a linear relationship between the d-band center energy of a TM or TM alloy (E_d) and its binding energy with a reactant molecule. Many studies have shown that the d-band center with respect to the Fermi energy (E_d-E_F) is a useful descriptor of the catalytic properties of TM systems. Originally established for TM surfaces, the d-band model has also been validated for particles with diameters of roughly 10 nm. However, the model has not yet been tested for sub-nanometer clusters and cluster alloys, in which the discrete nature of the energy-level spectrum becomes more prominent. We have calculated binding energies of four atom homogeneous TM clusters (M_4) and binary cluster alloys ($M_{4-x}N_x$, x=1,2,3) with propane and propene, for the purpose of a detailed study of propane dehydrogenation. We find that binding energy varies approximately linearly with d-band center for many $M_{4-x}N_x$ cluster alloys, in agreement with the d-band model. However, the agreement is much worse when the M_4 clusters formed by different TMs are compared. We will discuss possible reasons for these results, along with implications for dehydrogenation catalysis.

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