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FINAL REPORT

"SUPERSONIC BARE METAL CLUSTER BEAMS"

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Bare metal clusters. A major portion of the project involved elucidating the relation between reactivity and the electronic structure of transition-metal (TM) clusters of 2-200 atoms, which required the construction and continuous development of two principal apparati: the Fourier Transform-Ion Cylotron Resonance (FT-ICR) apparatus, and Ultraviolet Photoelectron Spectroscopy (UPS). Together, these machines have enabled the most detailed probing of the structure and chemical reactivity of TM clusters. In combination with calculations, UPS experiments have advanced understanding of TM cluster electronic structure, while the FT-ICR technique, with the direct injection from a supersonic cluster ion source, has allowed further characterization of structure and chemical reactivity, particularly chemisorption on TM cluster surfaces. Clusters of all the transition metals were included in these studies, with the principal focus on Fe, Co, Cu, Ag, Au, Pt, Sc, Y, La, Nb, V, Ta, Rh, Ni, and Ir. Fundamental aspects in chemisorption, reactivity, and heterogeneous catalysis have also become better understood as a result of these experiments for important classes of systems such as H_2, CO, and CO_2 adsorbed onto clusters of many of the metals listed above. In particular, a correlation was found between reactivity of H_2 with Fe, Co, and Ni clusters and differences between the cluster IP and EA. This was explained microscopically as resulting from a chemisorption barrier whose height is given by the excitation energy from the frontier orbital to the lowest unoccupied d-orbital. This is a general model that is likely to apply to any closed-shell species interacting with metal clusters.

Bare metal clusters in carbon cages. As recounted in a previous technical report, the DOE's role in the initial discovery of fullerenes at Rice was central, and from the start investigations were made into metal atoms trapped in the fullerenes cage. More recently, we have discovered that 2-4 atoms of La, Y, or Sc can be produced by laser vaporization of composite

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