

# Vortragsankündigung

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Es spricht: **Prof. Dr. Peter Armentrout**, Department of Chemistry, University of Utah, USA

Zeit: **Mittwoch, 16. Mai 2007**  
**17 Uhr c.t. – 19 Uhr**

Ort: **TU Berlin, Institut für Chemie**  
**Strasse des 17 Juni 115, 10623 Berlin**  
**Altes Chemiegebäude, Raum C264**

Thema: "Thermochemistry of Gas-Phase Reactions of Transition Metal Clusters Relevant for Catalysis"

Abstract: In our work, we have examined the kinetic energy dependences of the reactions of  $\text{Fe}_n^+$ ,  $\text{Co}_n^+$ , and  $\text{Ni}_n^+$  ( $n = 2 - 15$ ) with  $\text{D}_2$ ,  $\text{O}_2$ ,  $\text{N}_2$ ,  $\text{CD}_4$ , and  $\text{ND}_3$  in a guided ion beam tandem mass spectrometer over the energy range of 0 - 10 eV. Metal cluster cations are formed in a laser vaporization/supersonic expansion source and reactions are performed under single collision conditions. The kinetic energy dependences are analyzed to determine thresholds for various primary and secondary reactions. From these thresholds, bond energies for iron, cobalt, and nickel cluster cation bonds to D, O, N, C, CD,  $\text{CD}_2$ ,  $\text{CD}_3$ , ND,  $\text{ND}_2$ , and  $\text{ND}_3$  have been determined. For the atomic systems, e.g., D and O, bond energies to modest size metal clusters (10 – 15 atoms) rapidly converge to values equivalent to bulk phase values. Thus, values for the molecular fragments provide some of the very FIRST data for the thermochemistry of such species bound to surfaces, information that is largely non-existent even though these are key intermediates in a variety of catalytic processes. Recent extensions of this work have examined the collision-induced dissociation of  $\text{Fe}_x\text{O}_y^+$  ( $x = 1 - 6$ ) clusters, and have elucidated the thermochemistry of several non-stoichiometric combinations. Further, periodic trends in the CH bond activation of methane by atomic transition metal ions reveal the electronic requirements for this critical step in several catalytic processes.

Es sind alle Interessierten herzlich eingeladen.

Prof. Dr. M. Driess  
Koordinator der Cluster-Initiative „UniCat“