Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Influence of Charge State on the Reaction of $FeO_3^{+/-}$ with Carbon Monoxide J.U. REVELES, S.N. KHANNA, Virginia Commonwealth University, N.M. REILLY, G.E. JOHNSON, A.W. CASTLEMAN JR., Penn State University — A synergistic study combining experiments in molecular beams and first principles electronic structure calculations within a gradient corrected density functional approach is used to investigate the reactivity of charged FeO_3 clusters with CO. It is shown that highly oxidized iron clusters are able to readily effect the oxidation of CO to CO_2 at ambient temperature. Calculated energy profiles of the reaction demonstrate that the oxidation efficiency is governed by the strength of oxygen binding to the iron atom. Results for $FeO_3^{+/-}$ are presented and reveal that cation clusters are more efficient than the corresponding anion clusters at effecting the oxidation reaction due to different bond energies resulting from charge distribution.

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Date submitted: 15 Nov 2006 Electronic form version 1.4