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Dual reactivity of iron-oxide clusters: self-stimulated CO oxidation as well as NO reduction Y. MATSUDA, E.R. BERNSTEIN, Department of Chemistry, Colorado State University, Fort Collins, CO 80523, B.V. REDDY, F. RASOULI, Philip Morris USA Research Center, 4201 Commerce Road, Richmond, VA 23234, S.N. KHANNA, Physics Department, Virginia Commonwealth University, Richmond, VA 23284-2000 — It is shown that selected Fe_nO_m clusters can accomplish the dual task of oxidizing CO and reducing NO. Our studies are based on the neutral iron-oxide clusters obtained by laser ablation of iron metal and subsequent reaction of the gas phase metal atoms/ions/clusters with an O_2/He mixture. A mass spectra of the clusters after a laser ionization with 118 nm , 193 nm or 355 nm photons shows that the most dominant species in the beam have the composition Fe_nO_n, followed by $Fe_nO_{n+1,2}$ for increasing n. The neutral clusters generated in the beam were subsequently reacted with CO and NO introduced in the reaction cell. The relative intensity of the specific clusters exiting the reaction chamber as a function of reacting gas pressure was evaluated through standard ionization and detection procedures of time of flight (TOF) mass spectrometry. The results indicate that while Fe_2O, Fe_2O_2 and Fe_3O_3 are all active towards both CO and NO elimination, the relative intensity of other clusters remain largely unchanged. Results of the gradient corrected density functional calculations to reveal the possible mechanisms involved in the cluster activated conversion of CO to CO_2 and NO to N_2 will be presented.

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