Computational Study of Metal Oxide Nanocluster Interactions with Lewis Acidic Gas Molecules

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The production of Lewis acidic gases is a major pollution issue throughout the energy industry. Sequestering and converting these gases to safer or useable products requires catalysts and other materials which can resist chemical degradation long enough to be of practical use. To design practical catalysts, we must first answer some very fundamental questions about the chemistries of these materials. How do Lewis acidic gas molecules interact with metal oxide clusters? What role could these interactions play in the degradation of these materials? The physisorption and chemisorption interaction energies of CO_2, SO_2, or NO_2 with transition metal oxide nanoclusters have been calculated at the density functional theory and CCSD(T) levels. Comparisons of these interaction energies with fluoride affinities, electron affinities, and metal-oxygen bond strengths of the metal oxide nanoclusters have been made to develop correlations with the reducibility, Lewis acidity, and bond strengths of the metal oxide nanoclusters. This work is sponsored by the U.S. Department of Energy, Office of Science, Basic Energy Sciences.