

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Structure and Reactivity of $M_xS_y^+$ (M= Mo,W) Clusters with CO in the Gas Phase: an Experimental and DFT Study MELISSA PATTERSON, JAMES LIGHTSTONE, Stony Brook University, MICHAEL WHITE, Stony Brook University / Brookhaven National Laboratory — We have recently constructed a cluster deposition apparatus which employs a magnetron sputtering source for generating gas-phase cation clusters of pure metals and metallic compounds. Of particular interest are clusters of the transition metal sulfides, $M_xS_y^+$ (M = Mo, W), which are known in their bulk form to be active catalysts for a wide range of heterogeneous reactions. The work reported here examines the gas-phase reactivity of small transition metal sulfide clusters as a first step towards investigations of model catalysts prepared by size-selected deposition. Specifically, we have used density functional theory (DFT) along with mass spectroscopy and gas-phase collision studies to examine the structure and stability of small sulfide clusters, $M_xS_y^+$ ($x/y = 2/6, 3/7, 4/6, 5/7, 6/8, 7/10, 8/12$). The number of metal sites was probed through the formation of adducts with CO, which was introduced into a hexapole collision cell. Calculated binding energy curves for the addition of CO onto available metal sites were compared with experiment to give insight as to which geometry for the bare clusters fit best. Results will be presented for the calculated structures and stabilities of the prominent clusters as well as their adducts.

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Date submitted: 23 Nov 2005

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