Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Theoretical study of sulfur overlayers on transition metal surfaces DOMINIC ALFONSO, National Energy Technology Laboratory and Parsons Project Services Inc. — In the chemical and petrochemical industries, the deterioration of transition metal-based catalysts by sulfur poisoning incurs great cost to the economy. Investigation of the sulfur-metal interaction will help characterize the problem and may ultimately lend ideas for the development of sulfur-resistant materials. The structures formed by sulfur adsorbed on close-packed surfaces of Ag, Au, Cu, Ir, Ni, Pt, Rh, Co, Re, Ru, Fe and Mo were studied using first-principles calculations. At low coverage, sulfur forms a stable ($\sqrt{3} \times \sqrt{3}$) R30° ordered structure on the fcc (111) metal surfaces. In the case of hcp (0001) and bcc (110) metal surfaces, a stable (2×2) ordered structure was found. These results are in line with experimental findings. The adsorption energy of atomic sulfur varies between -3.58 and -6.30 eV. Notable decrease in the adsorption energy with increasing coverage was found. The lateral interactions among chemisorbed sulfur were investigated to find out what is responsible for the strong coverage effect. In order to explain the binding effects, the projected density of states were also studied in detail.

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Date submitted: 14 Nov 2006 Electronic form version 1.4