Abstract Submitted
for the OSS13 Meeting of
The American Physical Society

Sulfur adsorption on gold - an exercise in computational low-energy electron diffraction ASHLEY ERNST, NATHAN GRIESER, Ohio Northern University — Gold - one of the less reactive elements in nature - has recently sparked the interest of the scientific community through the properties of its surface. The Au(111) surface, under UHV conditions, reconstructs into a (22x$\sqrt{3}$) structure. Nevertheless, even a small amount of sulfur adsorbed on the Au(111) surface is enough to lift the reconstruction. As the amount of adsorbed sulfur increases, a succession of S/Au structures are formed, as recognized in low-energy electron diffraction (LEED) patterns. We report on the LEED computational analysis of one such phase: ($\sqrt{3}$x$\sqrt{3}$)R30^0 which corresponds, theoretically, to a 0.33ML sulfur coverage. Experimental evidence places this phase in coexistence with other phases on the Au substrate, therefore there is little expectation for a such a LEED investigation to answer the main question of the actual adsorption site of the atomic sulfur on the gold substrate. Still, as an exercise in computational LEED, we investigated several models for the ($\sqrt{3}$x$\sqrt{3}$)R30^0 structure, testing various adsorption sites for the sulfur atoms. We also considered the possibility of sulfur bonding to additional Au atoms, placed on top of the regular surface, forming Au-S entities.

Mellita Caragiu
Ohio Northern University

Date submitted: 01 Mar 2013 Electronic form version 1.4