

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

First-principles studies of the $\sqrt{7} \times \sqrt{7}$ R19.1° structure of sulfur on the Pd(111) surface DOMINIC ALFONSO, National Energy Technology Laboratory and Parsons Project Services Inc. — Density functional theory is used to investigate the $(\sqrt{7} \times \sqrt{7})$ R19.1° structure of sulfur on the Pd(111) surface. Applying the concepts of first-principles atomistic thermodynamics, we analyze the stability of various $(\sqrt{7} \times \sqrt{7})$ models in equilibrium with arbitrary H₂ and H₂S environment. Among the different models that were considered, the densely packed mixed sulfur-metal overlayer structure proposed by Berndt *et al.* [Surf. Sci. **393**, L119 (1997)] was found to be the most energetically favorable. This model consists of arrangement of Pd triangles and pentagons on top of Pd(111) with the sulfur atoms at 3/7 monolayer coverage. The dominant mechanism for sulfur interaction with Pd in the overlayer region is the rehybridization of sulfur 3 p and metal 4 d bands. Simulated scanning tunneling microscopy image for this structure shows some similarity with that obtained from experiment. Our study confirms that surface sulfide with no structural resemblance to its bulk counterparts can form on Pd(111).

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Date submitted: 02 Nov 2006

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