

Abstract Submitted  
for the MAR15 Meeting of  
The American Physical Society

**Theoretical investigation of oxygen adsorption on Pu-Ga alloy (111) surface**<sup>1</sup> SARAH C. HERNANDEZ, University of Texas at Arlington, THOMAS J. VENHAUS, Los Alamos National Laboratory, MUHAMMAD N. HUDA, University of Texas at Arlington — All electron density functional theory was implemented to study the adsorption of atomic oxygen on a 3.125 at. % Ga stabilized  $\delta$ -Pu (111) surface. A 4-layer periodic slab, with 8 atoms per layer, was used to model the surface, and the location of the Ga within the surface was considered. High symmetry on-surface and interstitials adsorption sites were explored, which also included the adatom placed in different local environments (i.e. oxygen coordinated with/without a Ga atom). Full relaxation of the atomic positions of the Pu-Ga slab and O atom were employed. The inclusion of spin-orbit-coupling was performed for the lowest energetic structure. The goal of these calculations was to probe the effects that Ga may have within the surface when O is adsorbed. We found that oxygen binds strongly at an on-surface site with chemisorption energy of -5.06 eV and prefers to be three-fold coordinated in a Pu-rich environment. However, when Ga is participating in chemical bonding with the O adatom chemisorption energies were unfavorable. Interstitials sites were also unfavorable, which implies that diffusion of O into the subsurface is an activated process. Furthermore, a geometric analysis of the slab after O adsorption showed local oxygen-induced distortions, which will be discussed in detail.

<sup>1</sup>We gratefully acknowledge support by the US Department of Energy through the Los Alamos National Laboratory LDRD Program.

Sarah Hernandez  
University of Texas at Arlington

Date submitted: 14 Nov 2014

Electronic form version 1.4