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A DFT Study of Atomic Hydrogen and Oxygen Chemisorption on the γ-U Surface[1] DAYLA MORRISON, ASOK RAY, Physics Department, University of Texas at Arlington — Generalized gradient approximation to density functional theory has been used to compute O and H atomic adsorption properties on the (100) surface of γ-U. The computational method used is the all-electron full-potential linearized augmented plane wave plus local orbitals basis method as implemented in the WIEN2k code. The adatom was allowed to approach the five-layer slab surface at the top, center and bridge sites. The bridge site was found to be most stable with chemisorption energies of 8.43 and 3.76 eV for O and H, respectively, spin-orbit coupling (SOC) included. The optimized distances to the surface for the O atom was 1.98 at the top, 0.75 at center and 1.32 Å and at the bridge sites. For H, these distances were found to be 2.07, 0.57, and 1.40 Å at the corresponding sites, respectively. Inclusion of SOC has significant effects on the energies, changing the chemisorption energy by as much as 0.63 eV for O and 0.43 eV for H. Possible changes in work function, magnetic moment, and charge density distributions have been investigated and will be presented. We will also present results on interstitial sites, by incorporation of O and H atoms inside the slab. Different properties were observed for the O adatom as compared to the H atom.

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Dayla Morrison
Physics Department, University of Texas at Arlington

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