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A Density Functional Study of Atomic Oxygen and Carbon Adsorptions on the (100) Surface of γ-Uranium[1] PRATIK DHOLABHAI, ASOK RAY, University of Texas at Arlington — Atomic oxygen and carbon adsorptions on the γ-U (100) surface have been studied using the generalized gradient approximation to density functional theory (GGA-DFT) with Perdew and Wang (PW) functionals. Different chemisorption sites at both non-spin-polarized and spin-polarized levels of theory have been thoroughly investigated. For O adsorption, the bridge position is the most favorable site with chemisorption energies of 7.887eV and 7.965eV for the non-spin-polarized and spin-polarized cases, respectively. The distances of the O adatom from the U surface are found to be 1.19Å and 1.22Å, respectively. For C adsorption, the center position is the most favorable site with a chemisorption energy of 7.816eV for the non-spin-polarized case, and 7.895eV for the spin-polarized case. The distances of the C adatom from the U surface are 0.62Å for the non-spin-polarized and 0.52Å for the spin-polarized cases. A study of the density-of-states (DOS) for O and C adsorbed uranium surfaces shows that the hybridization between U $5f$ orbitals and the O and C $2p$ orbitals is weak and the bonding is primarily ionic. Comparisons with published results will be presented.

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