A Density Functional Study of Atomic Oxygen and Carbon Ad- 
sorptions on the (100) Surface of γ-Uranium\textsuperscript{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 approxima-
tion to density functional theory (GGA-DFT) with Perdew and Wang (PW) func-
tionals. Different chemisorption sites at both non-spin-polarized and spin-polarized 
levels of theory have been thoroughly investigated. For O adsorption, the bridge po-
sition 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.

\textsuperscript{1}This work is supported by the Chemical Sciences, Geosciences and Biosciences 
Division, Office of Basic Energy Sciences, Office of Science, U.S. Department of 
Energy and the Welch Foundation, Houston, Texas.

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Date submitted: 23 Nov 2005
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