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**A Density Functional Study of Carbon Monoxide Adsorption on (100) Surface of $\gamma$-Uranium** ASOK RAY, PRATIK DHOLABHAI, University of Texas at Arlington — Adsorption of the CO molecule on the $\gamma$-U (100) surface has been studied at both non-spin-polarized and spin-polarized levels using the generalized gradient approximation to density functional theory (GGA-DFT) with Perdew and Wang (PW) functionals. The bridge position with the vert2 approach is found to be most favorable site with a chemisorption energy of 2.93eV for the non-spin-polarized case, and 3.19eV for the spin-polarized case. The distances of the carbon atom from the uranium surface are found to be 1.59Å and 1.72Å for the non-spin-polarized and spin-polarized cases, respectively. The inter-atomic distances between the carbon and oxygen atoms for the most favorable position are found to be 1.13Å and 1.21Å for the non-spin-polarized and spin-polarized cases, respectively. The magnetic moment for the most favorable site is found to be $0.04\mu_B$ per atom. A significant charge transfer from the first layer of the uranium surface to the carbon and oxygen atoms is found to occur, implying that the bonding is partly ionic. Significant hybridization between the U $5f$and CO $2p$ orbitals are also observed. 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 (Grant No. DE-FG02-03ER15409) and the Welch Foundation, Houston, Texas (Grant No. Y-1525).

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