Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

A First Principles Study of the Adsorption and Dissociation of CO_2 on the δ-Pu (111) Surface [1] RAYMOND ATTA-FYNN, ASOK RAY, Department of Physics, The University of Texas at Arlington — *Ab initio* calculations within the framework of density functional theory have been used to study the adsorption of molecular CO_2 and the corresponding partially dissociated (CO+O) and completely dissociated (C+O+O) products on the δ-Pu (111) surface. The completely dissociated C+O+O configurations exhibit the strongest binding with the surface (5.85 eV), followed by partially dissociated products CO+O (4.34 eV), with molecular CO_2 adsorption having the lowest binding energies (2.98 eV). For all initial vertically upright orientations the CO_2 molecule is physisorbed and its geometry and orientation does not change. For all initial flat lying orientations chemisorption occurs, with the final state corresponding to a bent CO_2 molecule with bond angles of 118^o-130^o except one case where spontaneous partial dissociation from the atop site occurs. The interactions of the CO_2 and CO with the Pu surface have been analyzed using the energy density of states and difference charge density distributions.

[1]This work is supported by the U. S. Department of Energy and the Welch Foundation

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Date submitted: 19 Nov 2008 Electronic form version 1.4