Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Density Functional Theory Investigation of Adsorption Properties of CO, CO_2 and H_2O on γ-Al_2O_3 Supported Pt Clusters[1] MEHMET GOKHAN SENSOY, HANDE USTUNEL, Department of Physics, Middle East Technical University, Ankara, Turkey, DANIELE TOFFOLI, Department of Chemistry, Middle East Technical University, Ankara, Turkey — The water-gas shift reaction is a key catalytic process for the production of clean H_2 gas for fuel cells.[2] In this study, we use plane wave pseudopotential density functional theory to study the adsorption properties and the activation of CO, CO_2 and H_2O on Pt clusters supported on the (001) surface of γ-Al_2O_3. A systematic study has been conducted to identify the most stable adsorption sites for both monoatomic and diatomic Pt clusters. Several stable adsorption geometries have been identified for the adsorbates, and their interaction with both the precious metal and the support is characterized in terms of adsorption energies and the nature of the bond between the adsorbed molecules and the precious metal.

[1]This work is supported by TUBITAK of Turkey (Grant No. 112T542), TR-GRID ULAKBIM and UHEM (Grant No. 1001942012)
[2]M. S. Dresselhaus and I. L. Thomas, Nature 414, 332 (2001)

Mehmet Sensoy
Middle East Tech Univ

Date submitted: 07 Nov 2013 Electronic form version 1.4