Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Activation of CO_2 on transition metal surfaces and oxide supported metal thin films SUJATA PAUL, MARCO BUONGIORNO NARDELLI, NC State Univ — Using first principles simulations based on Density Functional Theory, we have investigated the adsorption and activation properties of CO_2 on a variety of transition metal surfaces and oxide supported metal thin films. We intend to focus on the chemical conversion of CO_2 through heterogeneous catalysis using surfaces and interfaces where there is nanoscale control over charge density at the reactive sites. The activation of CO_2 on clean metal surfaces is possible at very high temperatures and the situations changes drastically when reaction happens on oxide supported metal thin film. The chemical reactivity of the molecule on the surface depends on the charge rearrangement at the metal-alkaline earth oxide interface. We want to understand the possible catalytic systems and characterize the relevant geometrical and electronic parameters related to the reaction mechanisms, rates and yield.

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Date submitted: 22 Nov 2008 Electronic form version 1.4