Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Theoretical Design of Nanostructured Materials for CO_2 Adsorption, Activation and Reduction SUJATA PAUL, ERIK E. SANTISO, MATIAS NUNEZ, NC State University, Raleigh, NC, MARCO B. NARDELLI — Using first principles simulations based on Density Functional Theory, we have investigated the adsorption and activation properties of CO2 on a variety of materials both in bulk and in nanostructured form. In particular, we will discuss the interaction of CO2 with elemental transition metal surfaces, oxide-supported nanoparticles, artificial molecular systems and nanoporous materials. Particular emphasis is given to the construction of complex systems where interfaces between heterogeneous materials are the active site for catalytic reactions. Our investigation is focused on the prediction of possible techniques to tune the properties of the interfaces in order to enhance the desired chemical activity. A preliminary study on bulk systems already showed promising results for possible applications to catalytic processes.

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Date submitted: 17 Nov 2006 Electronic form version 1.4