Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

***Ab initio* Molecular Dynamics Study of Carbon Dioxide Adsorption on the Ni Catalyst Surface** JI IL CHOI, YONG-HOON KIM[1], Korea Advanced Institute of Science and Technology — The first-principles molecular dynamics simulations can provide insight into the surface reaction mechanisms by including thermodynamic environments and rigorously determining the transition states between reactants and products, which are not available from the static study of the species already adsorbed on the surface. In view of its importance in various energy applications, we here report on the first-principles molecular dynamics study of the chemical reaction of CO_2 molecules on the representative atomicallyflat lowMiller-index Ni(111) surface. We adopted the DFT-D2 scheme to properly describe the van der Waals interactions, and considered various thermodynamic conditions including the temperature, pressure, and number of additional molecular species. To analyze the reaction mechanisms, in addition to the change of the electronic structure of CO_2 upon adsorption on the Ni surface the energy barriers between the initial and final stages of CO_2 deposition were calculated with and without the interactions with neighboring molecules.

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Date submitted: 15 Nov 2013 Electronic form version 1.4