Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Controlled Catalytic Properties of Platinum Clusters on Strained Graphene GYUBONG KIM, Korea Institute of Science and Technology, YOSHIYUKI KAWAZOE, Tohoku University, KWANG-RYEOL LEE, Korea Institute of Science and Technology —
We employed biaxially strained graphene as the supporting material for Pt clusters (Pt_x, x=1, 4 or 6) and studied the molecular adsorption behaviors of H_2, CO and OH on the cluster using ab initio calculations. It was shown that the applied strain enhances binding of the Pt cluster on the graphene, which lowers the average energy of Pt d electron (d-band center). The binding energies of H_2, CO and OH on Pt_1/graphene are strongly correlated with the d-band center modulated by the graphene strain. The calculations with small Pt clusters (Pt_4 and Pt_6) also show that the d-band center is a substantial factor for the catalytic activity of the Ptx/graphene system. We also found that the stability of the Pt clusters was enhanced by applying the strain on the graphene support.

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Date submitted: 08 Nov 2011 Electronic form version 1.4