Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Controlled catalytic properties of iron nanoparticles on doped graphene: A first-principles study SOL KIM, SEUNG-HOON JHI, Pohang Univ of Sci & Tech — Iron is an important catalyst in Fischer-Tropsch synthesis (FTS). Recently carbon-material- supported iron nanoparticles were reported as a good catalyst better than bulk iron surface. Here we employed B- and N-doped graphene as supporting materials for iron nanoparticles and studied the change in d-band center of iron nanoparticles which is a key factor in gas adsorption. We then investigated the molecular adsorption of H_2 and CO on the nanoparticles using first-principle calculations. It was found that B doping enhances the binding energy of the Fe_{13} on the graphene, which lowers the d-band center of Fe_{13}, but N doping reduces it. Difference in the work-function and subsequently in the charge transfer causes such behavior in the binding energies. We showed that the adsorption of H_2 and CO on the Fe-graphene substrate is strongly correlated with the d-band center modulated by the doping concentration. We also found that the stability of Fe nanoparticle was enhanced by graphene doping.

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Date submitted: 13 Nov 2013 Electronic form version 1.4