Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Quantum Monte Carlo studies of surface adsorptions CHING-MING WEI, CHENG-RONG HSING, IAMS, Academia Sinica, Taipei 10617, Taiwan — Surface adsorption is the first step to the study of surface catalytic reaction. The most common used tool is the Density Functional Theory (DFT) based on exchange-correlation approximations and the accuracy usually has not been checked carefully by highly accurate quantum many-body approaches. We have performed calculations of the surface adsorptions using the state-of-the-art diffusion quantum Monte Carlo (QMC) method to examine the accuracy of LDA and GGA (PBE) functionals in the study of surface adsorptions. The systems examined include the H_2O and OH adsorptions on various types of surfaces such as NaCl(100), MgO(100), TiO_2(110), graphene, Si(100)-(2x2) and Al(100). By comparing GGA (PBE) results with DMC, our results indicate that (i) for the H_2O adsorption, PBE predicts the correct adsorption energies; (ii) for the OH adsorption, PBE has predicted a large over-binding effect except on graphene and Si(100) surfaces. This fact indicates that one needs to be cautious when using DFT to study the surface adsorptions of OH free radical.

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Date submitted: 16 Dec 2011 Electronic form version 1.4