Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

First Principles Study of Adsorption of O_2 on Al Surface with Hybrid Functionals HENGRUI LIU, HONGJUN XIANG, XIN GAO GONG, Key Laboratory for Computational Physical Sciences (MOE) and Surface Physics Laboratory, Fudan University — Adsorption of O_2 molecule on Al surface has been a long standing puzzle for the first principles calculation. We have studied the adsorption of O_2 molecule on the Al(111) surface using hybrid functionals.In contrast to the previous LDA/GGA, the present calculations with hybrid functionals successfully predict that O_2 molecule can be absorbed on the Al(111) surface with a barrier around 0.2$\sim$0.4 eV , which is in good agreement with experiments. Our calculations predict that the LUMO of O_2 molecule is higher than the Fermi level of the Al(111) surface, which is responsible for the barrier of the O_2 adsorption.

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Date submitted: 17 Nov 2011 Electronic form version 1.4