Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Theoretical Study of Hydrogen Dissociation on the $TiAl_3$ Surface[1]

YAN WANG, M. Y. CHOU, School of Physics, Georgia Institute of Technology — In order to better understand the catalytic role played by Ti in enhancing the reaction kinetics of sodium alanate, we present a first-principles investigation of hydrogen dissociation and adsorption on the pure Al surface as well as on the Ti doped surface with a local alloy composition of $TiAl_3$. The most energetically favorable location for Ti near the surface is identified. It is found that the presence of Ti promotes H adsorption on the surface with the H atom sitting on top of an Al atom. The binding between Ti and Al modifies the surface charge distribution near the adsorption site and facilitates the adsorption process. The potential energy surface for H_2 dissociation over both pure Al and the alloy surfaces are also discussed.

[1]Supported by the Department of Energy.

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Date submitted: 29 Nov 2005 Electronic form version 1.4