Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

First principles study of ammonia decomposition on Ni and Pd surfaces[1] TALAT S. RAHMAN, SERGEY STOLBOV, Kansas State University — Ammonia is considered as an efficient storage for hydrogen. It can be converted to hydrogen on board vehicle by decomposition. The decomposition requires efficient catalyst that still has to be designed based on systematic understanding of the reaction mechanisms. We present results of first principles electronic structure calculations based on density functional theory and the generalized gradient approximation of various stage of the decomposition of NH_3 on Ni and Pd surfaces. It is known that the ammonia decomposition rate is much higher on Ni that on Pd. The reaction mostly occurs on surface steps and defects. We calculate, compare and contrast adsorption energies, the paths and energy barriers for NH_3 diffusion and dissociation on singular and stepped Ni and Pd surfaces, as well as on those with vacancies. The differences in the characteristics of the energy landscape on the various surfaces are explained through analysis of the local densities of electronic states and valence charge densities calculated for the molecule located at preferred adsorption sites and saddle points on the reaction paths. Contact will be made with available experimental data.

[1]We acknowledge financial support from DOE under grant No. DE-FGO3-03ER15445.

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Date submitted: 30 Nov 2004 Electronic form version 1.4