Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Hydrogen Multicenter Bonds on Small Metal Clusters[1] P. TARAKESHWAR, T.J. DHILIP KUMAR, N. BALAKRISHNAN, Department of Chemistry, University of Nevada Las Vegas, 4505 Maryland Parkway, Las Vegas, NV 89154, USA — We investigate the saturation of hydrogen on metal clusters employing *ab initio* calculations. Our calculations reveal that energetically the most preferred configuration of the hydrogen saturated metal clusters exhibit hydrogen multicenter bonds. The strength of these hydrogen multicenter bonds can be modulated either by changing the extent of hydrogen saturation or using different metal clusters. In the context of hydrogen storage materials, our calculations indicate that early first-row transition metals have the best propensity to form hydrogen multicenter bonds. The relevance of this work in the context of hydrogenation and dehydrogenation kinetics of complex metal hydrides will be discussed.

[1]This work is supported by DOE Grant DE-FG36-05GO85028.

T.J. Dhilip Kumar
Department of Chemistry, University of Nevada Las Vegas

Date submitted: 30 Nov 2007 Electronic form version 1.4