Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Metallacarboranes: Towards promising hydrogen storage metal organic framework ABHISHEK SINGH, Materials Research Centre, Indian Institute of Science, Bangalore 560012, India, ARTA SADRZADEH, BORIS YAKOBSON, Department of Mechanical Engineering and Materials Science, Rice University, Houston, Texas 77005, USA — Using first principles calculations we show the high hydrogen storage capacity of metallacarboranes,[1] where the transition metal (TM) atoms bind hydrogen via Kubas interaction. The average binding energy of $\sim$0.3 eV/H favorably lies within the reversible adsorption range The Sc and Ti are found to be the optimum metal atoms maximizing the number of stored H_2 molecules. Depending upon the structure, metallacarboranes can adsorb up to 8 wt% of hydrogen, which exceeds DOE goal for 2015. Being integral part of the cage, TMs do not suffer from the aggregation problem. Furthermore, the presence of carbon atom in the cages permits linking the metallacarboranes to form metal organic frameworks (MOF), thus able to adsorb hydrogen via Kubas interaction, in addition to van der Waals physisorption.

[1]A. K. Singh, A. Sadrzadeh, and B. I. Yakobson, Metallacarboranes: Toward Promising Hydrogen Storage Metal Organic Frameworks, JACS 132,14126 (2010).

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Date submitted: 11 Nov 2010 Electronic form version 1.4