Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Hydrogen Storage Investigation on Nanotube, Graphene and Organo-metallic Complexes HONG ZHANG, Sichuan University, China — New materials and methods for storing hydrogen at high gravimetric and volumetric densities are required because of the widely use of hydrogen for clean fuel. With exceptionally high surface areas, porous materials based on carbon have recently emerged as some of the most promising candidate materials. Here I reviewed our former work on hydrogen storage based on several kinds of organometallic Complexes. Maximum capacities of the hydrogen storage in organometallic compounds consisting of Co and Ni atoms bound to C_mH_m ring were found 3.48 wt % and 3.49 wt %, respectively; for the structures having a transition metal (TM) Co and Ni inserted in C_mH_m ring, the maximum number of H_2 molecule bound to the inserted-type CoC_mH_m and NiC_mH_m complexes is three, and the largest hydrogen storage density is 5.13 wt % and 3.49 wt % for CoC_4H_4 and NiC_4H_4, Meanwhile, the ionic ($C_4H_4^+$ and $C_5H_5^+$) improves the capability of hydrogen storage and makes all H_2 adsorbed to the charged compounds in molecular form. With the CH_3 ligand bound to the compounds, the adsorption energy of H_2 decreases to an ideal range, and stability of the compounds are improved. At last, the hydrogen adsorption properties on the complex structures $TiRH_7Si_8O_{12}$ are investigated, and the kinetic stability when H_2 was added to organometallic compounds is also discussed by analyzing HOMO-LUMO gaps. Here we also mentioned our results of hydrogen storage based on nanotubes and graphene.

Hong Zhang
Sichuan University, China

Date submitted: 17 Oct 2012 Electronic form version 1.4