Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

**The effect of metal clustering on hydrogen storage** PURU JENA, Virginia Commonwealth University, QIAN WANG, Virginia Commonwealth University, QIANG SUN, Virginia Commonwealth University, YOSHIYUKI KAWAZOE, IMS, Japan — Hydrogen has been recognized as an ideal energy carrier and has the potential to reduce our dependence on fossil fuels which are not only limited but also are harmful to the environment. The success of a new hydrogen economy, however, depends upon our ability to find materials that can store hydrogen reversibly with high gravimetric and volumetric density and operate under moderate temperatures and pressures. Although a great deal of effort has recently been devoted to searching of such materials, none are known to meet the above conditions. Nanostructures offer new possibilities for hydrogen storage due to the novel chemistry. It has been shown very recently that coating of carbon nanostructures with ***isolated transition metal atoms*** such as Sc and Ti can increase the binding energy of hydrogen and lead to high storage capacity up to 8 wt% hydrogen, However, this prediction depends on the assumption that the metal atoms coated on the fullerene surface will remain isolated. Using first principles calculations based on density functional theory, and we show that Ti atoms would prefer to cluster on the $C_{60}$ surface which can significantly alter the nature of hydrogen bonding, thus affecting not only the amount of stored hydrogen but also their thermodynamics and kinetics.

Anil Kandalam
Virginia Commonwealth University

Date submitted: 02 Dec 2005 Electronic form version 1.4