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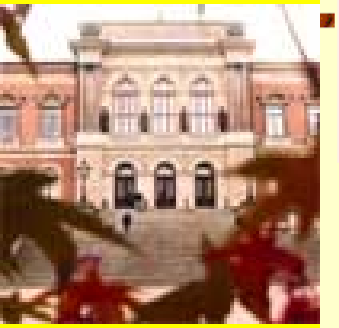


COST Action no. MP1103

Action Title: Nanostructured materials for solid-state hydrogen storage

Agenda – Working Groups Meeting
Warsaw, Poland, 17/09/2015

WG4

**Rajeev Ahuja**

**Uppsala Univ.**
**Sweden**

Condensed Matter Theory Group
UPPSALA UNIVERSITET

Theory Group
UPPSALA UNIVERSITET

## Theory and Simulations : WG4

# Nanostructures with enhanced hydrogen storage capacity

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# Improvement in Hydrogen Desorption from β- and γ-MgH2 upon Transition-Metal Doping

Tanveer Hussain, Tuhina Adit Maark, Sudip Chakraborty and Rajeev Ahuja

ChemPhysChem 16, 634 (2015).


The thermodynamics and kinetics of hydrogen adsorption and desorption from materials can be enhanced through doping. In their Full Paper Hussain et al. performed a systematic study based on density functional theory to explore the effect of various transition metals as dopants on the hydrogen-storage properties of the high-pressure phases (β and γ) of magnesium hydride (MgH2). Upon substituting Mg with small fractions of dopants, the Mg--H bond strength decreased compared with that of the pure form; this ultimately improves the H2 desorption from these phases of MgH2.

# Hydrogen Storage Properties of Light Metal Adatoms (Li, Na) Decorated Fluorographene Monolayer

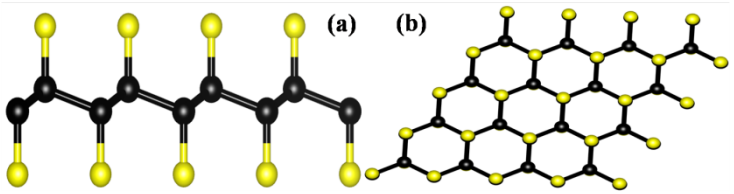
2D materials can solve the $H_2$ storage problem efficiently

Fluorographene (FG) has exceptional mechanical and optical properties with pronounced stability

FG withstand a higher temperature up to ~670 K

Light metal adatoms bind strongly on FG than graphene and BN sheets.

Li and Na adsorption on FG studied computationally




**Pure FG monolayer**

*Hussain et al. Nanotechnology 26, 275401 (2015)*

nature INDIA

doi:10.1038/nindia.2015.85 Published online 24 June 2015

# Metal-modified fluorographene stores hydrogen

Using a computer model, researchers have shown that fluorographene modified with light metals can be used to store hydrogen molecules1. Their calculations indicate that the materials obtained by attaching light metals such as lithium and sodium to either side of fluorographene efficiently adsorb hydrogen. Hydrogen stored in this manner could be used as an eco-friendly fuel.

To find an effective hydrogen-storage material, the researchers used the computer model to simulate structures of fluorographene monolayers in which light metal atoms replaced a few of the fluorine atoms.

The fluorographene monolayer consisted of eight carbon and eight fluorine atoms, two of which atoms (one each from either side) were substituted by atoms of lithium or sodium. Since both lithium and sodium atoms have a lower electronegativity than the carbon atoms to which these metal atoms were attached, charge could be transferred from the metal atoms to fluorographene.

The scientists found that the carbon atoms acquired a most of this transferred charge and the remaining charge went to the fluorine atoms, generating positive charges in the metal atoms. These positively charged metal atoms then bound to hydrogen molecules through weak electrostatic interactions and van der Waals forces.

“Each metal atom can bind to four hydrogen molecules on either side of the fluorographene, making it an excellent hydrogen-storing material,” says Rajeev Ahuja, one of the researchers.

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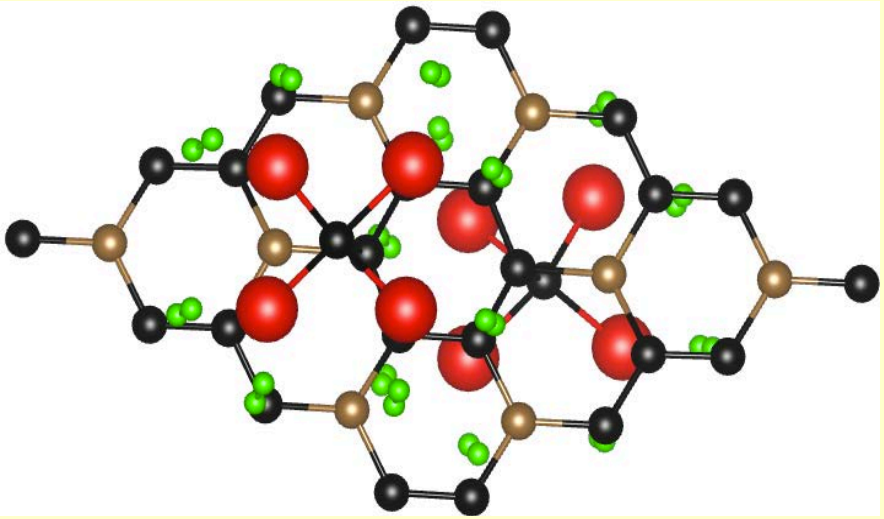
# Highlight : BC3 Sheet Functionalized with Lithium Rich Species Emerging as a Reversible Hydrogen Storage Material

**The present investigation deals with the functionalization of BC3 monolayer with two important members of polylithiated family, CLi4 and OLi2. The calculated binding energies for both the dopants CLi4 and OLi2 over the BC3 monolayer are much higher than their corresponding dimerization energies ensuring the stabilities of BC3-CLi4 and BC3-OLi2 systems. A large distance between the dopants ensures strongly their uniform distribution over the substrate and made the possibility of clustering negligibly small. Due to the difference in electronegativities, a significant amount of charge has been transferred from Li to C and O in both CLi4 and OLi2 resulting in the formation of Li+ ion. The adsorption of H2 molecules around Li+ has been resulted by the electrostatic and weak van der Waals interaction. The H2 storage capacities for two-sided coverage of CLi4 and OLi2 are found to be 11.88wt% and 8.70 wt% respectively with optimum adsorption energies for the practical H2 storage systems. Thus, we have presented computationally engineered stable systems for high capacity storage of hydrogen at ambient conditions, which can certainly be beneficial for practical energy applications.**



**Optimized structure of fully hydrogenated BC3-CLi4. Brown, black, red and green balls represent B, C, Li and H atoms**

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# Some Publications on Hydrogen Storage in 2015

1.BC3 Sheet Functionalized with Lithium Rich Species Emerging as a Reversible Hydrogen Storage Material
Tanveer Hussain, Sudip Chakraborty, T. W. Kang, Börje Johansson and Rajeev Ahuja
Accepted in ChemPhysChem, 16, 634 (2015).

2. R. Johansson, R. Ahuja, O. Eriksson, B. Hjörvarsson, and R. Scheicher
Effect of uniaxial strain on the site occupancy of hydrogen in vanadium from density-functional calculations
Nature-Scientific Reports 5, 10301 (2015).

3. Q. Lai, A.Thornton, M.Hill, Z. Haung, H.K. Lui., Z. Guo, M.Paskevicius, D. Sheppard, C.Buckely, A. Banerjee, S. Chakraborty, R.Ahuja and K.F. Aguey-Zinsou
Hydrogen storage materials for mobile and stationary applications: Current state of the art
ChemSusChem 8, 2789 (2015).

4. (a) T. Hussain, T. A. Maark, S. Chakraborty and R. Ahuja
Improvement in Hydrogen Desorption from β- and γ-MgH2 on Selected Transition Metal Doping
ChemPhysChem 16, 634 (2015).
(b) Cover page of the issue.

5. (a) T. Hussain, M.Islam, S.G. Rao, P. Panigrahi, D. Gupta and R. Ahuja
Hydrogen Storage Properties of Light Metal Adatoms (Li, Na) Decorated Fluorographene Monolayer
Nanotechnology 26, 275401 (2015).

(b) Nature has mentioned it in their highlights. Please see the following website :
http://www.natureasia.com/en/nindia/article/10.1038/nindia.2015.85

6. Q.Tay, P. Kanhere, CF. Ng, S. Chen, S. Chakraborty, A. Huan, CT. Sum, R. Ahuja & Z. Chen
Defect Engineered g-C3N4 for Efficient Visible Light Photocatalytic Hydrogen Production
Chemistry of Materials 27, 4930 (2015).

7. C. J. Rupp, S. Chakraborty, R. Ahuja & R. J. Baierle
Impurity effect in ultra-thin hydrogenated silicene and germanene. A first principles study
Phys.Chem.Chem.Phys. 17, 22210 (2015).