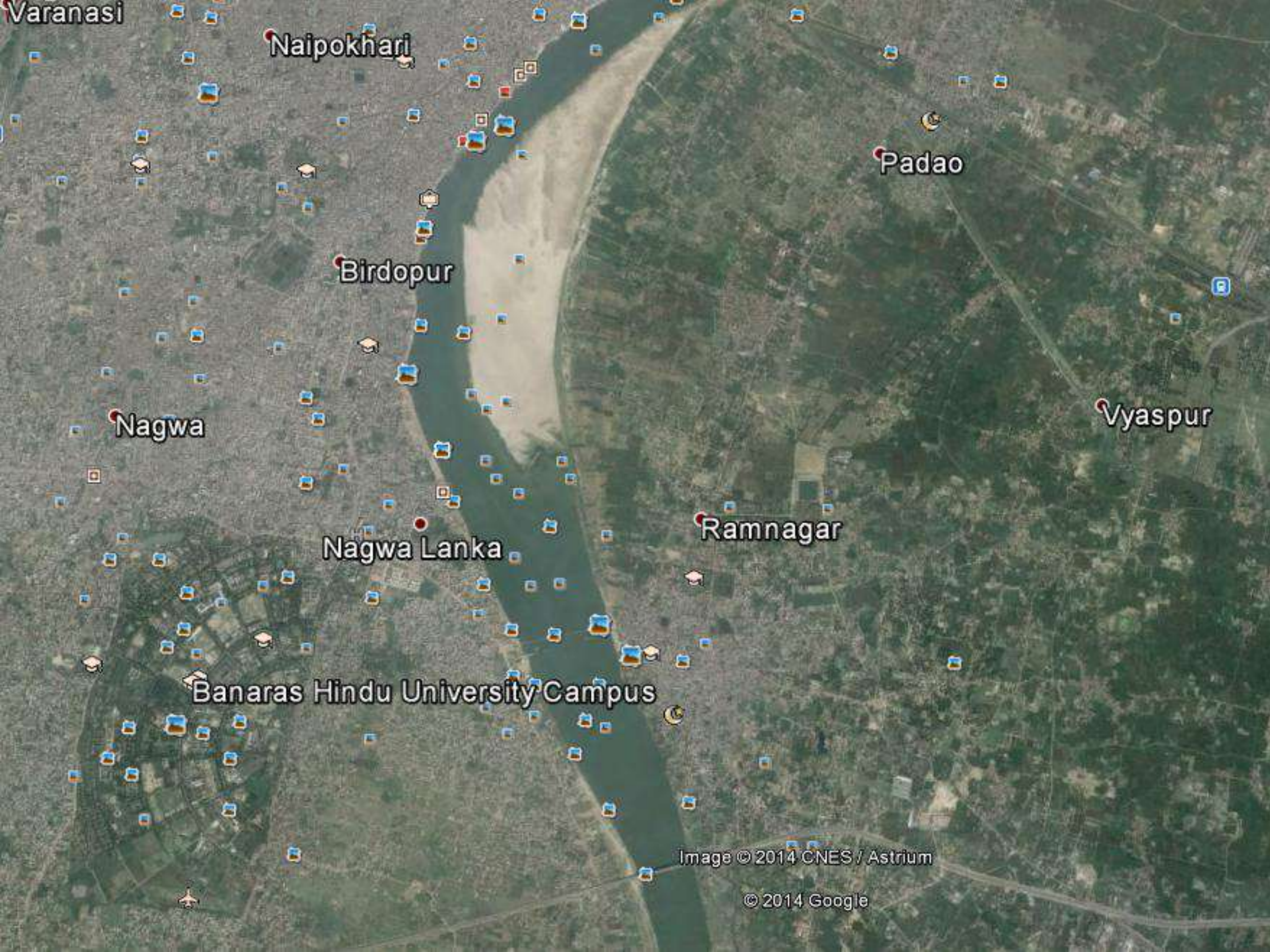
BRICS… ENERGY c/o Dr. S.V. Shirinskii MPEI Russia (25 JUNE 2020)

Banaras Hindu University

INDIA


Varanasi
Naipokhari
Padao
Birdopur
Vyaspur
Nagwa
Ramnagar
Nagwa Lanka
Banaras Hindu University Campus
Image © 2014 CNES / Astrium
© 2014 Google

- **Banaras Hindu University is situated in the holy city of Varanasi**
- **Founded: in 1916 ,by the great visionary, Pandit Madan Mohan Malviya,.**
- **Area of the main campus is about 1400 acres**
- **A satellite campus of the university - area of 2700 acres.**
- **The university comprises:**
- **5 Institutes**
- **16 Faculties**
- **150 Departments, spanning a vast range of subjects pertaining to most of the branches of humanities, social science, technology, medicine, science, fine arts and performing arts.**

- **It has 6 centres of Advanced Studies, 10 Departments under Special Assistance Programme and a large number of specialized Research Centers.**
- **BHU houses the largest museum among the Indian universities, which is a treasure trove of exhibits**
- **The Institute of Medical Sciences of the University houses the largest trauma centre of the country and an additiona ¬ 1000 bed hospital.**
- **The University family consists of about 32000 students, (including students from developed countries)**
- **About 2000 teachers.**
- **A large number of students from about 60 countries all over the world come to study**

- **Number of students:**
- **Undergraduates: 14,649**
- **Postgraduates: 9,120**
- **M.Phil: 41**
- **Ph.D.: 3,497**
- **Diploma: 2,998**
- **Certificate: 362**

- **Total:**
- **Students (Male); 19,392**
- **Students (Female): 11,275**
- **Total no. Of students: 30,667**

- **International Students:**
- **Male: 417**
- **Female: 186**
- **Total: 603 (from 54 countries)**
- **url of the Web page of the University: http://www.bhu.ac.in/**

- **Theme: ENERGY**
- **Banaras Hindu University(INDIA)**

- **Summary:**
- **The details about BHU have been uploaded to the BRICS NU website and are now accessible**

- **BHU has floated 4 courses on Energy for BRICS NU partners:**

1. **Post Graduate Diploma in Non Conventional Energy sources**
2. **Certificate Course on Clean Coal Technology**
3. **Energy Resource Management**
4. **Post Graduate Course in Energy Economics**
5. **RESEARCH…..including collaborative efforts with BRICS**

15 PROJECTS

- **The progress of project proposals on Energy is summarized below**

  Total projects Prepared :08

  Projects Agreed upon by BRICS partners :05

  Projects under Consideration/ Being Explored :03

- **The BHU Energy Group attended the various web conference hosted by BRICS NU**
- **BHU will be solar energy driven campus/ zero energy campus shortly and this project is already in place**
- **In addition numerous emails have been sent by the interested BHU faculty to potential BRICS NU partners abroad but most of them have not been responded to. It is requested to develop structures to facilitate the collaborations among BRICS nations.**

Points of Discussions

- **To find interested potential universities for the courses we have floated**
- **To explore the possibility of making our courses more meaningful of attractive**
- **To find potential collaborators among the BRICS NU programme in the various fields of energy that we have competence and we also have interested faculty for joint bilateral and multilateral projects**
- **To explore possibility for student and faculty exchange. Possibility of student exchange at various levels, viz. undergraduate, post graduate and research levels to be explored**
- **To explore possibilities of joint research supervision among the partners of BRICS NU**

Collaborative projects proposed:

- Eight Projects

Collaborative projects proposed:

- EightProjects
  1st Project:
  Hydrogen Energy:
  Production ,Storage and
  Applications

1.Collaborative project proposed:

HYDROGEN AS A NEW RENEWABLE, CLEAN AND CLIMATE FRIENDLY FUEL;ITS PRODUCTION;STORAGE; AND APPLICATIONS.

PI:Prof ONSrivastava BHU..Varanasi INDIA

Collaborating Institution:Prof

1AlexenderY.Ramenskiy Moscow ..Russia

2.Prof.Helton Jose Alves..Universida Federal do Parana Brazil.

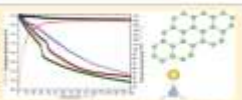
Available online at www.sciencedirect.com
SciVerse ScienceDirect
journal homepage: www.elsevier.com/locate/he

Effects of nano size mischmetal and its oxide on improving the hydrogen sorption behaviour of MgH_2

T. Sadhasivam[a,b], M. Sterlin Leo Hudson[a,c], Sunita K. Pandey[a], Ashish Bhatnagar[a], Milind K. Singh[a], K. Gurunathan[b], O.N. Srivastava[a,*]
[a] Hydrogen Storage Mission Mode MNRE Project Unit, Hydrogen Energy Centre, Department of Physics, Banaras Hindu University, Varanasi 221005, India
[b] Department of Nanoscience and Technology, Alagappa University, Karaikudi 630003, India
[c] Department of Physics, Central University of Tamil Nadu, Thiruvarur 610004, India

The Journal of Physical Chemistry C

Excellent Catalytic Effects of Graphene Nanofibers on Hydrogen Release of Sodium alanate



Available online at www.sciencedirect.com
SciVerse ScienceDirect
journal homepage: www.elsevier.com/locate/he

Effects of nano size mischmetal and its oxide on improving the hydrogen sorption behaviour of MgH_2

T. Sadhasivam[a,b], M. Sterlin Leo Hudson[a,c], Sunita K. Pandey[a], Ashish Bhatnagar[a], Milind K. Singh[a], K. Gurunathan[b], O.N. Srivastava[a,*]

Available online at www.sciencedirect.com
ScienceDirect
journal homepage: www.elsevier.com/locate/he

Carbon nanostructures as catalyst for improving the hydrog[en] storage behavior of sodium aluminum hydride

M. Sterlin Leo Hudson, Himanshu Raghubanshi, D. Pukazhselvan, O.N. Srivastava*
Nanoscience and Technology Unit, Department of Physics, Banaras Hindu University, Varanasi 221005, India

Available online at www.sciencedirect.com
ScienceDirect
journal homepage: www.elsevier.com/locate/he

[D]irect synthesis of sodium alanate using mischmetal [n]anocatalyst

[D.] Pukazhselvan, M. SterlinLeo Hudson, O.N. Srivastava*
[Hydr]ogen Energy Centre, Dept. of Physics, Banaras Hindu University, Varanasi, UP 221 005, India

Available online at www.sciencedirect.com
ScienceDirect
journal homepage: www.elsevier.com/locate/he

Studies on the de/re-hydrogenation characteristic of $Mg(NH_2)_2$/LiH mixture admixed with carbon nanofibres

Rohit R. Shahi, Himanshu Raghubanshi, M.A. Shaz, O.N. Srivastava*
Department of Physics, Hydrogen Energy Centre, Banaras Hindu University, Varanasi 221005, India

Available online at www.sciencedirect.com
ScienceDirect
journal homepage: www.elsevier.com/locate/he

Structural and hydrogenation studies of ZnO and Mg doped ZnO nanowires

Jai Singh, M.S.L. Hudson, S.K. Pandey, R.S. Tiwari, O.N. Srivastava*

Available online at www.sciencedirect.com
ScienceDirect
journal homepage: www.elsevier.com/locate/he

Synthesis, characterization and hydrogen storage behaviour of AB_2 ($ZrFe_2$, $Zr(Fe_{0.75}V_{0.25})_2$, $Zr(Fe_{0.5}V_{0.5})_2$) type materials

T.P. Yadav*, Rohit R. Shahi, O.N. Srivastava

One step high pressure mechanochemical synthesis of reversible alanates $NaAlH_4$ and $KAlH_4$

D. Pukazhselvan [a,*], Duncan Paul Fagg [a], O.N. Srivastava [b]

Hydrogen uptake of reduced graphene oxide and graphene sheets decorated with Fe nanoclusters

M. Sterlin Leo Hudson [a,*], Himanshu Raghubanshi [b], Seema Awasthi [c], T. Sadhasivam [d], Ashish Bhatnager [e], Satoru Simizu [f], S.G. Sankar [f], O.N. Srivastava [e]

Catalytic effect of carbon nanostructures on the hydrogen storage properties of $MgH_2-NaAlH_4$ composite

Ashish Bhatnagar [a], Sunita K. Pandey [a], Viney Dixit [a], Vivek Shukla [a], Rohit R. Shahi [b], M.A. Shaz [a], O.N. Srivastava [a,*]

$MgH_2-ZrFe_2H_x$ nanocomposites for improved hydrogen storage characteristics of MgH_2

Rohit R. Shahi [a,*], Ashish Bhatanagar [b], Sunita K. Pandey [b], Vivek Shukla [b], T.P. Yadav [b], M.A. Shaz [b], O.N. Srivastava [b]

Effects of Ti-based catalysts and synergistic effect of SWCNTs-TiF_3 on hydrogen uptake and release from MgH_2

Rohit R. Shahi [a,b,*], Ashish Bhatnagar [a], Sunita K. Pandey [a], Viney Dixit [a], O.N. Srivastava [a]

Effects of Ti-based catalysts and synergistic effect of SWCNTs-TiF_3 on hydrogen uptake and release from MgH_2

Rohit R. Shahi [a,b,*], Ashish Bhatnagar [a], Sunita K. Pandey [a], Viney Dixit [a], O.N. Srivastava [a]

On the synthesis, characterization and hydrogen storage behavior of $ZrFe_2$ catalyzed Li–Mg–N–H hydrogen storage material

Vivek Shukla [a], Ashish Bhatnagar [a], Sunita K. Pandey [a], Rohit R. Shahi [b], T.P. Yadav [a], M.A. Shaz [a], O.N. Srivastava [a,*]

HYDROGEN STORAGE IN CARBON DERIVED FROM SOLID ENDOSPERM OF COCONUT

Viney Dixit, Ashish Bhatnagar, R. R. Shahi, T. P. Yadav, O. N. Srivastava*
Hydrogen Energy Center, Department of Physics, Banaras Hindu University, Varanasi-221005, India
* Corresponding author: E-mail: hepomphy@gmail.com; Tel: 00915422368468

Abstract

Carbons are being widely investigated as hydrogen storage material owing to their light weight, fast hydrogen adsorption kinetics and cost effectiveness. However, these materials suffer from low hydrogen storage capacity, particularly at room temperature. The aim of the present study is to develop carbon-based material from natural bio-precursor which shows at least moderate hydrogen storage at room temperature. For this purpose, hydrogenation characteristics of carbon derived from solid endosperm of coconut is studied. Solid endosperm and its carbonized version have a native grown distribution of light elements like K (from KCl), Na, Mg, etc. The hydrogen storage measurements reveal that the as synthesized materials have good hydrogen adsorption and desorption capacity with fast kinetics. The synthesized material adsorbs 2.30 wt. % at room temperature and 8.00 wt.% at liquid nitrogen temperature under 70 atm pressure. The present work is likely to initiate research on native light metal bearing carbon derived from natural precursors.

Keywords: Coconut endosperm; Carbonization; Hydrogenation; KCl; Mg.

Hydrogen storage by reduced graphene oxide and graphene-like nanosheets decorated with Fe nanoclusters

Authors: M.S.L. Hudson, O.N. Srivastava, S. Simizu, S.G. Sankar
Affiliation: Central University of Tamil Nadu, W

Pages: 423 - 427
Keywords: helium isotherm, nitrogen isotherm, thermal reduction, chemical reduction, pore size analysis

Abstract: Here, we present the high pressure hydrogen sorption isotherm up to 50 bar of graphene oxide (GO) reduced by thermal reduction (TR-GO), chemical reduction (CR-GO) and graphene like nanosheets decorated with Fe nanoclusters (Fe-GS). GO was first derived by thermal exfoliation of graphite oxide, prepared by modified Staudenmaier method; further reduction at 623K under high vacuum yields TR-GO. CR-GO has been produced by reduction of GO using hydrazine. Fe-GS has been synthesized through arc discharge between the ends of two graphite rods with one rod carrying Fe nanoparticles. The surface area calculated from nitrogen adsorption isotherm at 77 K using BET method for GO, TR-GO, CR-GO and Fe-GS are 304, 357, 80 and 185 m2g-1, respectively. The skeletal density of TR-GO, CR-GO and Fe-GS determined through He gas pycnometry are 1.8, 2.0 and 1.05 gcm-3, respectively. High pressure hydrogen PCT isotherm of TR-GO, CR-GO and Fe-GS has been determined at 300 K and 77 K. The volume of hydrogen adsorbed by TR-GO, CR-GO and Fe-GS at 77 K and 50 bar is 230 ccg

Publication of hydrogen energy 2019-20

Dalton Transactions

PAPER

View Article Online
View Journal

Check for updates

Cite this: DOI: 10.1039/c9dt02270h

A dual borohydride (Li and Na borohydride) catalyst/additive together with intermetallic FeTi for the optimization of the hydrogen sorption characteristics of $Mg(NH_2)_2$/2LiH†

Vivek Shukla,[a] Ashish Bhatnagar,[a] Sweta Singh,[a,b] Pawan K. Soni,[a] Satish K. Verma,[a] T. P. Yadav,[a] M. A. Shaz[a] and O. N. Srivastava *[a]

The present study deals with the material tailoring of $Mg(NH_2)_2$–2LiH through dual borohydrides: the reactive $LiBH_4$ and the non-reactive $NaBH_4$. Furthermore, a pulverizer, as well as a catalyst FeTi, has been added in order to facilitate hydrogen sorption. Addition of $LiBH_4$ to $LiNH_2$ in a 1 : 3 molar ratio leads to the formation of $Li_4(BH_4)(NH_2)_3$ which also acts as a catalyst. However, the addition of $NaBH_4$ doesn't lead to any compound formation but shows a catalytic effect. The onset dehydrogenation temperature of thermally treated $Mg(NH_2)_2$–2LiH/$(Li_4(BH_4)(NH_2)_3$–$NaBH_4)$ is 142 °C as against 196 °C for the basic material $Mg(NH_2)_2$–2LiH. However, with the FeTi catalyzed $Mg(NH_2)_2$–2LiH/$(Li_4(BH_4)(NH_2)_3$–$NaBH_4$, it has been reduced to 120 °C. This is better than other similar amide/hydride composites where it is 149 °C (when the basic material is catalyzed with $LiBH_4$). The FeTi catalyzed $Mg(NH_2)_2$–2LiH/$Li_4(BH_4)(NH_2)_3$–$NaBH_4$ sample shows better de/re-hydrogenation kinetics as it desorbs 3.9 ± 0.04 wt% and absorbs nearly 4.1 ± 0.04 wt% both within 30 min at 170 °C (with the H_2 pressure being 0.1 MPa for desorption and 7 MPa for absorption). The eventual hydrogen storage capacity of $Mg(NH_2)_2$–2LiH/$Li_4(BH_4)(NH_2)_3$–$NaBH_4$ together with FeTi has been found to be ~5.0 wt%. To make the effect of catalysts intelligible, we have put forward in a schematic way the role of Li and Na borohydrides with FeTi for improving the hydrogen sorption properties of $Mg(NH_2)_2$–2LiH.

Received 29th May 2019,
Accepted 27th June 2019

DOI: 10.1039/c9dt02270h

rsc.li/dalton

1. Introduction

The increase in the demand for energy and use of fossil fuels to fulfill this demand has now become a potential threat to the society. Hydrogen is a promising energy vector,[1] has the highest energy density (142 MJ kg^{-1}) and is clean, renewable & environmentally friendly.[2,3] Devices based on H_2 fuel could not be readily developed due to technical challenges in areas such as hydrogen production, storage, and application. Among these three issues, storage of hydrogen in a safe, efficient and economical manner is a huge challenge.[4,5] The US DOE 2020 has set the target (gravimetric capacity: 4.5 wt%, volumetric capacity: 30 g per H_2) which has to be satisfied by the hydrogen storage material for application in vehicular transportation.[6] As a result of tremendous R&D efforts on hydrogen storage materials, it is expected that light weight hydrides will emerge as a potential candidate capable of fulfilling the above-said criteria.[7] Recently, special attention has been paid to such hydrides which are composed of light metal elements and have a high hydrogen content such as amides,[8,9] alanates,[10,11] and borohydrides.[12] One category of these materials which seems very promising is the combination of amide/hydride composites, which show a relatively high hydrogen content and also possess good reversibility.[13,14] However, some issues need to be addressed before it can be used for practical application. These include: (i) a higher desorption temperature to release hydrogen (~250 °C). (ii) Slow hydrogen sorption kinetics (<1 wt% min^{-1}). (iii) Limitations of high enthalpy (>45 kJ mol^{-1}) and lack of good cyclability.[15–21]

Out of the various amide/hydride composites, $Mg(NH_2)_2$: 2LiH (molar ratio 1 : 2), which has a hydrogen storage capacity of 5.5 wt% and a working temperature of ~220 °C, is an optimum material.[22–24] For brevity, this will henceforth be written as 1 : 2 $Mg(NH_2)_2$–LiH. To improve the hydrogen storage characteristics of this material, various catalysts/additives[25,26] have been employed. For example, Yang et al.[25] first introduced $LiBH_4$ in the Li–Mg–N–H system where

[a] Hydrogen Energy Centre, Department of Physics, Banaras Hindu University, Varanasi 221005, India. E-mail: hepons@yahoo.com; Tel: +91 0542 2368468
[b] Department of Physics, School of Physical and Material Sciences, Mahatma Gandhi Central University, Bihar, 845401, India

† Electronic supplementary information (ESI) available: Fig. S1–S9. See DOI: 10.1039/c9dt02270h

PCCP

PAPER

View Article Online
View Journal | View Issue

Check for updates

Cite this: Phys. Chem. Chem. Phys., 2017, 19, 9444

Enhanced hydrogen sorption in a Li–Mg–N–H system by the synergistic role of $Li_4(NH_2)_3BH_4$ and $ZrFe_2$†

Vivek Shukla, Ashish Bhatnagar, Pawan K. Soni, Alok K. Vishwakarma, M. A. Shaz, T. P. Yadav and O. N. Srivastava *

The present investigation describes the synergistic role of $Li_4(BH_4)(NH_2)_3$ and $ZrFe_2$ in the hydrogen storage behaviour of a Li–Mg–N–H hydride system. The onset desorption temperature of $ZrFe_2$-catalysed $Mg(NH_2)_2$–LiH–$Li_4(BH_4)(NH_2)_3$ is ~122 °C, which is 83 °C, 63 °C, and 28 °C lower than that of thermally treated 2$LiNH_2$–1MgH_2, 2$LiNH_2$–1MgH_2–4 wt%$ZrFe_2$, and 2$LiNH_2$–1MgH_2–0.1$LiBH_4$ composites, respectively. Native $Mg(NH_2)_2$–LiH–$Li_4(BH_4)(NH_2)_3$ absorbed only 2.78 wt% of H_2 within 30 min. On the other hand, the $ZrFe_2$-catalysed $Mg(NH_2)_2$–LiH–$Li_4(BH_4)(NH_2)_3$ sample absorbed 3.70 wt% of hydrogen within 30 min and 5 wt% of H_2 in 6 h at 180 °C and 7 MPa H_2 pressure. $Mg(NH_2)_2$–LiH–$Li_4(BH_4)(NH_2)_3$ catalyzed with $ZrFe_2$ shows negligible degradation of the storage capacity even after repeated cycles of de/rehydrogenation. The effect of $ZrFe_2$ and $Li_4(BH_4)(NH_2)_3$ on a $Mg(NH_2)_2$/LiH composite has been described and discussed with the help of structural (X-ray diffraction), microstructural (electron microscopy), and vibrational modes of molecules through FTIR studies. The present results suggest that an optimum catalysis may originate from the synergistic action of an in situ formed quaternary hydride ($Li_4(BH_4)(NH_2)_3$) and an intermetallic-like $ZrFe_2$, which acts as a pulverizer cum catalyst.

Received 6th December 2016,
Accepted 7th March 2017

DOI: 10.1039/c6cp08333a

rsc.li/pccp

1. Introduction

Because of the enhanced emphasis on the detrimental effects of global warming, the worldwide demand for renewable energy is quickly increasing.[1] Hydrogen may be an ideal renewable energy carrier if it can be safely and efficiently stored. Hydrogen is a totally carbon-free fuel and it has the highest energy density of 142 MJ kg^{-1} compared to other fossil fuels.[2] Thus, when used as a fuel, it can mitigate global warming. Many efforts have been made in the development of new hydrogen storage materials worldwide. After these extensive efforts, it has been found that solid state storage of hydrogen in the form of hydride is one of the best options for storing hydrogen.[3–5] However, after decades of research, no hydride has been found that satisfies all the requirements for H_2 storage (United States Department of Energy (US DOE) target-2015).[6] In the last few years, complex hydrides such as alanates, amide-hydrides, and borohydrides have been considered as promising materials for safe and efficient hydrogen storage. The Li-Mg-N-H system is the one of most propitious candidates for hydrogen storage because of its favorable thermodynamics, high hydrogen content, and good reversibility at moderate operating temperatures.[7,8] Out of various metal N-H systems, 1 : 2 $Mg(NH_2)_2$/LiH has a theoretical storage capacity of 5.5 wt% in the mild temperature range of sorption (>200 °C). The metal-NH system can be a storage material of great interest if its unfavorable thermodynamics, slow kinetics, and inability to rehydrogenate or comparatively low hydrogen storage capacity can be resolved.[9–12] Thus, it is necessary to improve the thermodynamics and kinetics of the Li-Mg-N-H system. In this regard, V, V_2O_5, VCl_3, $TiCl_3$, Pb_3PO_4, TiN, KF, RbF, NaH, and KH have been used as catalysts to improve the thermodynamics and kinetics of the Li–Mg–N–H system.[13–20] However, it is still not good for practical purposes, which restricts its application. It has been found that metal borohydrides such as $LiBH_4$, $NaBH_4$, $Ca(BH_4)_2$, and $Mg(BH_4)_2$ are also effective dopants for improving the hydrogen sorption (de/rehydrogenation) reaction kinetics of the Li–Mg–N–H system.[21–27] Yang et al.[25] observed a ternary composite system $LiNH_2$/MgH_2/$LiBH_4$ and explained that in this system, $LiNH_2$

Hydrogen Energy Centre, Department of Physics, Banaras Hindu University, Varanasi-221005, India. E-mail: hepons@yahoo.com; Tel: +91 0542 2368468

† Electronic supplementary information (ESI) available: Fig. S1: Gas chromatography (GC) measurements using Carbosphere and Chromosorb columns (i and ii) detection of pure H_2 in Chromosorb column (iii and iv) detection of evolved gases on the dehydrogenation of the TT L-M-B-Z sample in a Chromosorb column. Fig. S2: Storage capacity upon cycling (180 °C) of the catalysed TT L–M–B–Z composite. Fig. S3: (i) XRD of the L-M-Q and TT L-M-Q sample and (ii) TPD of the TT L-M-Q sample. Fig. S4: Transmission electron microscopy images of (a) the L-M-B-Z sample, (b) selected area diffraction pattern (SAED) of the L-M-B-Z sample, (c) after cycling TT L-M-B-Z and (d) selected area diffraction pattern (SAED) of the after cycled TT L-M-B-Z sample. See DOI: 10.1039/c6cp08333a

Publication of hydrogen energy 2019-20

ARTICLE IN PRESS
INTERNATIONAL JOURNAL OF HYDROGEN ENERGY XXX (XXXX) XXX
Available online at www.sciencedirect.com
ScienceDirect
journal homepage: www.elsevier.com/locate/he

Multiple improvements of hydrogen sorption and their mechanism for MgH_2 catalyzed through TiH_2@Gr

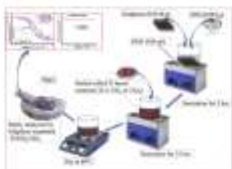
Satish Kumar Verma [a], *Ashish Bhatnagar* [b], *Vivek Shukla* [a], *Pawan Kumar Soni* [a], *Anant Prakash Pandey* [a], *Thakur Prasad Yadav* [a], *Onkar Nath Srivastava* [a,*]

[a] Hydrogen Energy Centre, Department of Physics, Institute of Science, Banaras Hindu University, Varanasi, 221005, India
[b] Department of Physics and Materials Science and Engineering, Jaypee Institute of Information Technology, Noida, 201309, India

HIGHLIGHTS

- Onset dehydrogenation temperature of 204 °C for MgH_2 catalyzed by TiH_2@Gr.
- Good cyclic stability and improved thermodynamics for MgH_2 catalyzed by TiH_2@Gr.
- Mechanism for catalytic action of TiH_2@Gr on MgH_2.
- Comparison of catalytic effect of Ti@Gr, TiO_2@Gr and TiH_2@Gr on MgH_2.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 4 January 2020
Received in revised form
2 May 2020
Accepted 4 May 2020
Available online xxx

Keywords:
Hydrogen storage
Magnesium hydride
Graphene templated Ti-based

ABSTRACT

The present investigation reports the effect of TiH_2 templated over graphene (TiH_2@Gr) on the hydrogen sorption characteristics of MgH_2/Mg. The as synthesized TiH_2@Gr leads to significant effect on sorption in MgH_2 by the following effects: the first is dehydrogenation of MgH_2–TiH_2@Gr, which leads to the conversion of some part of TiH_2 into $TiH_{1.924}$. TiH_2 together with $TiH_{1.924}$ works as a better catalyst than TiH_2 alone. The second is ball-milling of TiH_2@Gr, which produces defective graphene, which also works as co-catalyst. The third is anchoring of TiH_2 on graphene, which does not allow the catalyst to agglomerate. The catalytic effect of TiH_2@Gr on MgH_2 is found to be better than Ti@Gr and TiO_2@Gr. The onset desorption temperature for MgH_2–TiH_2@Gr is ~204 °C, which is 31 °C and 36 °C lower than MgH_2–Ti@Gr, MgH_2–TiO_2@Gr respectively. The better catalytic behavior of TiH_2@Gr

* Corresponding author.
E-mail addresses: heponsphy@gmail.com, heponsphy.bhu@gmail.com (O.N. Srivastava).
https://doi.org/10.1016/j.ijhydene.2020.05.031

Please cite this article as: Verma SK et al., Multiple improvements of hydrogen sorption and their mechanism for MgH_2 catalyzed through TiH_2@Gr, International Journal of Hydrogen Energy, https://doi.org/10.1016/j.ijhydene.2020.05.031

ARTICLE IN PRESS
INTERNATIONAL JOURNAL OF HYDROGEN ENERGY XXX (XXXX) XXX
Available online at www.sciencedirect.com
ScienceDirect
journal homepage: www.elsevier.com/locate/he

Ternary transition metal alloy FeCoNi nanoparticles on graphene as new catalyst for hydrogen sorption in MgH_2

Sweta Singh [b], *Ashish Bhatnagar* [c], *Vivek Shukla* [a], *Alok K. Vishwakarma* [a], *Pawan K. Soni* [a], *Satish K. Verma* [a], *M.A. Shaz* [a], *A.S.K. Sinha* [d], *O.N. Srivastava* [a,*]

[a] Hydrogen Energy Centre, Department of Physics, Banaras Hindu University, Varanasi 221005, U.P, India
[b] Department of Physics, Mahatma Gandhi Central University, Motihari, 845401, Bihar, India
[c] Department of Physics and Materials Science and Engineering, Jaypee Institute of Information Technology, Noida, 201309, India
[d] Department of Chemical Engineering and Technology, Indian Institute of Technology, Banaras Hindu University, Varanasi, 221005, India

HIGHLIGHTS

- Synthesis of FeCoNi@GS by one pot method.
- FeCoNi@GS has been used as catalyst for MgH_2.
- MgH_2 catalyzed by FeCoNi@GS show excellent cyclability.
- Formation enthalpy of MgH_2: FeCoNi@GS is reduced by 19.26 kJ/mol of H_2 as compared to ball milled MgH_2.

GRAPHICAL ABSTRACT

ARTICLE INFO

Article history:
Received 26 June 2019
Received in revised form
22 September 2019
Accepted 25 October 2019
Available online xxx

Keywords:
Ternary alloy FeCoNi
Graphene templated FeCoNi
MgH_2
Hydrogen storage

ABSTRACT

The present investigation deals with the synthesis of ternary transition metal alloy nanoparticles of FeCoNi and graphene templated FeCoNi (FeCoNi@GS) by one-pot reflux method and there use as a catalyst for hydrogen sorption in MgH_2. It has been found that the MgH_2 catalyzed by FeCoNi@GS (MgH_2: FeCoNi@GS) has the onset desorption temperature of ~255 °C which is 25 °C and 100 °C lower than MgH_2 catalyzed by FeCoNi (MgH_2: FeCoNi) (onset desorption temperature 280 °C) and the ball-milled (B.M) MgH_2 (onset desorption temperature 355 °C) respectively. Also MgH_2: FeCoNi@GS shows enhanced kinetics by absorbing 6.01 wt% within just 1.65 min at 290 °C under 15 atm of hydrogen pressure. This is much-improved sorption as compared to MgH_2: FeCoNi and B.M MgH_2 for which hydrogen absorption is 4.41 wt% and 1.45 wt% respectively, under the similar condition of temperature, pressure and time. More importantly, the formation enthalpy of MgH_2: FeCoNi@GS is 58.86 kJ/mol which is 19.26 kJ/mol lower than B.M: MgH_2 (78.12 kJ/mol).

* Corresponding author.
E-mail address: heponsphy@gmail.com (O.N. Srivastava).
https://doi.org/10.1016/j.ijhydene.2019.10.204

Please cite this article as: Singh S et al., Ternary transition metal alloy FeCoNi nanoparticles on graphene as new catalyst for hydrogen sorption in MgH_2, International Journal of Hydrogen Energy, https://doi.org/10.1016/j.ijhydene.2019.10.204

.2nd Project :.BIOFUEL FROM MICROALGAE

Status: Collaborator: Prof. Dr. Eduard Jacob-Lopes, Univeridade Federal de Santa Maria, Centro de Ciencias Rurais Av. Roraima 1000, Camboi Santa Maria, Brazil

- Prof. R.K. Asthana, Dept. of Botany

TiO2 thin film photoanode based dye-sensitized solar cells (DSSCs) for harvesting solar radiation (light energy)

- Status: Collaborators being explored
-
- Dr. Pankaj Srivastava, Assistant Professor, Department of Chemistry, Institute of Science, BHU Varanasi 221005

3rd Project New materials for fuel cells, super capacitors, electrochemical sensor and for the removal of organic/inorganic contaminants from natural water sources

- **Status: Collaborators being explored**
- ***Dr. V. Ganesan***
- ***Assistant Professor, Department of Chemistry, Institute of Science6***

5.4th Project. TiO2 thin film photoanode based dye-sensitized solar cells (DSSCs) for harvesting solar radiation (light energy)

- **Status: Collaborators being explored**
- **Dr. Pankaj Srivastava, Assistant Professor, Department of Chemistry, Institute of Science, BHU Varanasi 221005 Uttar Pradesh, India**
- **Collaborators being explored**

.5 th Project:.Title of the Project: "**Graphene Based Hierarchically Nanostructured Composites as Multi-Functional Materials for Energy Storage, Actuator and Sensing Applications**"

- **Proposal submitted by us under the project BRICS PILOT Call 2016Collaborators:**
- **From India: Dr. Anchal Srivastava, BHU**
- **From China: Prof. Li Song,** Synchrotron Radiation National Lab, University of Science and Technology of China.
- **From South Africa: Dr. Patric Ndungu,** Department of Applied Chemistry, University of Johannesburg.

- **6TH PROJECT:. DEVELOPMENT OF NEW GENERATION - BIOFERTILIZERS/BIOPESTICIDES FOR CLIMATE RESILIENT AGRICULTURE**
-
- **Collaborators: Prof. Leonardo F. Fraceto** - Institute of Science and Technology - São Paulo State University, Brazil) and **Prof. Renata de Lima** (University of Sorocaba, Brazil).
- **Collaborators from India:**
- **Prof. H. B. Singh** and **Prof. B K Sarma**
- Department of Mycology & Plant Pathology, I.Ag.Sci., BHU, Varanasi
- **Prof. Bandana Bose** and **Prof. PadmanabhDwivedi**
- Department of Plant Physiology, I.Ag.Sci., BHU, Varanasi
- **Dr. AmitavRakshit**, Sr. Asstt. Professor
- Department of Soil Science & Agric. Chemistry, I.Ag.Sci., BHU, Varanasi

- **7^{th} Project: Project Details:**

1. Development of thin film Solar cell using thermal/e-beam evaporation technique

- **Status:** Agreed upon by BRICS partner
- **Participating Faculty: Prof B.K. Singh, Department of Physics**
- **Theme: Energy (Sub theme: Solar Cell)**
- **The group has agreement with a Russian group headed by Prof. V. F. Markov of Ural Federal University (Russia) under BRICS Network.**

8th Project :. A Project proposal on Energetic materials for submission to BRICS Network University (consideration under "Nanomaterials and meta materials for energetics for MISIS, Moscow)

- **Status: Collaborators being explored**
- **Dr. Satyen Saha, Assistant Professor, Department of Chemistry, Banaras Hindu**
- **University, Varanasi 221005, India.**

- **COURSES FLOATED (four courses)**
- **BY …BHU (INDIA) UNDER BRICS**

FOR BRICGS NU ENERGY ITG

Course flotted

Course name: **M A (Masters) in Energy Economics**

Basic university: **Banaras Hindu University,** A Comprehensive University, as Institute of Eminence, of International Repute and of more than Hundred Years Old.

URL of the University: **www.bhu.ac.in**

Educational program / degree: **Master's Degree in Energy Economics (M. A in Energy Economics).**

Duration: **Two years full time duration with 4 semesters** emphasizing both on class room teaching and field work.

Eligibility: Eligibility: B.A. (Hons.) Economics/ B.Com./B.Sc./B.A. Programme with Economics or B.Tech. or MBA with minimum of 50% aggregate marks from a recognized University/Institute. The course will be taught in English Medium only.

NOTE: In addition to the above that the candidates must have minimum 50% marks at Higher and Senior Secondary level with Mathematics as one subject. However, this course requires advance knowledge of mathematics.

Responsible person (with contact details): **Prof. Mrutyunjaya Mishra, Course Coordinator**, Professor of Economics (Environmental Economics), Department of Economics, Faculty of Social Sciences, Banaras Hindu University, Varanasi-221005, Mobile No: +91 9838419845, email: coordinator.energyeco@bhu.ac.in; mmishrabhu@gmail.com.

Program description: **Background to the Course:**

This course owes its Origin to the BRICS-NU programme to which Banaras Hindu University is an International Partner. Of few selected Core Areas of Research and Higher Study Energy is an important part and Energy Economics is one among the cores. Its our proud privilege that the Esteemed Banaras Hindu University happens to be a lead partner of this Core Area and Group. On the initiation of the Hon'ble Vice Chancellor and the guidance of the Dean of Faculty of Social Sciences, Department of Economics decided to launch this course, **Master of Arts in Energy Economics.**

Course preamble:

Efficiency and sustainability of energy system are pre-requisites for Sustainable Development and the challenges to achieve this lie at the interface of technology, innovation and human behavior. This course is tailored for the student desiring an understanding of the relationship between the energy sector and the wider economy. It covers additional topics in related and associated fields of Management, Commerce, Engineering, Mining and Natural Resources with emphasis on tracing the national and Global impacts and implications of energy sector decisions. This course provides an overview of the economic, technological, and political forces that shape the global energy industry, the methods governments use to regulate the industry, and the business models that emerge.

The course aims at broadening the vision of students while making any energy related decision as a technology developer, energy manager, entrepreneur, policy maker, researcher in future or simply for personal energy use in day to day activities.

Topics to be covered include, resource based energy activities, depletion policy and environmental issues, pricing security and sustainability.

The course begins by framing the industry in its microeconomic context and uses that framework to explore the role of technology and innovation, global markets and geopolitics, and the regulation of externalities including climate change. The readings and coursework will use specific examples from the power, renewables, oil & gas, and environmental sectors from the both developing and developed countries and other select geographies to illustrate these forces in context. Students can tailor their final policy memo towards their topics of interest.

Objectives

The aim of the of the Masters in Energy Economics programme is to prepare the students for managerial , advisory and academic position in the energy sector. The programme aims to provide an intellectually challenging academic programme which will strengthen the ability of students to analyse, synthesise and evaluate key theoretical concepts and practical applications in energy with emphasis on the economic dimensions of the subject. Since the world's long term economic development depends on the existence of efficient, innovative and creative energy industries individuals who possesses sound knowledge on various aspects like economic, commercial, technical, management and environmental aspects will be of high demand and cater to the need of both at national and international level.

Curriculum: **Course Curriculum of Energy Economics**

All papers covered under the course are Core courses of 4 credits each and dissertation is 4 credits. The internship is assigned with 4 credits. So total credit score is 84 credit.

Sl.No	Course No	Course Title	Course No	Course Title
	SEMESTER I		SEMESTER II	
1	MEE-101	Microeconomics	MEE -201	Macroeconomics
2	MEE -102	Energy Economics	MEE -202	Basic and Applied Econometrics
3	MEE -103	Environmental Economics	MEE -203	Advanced Resource Economics
4	MEE -104	Mathematical Economics	MEE -204	Investment and Portfolio Management
5	MEE -105	Applied Statistics	ECM-205	Advanced Mining and Evaluation
	SEMESTER III		SEMESTER IV	
6	MEE-301	Operations Research	MEE -401	Economic Evaluation and Project Management
7	MEE-302	Research Methods for Energy Analysis	MEE-402	Management of Technology for Energy
8	MEE-303	International Trade in Energy resources	MEE -403	International Business Strategy and Energy Sector
9	MEE -304	Energy ,Economy and Society	MEE -404	Energy, Climate Change and Global Politics
10	MEE-305	Accounting and Finance	MEE -405	Field Work based Dissertation

Presentation: Students are required to undergo **Summer Internship** during the summer vacation between II and III semester and prepare reports about their learning, education and training during summer internship.

Further students submit a Master Dissertation at the end of the Semester as a partial fulfillment of the course and the dissertation is of 4 credits.

Other materials: Course and Source Materials provided to students by teachers and resource persons from time to time. Standard books and study materials prescribed for reference as study and reference materials.

COURSE ON HYDROGEN ENERGY

Hydrogen Energy Centre, Department of Physics, Banaras Hindu University, Varanasi, India

Academic plan showing the courses proposed: Proposed Courses

The PG special course will run for one year. The student to be admitted will be PG students from Science / Engineering stream. The one year course will be divided in two semesters. Also the teaching will be in research ambience. This will be achieved through a project which will be research oriented and will form essential part of the syllabus and will carry 4 credits and will be carried out in the second semester (out of total 10 credits where 6 will be from theory for each semester).

The courses will run for five years, midterm changes will be made to bring new relevant topics covering emerging areas. The five year course will be based on feedback from the first five year PG students who would have undergone the special course in Hydrogen Energy. Besides this the next five year course will bring in such new topics which will be in conformity with societal need relating to use of clean, renewable and environment friendly energy (only hydrogen fulfill all these requirements) for which the country is committed (India has signed 2015 Paris Agreement). The last five years course schedule will be based on new and innovative areas in Hydrogen Energy which would have emerged by then. It will also cover academic strategies and research perspectives for adoptability of Hydrogen Energy for the country. A tentative academic plan showing the course proposed is given in the following.

COURSE ON HYDROGEN ENERGY

1st Semester (III Semester as per present PG teaching schedule)

Course 1 (Theory) (a) Hydrogen vis-a-vis other Renewable Energies

(b) Present route of hydrogen production from Hydrocarbon and its limitations.

(c) The solar Resource

(d)Introduction to Hydrogen Production through splitting of water using solar energy various Solar Routes

Course 1 (Laboratory).

Basic experiments on Hydrogen Production.

Course 2 (Theory) (a) Why storage? The logic of storage

(b) Various Techniques of Hydrogen Storage (High Pressure Gaseous, Liquid and Solid (Hydride))

(c) Advantages and preference for solid state hydrogen storage route.

(d) The safety aspects of various storage routes.

Course 2 (Laboratory)

Basic experiments of Hydrogen Storage including known intermetallic hydrides for Hydrogen Storage.

4. Hydrogen Energy Centre, Department of Physics, Banaras Hindu University, Varanasi, India
Academic plan showing the courses proposed : Proposed Courses

2nd Semester (IV Semester as per present PG teaching schedule)

Course 1 (Theory)

Various Routes of Production of Solar Hydrogen in
(a) Solar energy driven pathways through water splitting.
(b) The role of nanomaterials in PV driven hydrogen production
(c) Hydrogen production using solar energy induced water splitting employing nanocatalyst e.g. Cds TiO_2.
(d) Photo biological methods of renewable hydrogen production.
(e) Photoelectrochemical Electrolysis (use of Photoanodes of nanostructured oxide TiO_2 , Fe_2O_3, WO_3 etc.
(f) Photocatalytic Electrolysis (deploying semiconductors nanoparticles e.g. nano Cds and hybrid materials).

Course 1 (Laboratory)

Hydrogen Production Experiments using nanomaterials.

Course 2 (Theory)

(a) Various types of hydrogen storage materials (hydride).
(b) Hydrogen storage modes: Physisorption and chemisorption.
(c) Mechanism of hydrogen storage.
(d) Understanding Hydrogen Storage in Hydrides in regard to optimizing.

Course 2 (Laboratory)

Synthesis and Characterization of Large Scale Hydride (Kg Level) for Hydrogen Application and Demonstration for Electricity and Automotive Power Applications.

- **The University has floated the following courses**

Post Graduate Diploma in Non Conventional Energy sources

- Development and economic growth of societies depends on the energy inputs. Growth of energy sector is particularly critical for socioeconomic development of rural areas. Globally the need for energy is only bound to increase. Unsustainability of fossil fuels due to their limited nature leaves no option but to harness non-conventional energy to overcome the barriers to development posed by energy security in the rural areas. In view of the anthropogenic global warming threat driving climate change coupled with scarcity of fossil fuels, the Post Graduate Diploma Programme in the Non-conventional Energy Sources is timely to enable students with varied backgrounds to appreciate various aspects of the energy sources. Students will be exposed to the different kinds of non-conventional energy sources and their applications to different aspects. The course is aimed at providing an understanding of the non conventional energy sources and their applications in different areas. The modules would include units on Solar Energy, Solar Energy Applications, Hydrogen Energy & Fuel Cells, Wind Energy and Biomass, Geothermal Energy, Batteries, Supercapacitors and Nuclear Energy. Lab training with credits would form an integral part of the course

- **Duration : 2 Semesters**
- **Eligibility Qualifications : B.Sc. in Science Discipline**

- **Certificate Course on Clean Coal Technology**
- Clean coal technologies focus on efficient combustion of coal with reduced emissions of sulfur dioxide, nitrogen oxide, particles and mercury, and reducing carbon dioxide emissions through carbon capture and storage. Other technologies such as coal liquefaction and gasification are being pursued to produce low cost, secure alternatives to oil and natural gas for use in electricity generation and transportation. The Department of Geology, B.H.U proposes a certificate course to educate, encourage and support public/private organisations to be aware of the intricacies of coal constitution and its bearing on the clean coal technologies that ultimately can be brought to large-scale commercial deployments. The takers of this certificate course would not only be the Thermal Power Generation plants but also other coal consumers like, steel plants, cement plants and other industries including post graduate students. The course structure would include coal as rock and fuel, environmental pollution and assessment, clean coal technologies (CCT) and coal preparation. There would be credits for lab training.

- **Duration : 1 Semester**
- **Eligibility Qualifications : B.Sc. in Science Discipline**

SOME DETAILS OF MAJOR RESEARCH 1ST PROJECT

Hydrogen Energy: Production ,Storage and Applications

Energy (Electricity) Scenario In India

WHY HYDROGEN FOR INDIA?

India is 3rd largest electricity producer

China 6015 (TWh)

USA 4327 (TWh)

India 1423 (TWh)

Russia 1038 (TWh)

India's electricity consumption is very low 1/3rd of world's consumption i.e. 1213 kWh per capita (This has to be increased for improving the life quality).

Various Sources of Electrica

Coal (63.90%)

Hydro (13.00%)

Wind (3.70%)

Solar (15.30 %)

Biomass (1.10%)

Nuclear (3.00%)

India expanded its solar-generation capacity 8 times from 2,650 MW on 26 May 2014 to over 20 GW as on 31 January 2018.

Installed capacity of electricity generation in India was 344 GW on 31 may 2018

Renewable Energy Component for India ~17%.

India will continue to depend on Coal for future production but the Renewable and Nuclear Energy component is planed to be increased up to ~30% in coming~10 years

Energy (Oil) Scenario In India

Total Oil Production

India 856 Tbd (Thousand barrel daily)
China 3999 Tbd ………………………
Russia 11227 Tbd……………………
Brazil 2605 Tbd………………………
South Africa 169 Tbd………………

Total Oil Consumption

India 4,69,0000 Bbd (Billion barrel daily) (Per Capita one of the lowest world
China 1,32,26,000 Bbd
Russia 3,22,4000 Bbd
Brazil 30,17,000 Bbd
South Africa 5,90,900 Bbd

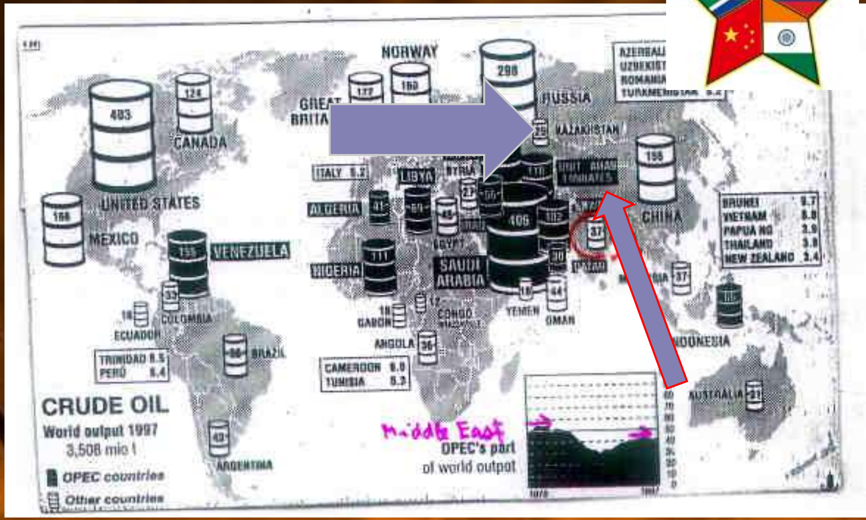
India has therefore very precarious position in regards to Oil. It is almost a total oil importing country and has to spent about 50% of its foreign exchange reserve on oil imports.

Therefore it is looking for a indigenous replacement of oil. It has been found that based on logistics Hydrogen is the best option.

Why Hydrogen for INDIA?

Indigenous oil production in 1997

India 46MT (1992) 37MT (1997)
32MT (1999)
China 155MT (1999)
Saudi Arabia 406MT
USA 403MT
Russia 298MT



Decreasing Indigenous oil supply but ever increasing demand

Large Gap between Demand &Supply
1$=Rs.17; 0,000Crores

World Resources 1052.7 Billion US Baralls

Middle East	USA	China	India
69%	15% ?	5%	0.9%

India is importing about 156--180 MT Indigenous oil (30MT Indigenous)

	Country	Production (bbl/day)	Share of World %	Date of Information
	World	84,820,000[6]	100%	—
1	Russia	10,900,000	13.28%	2013 est.[7][8]
2	Saudi Arabia	9,900,000	12.65%	2013 est.[7][9]
3	United States	8,453,000	9.97%	2013 est.
4	Iran	4,231,000	4.77%	2013 est.
5	China	4,073,000	4.56%	2013 est.
6	Canada	3,592,000	3.90%	2013 est.
7	Iraq	3,400,000	3.75%	2013 est.
8	United Arab Emirates	3,087,000	3.32%	2013 est.
9	Venezuela	3,023,000	4.74%	2013 est.
10	Mexico	2,934,000	3.56%	2013 est.
11	Kuwait	2,682,000	2.96%	2013 est.
12	Brazil	2,633,000	3.05%	2013 est.
13	Nigeria	2,525,000	2.62%	2013 est.
14	Norway	1,998,000	2.79%	2013 est.
15	Algeria	1,885,000	2.52%	2013 est.
16	Angola	1,840,000	2.31%	2013 est.
17	Kazakhstan	1,635,000	1.83%	2013 est.
18	Qatar	1,631,000	1.44%	2013 est.
19	United Kingdom	1,099,000	1.78%	2011 est.
20	Colombia	1,011,992	0.97%	2013 est.
21	Azerbaijan	987,000	1.20%	2011 est.
22	Indonesia	982,900	1.66%	
23	India	897,300	1.04%	2013 est.

INDIA IS LOOKING FOR A FUEL WHICH CAN REPLACE OIL(PETROLEUM) ,WHICH IS INDIGENOUS, RENEWABLE ,CLEAN AND CLIMATE FRIENDLY.

VARIOUS LOGISTICS SUGGEST THAT FOR INDIA SUCH A FUEL MAY BE HYDROGEN….PLENTY OF WATER AROUND BAY OF BENGAL..ARABIAN SEA …INDIAN OCEAN…~200RIVERS INCLUDING ,BRHMAPUTRA&GANGA

PLENTY OF SOLAR INSOLATION …NEXT ONLY TO AFRICA

WHY HYDROGEN FOR INDIA?

1. HUGE DIFFERENCE BETWEEN OIL PRODUCTION AND ONSUMPTION
2. CLIMATE CHANGE EFFECTS
3. Urban AIR POLLUTION

Types of damage	Coal	Petroleum	N. Gas
on Humans	5.54	4.51	3.33
on Animals	0.82	0.67	0.48
on Plants and Forests	2.15	1.74	1.29
on Aquatic Systems	0.29	1.68	0.18
on Man-Made Structures	1.78	1.43	1.07
other Pollutants Costs	1.56	1.26	0.94
by Strip Mining	0.79	-	-
by Climatic Change	2.22	1.80	1.34
by Sea Level Rise	0.51	0.41	0.31
Total Environmental Damage	*15.66*	*13.50*	*8.94*

Environmental and health damage by Fossil Fuels

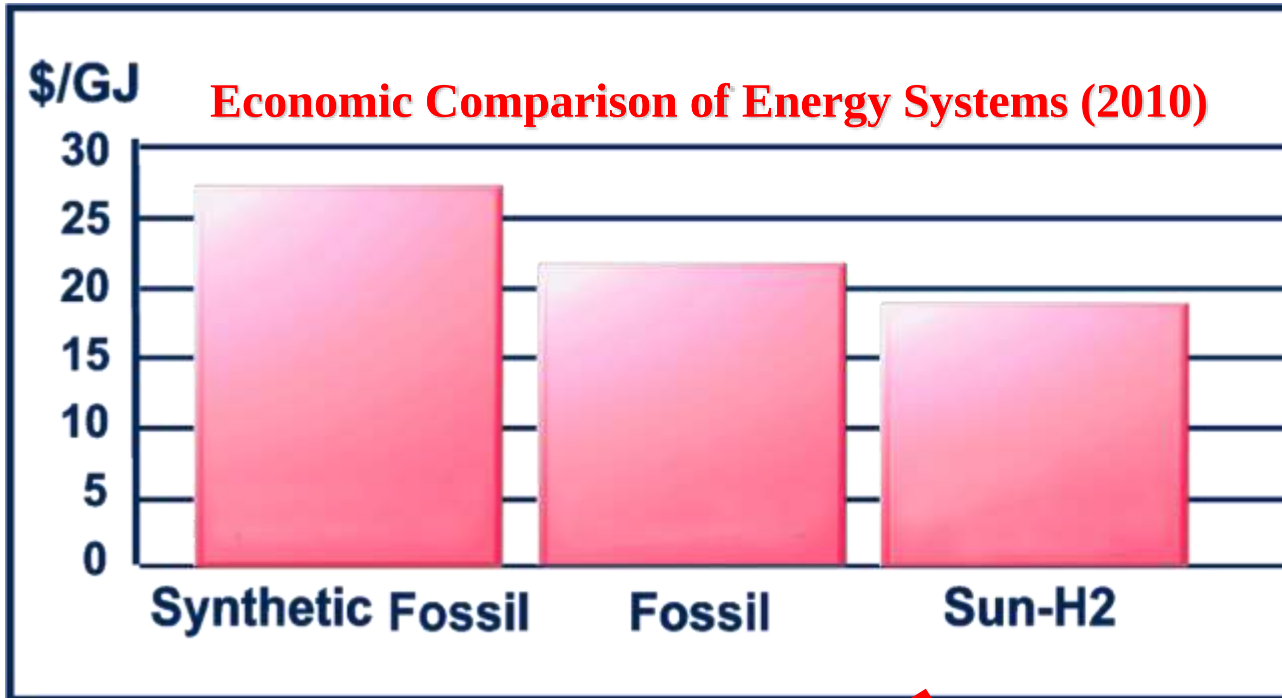
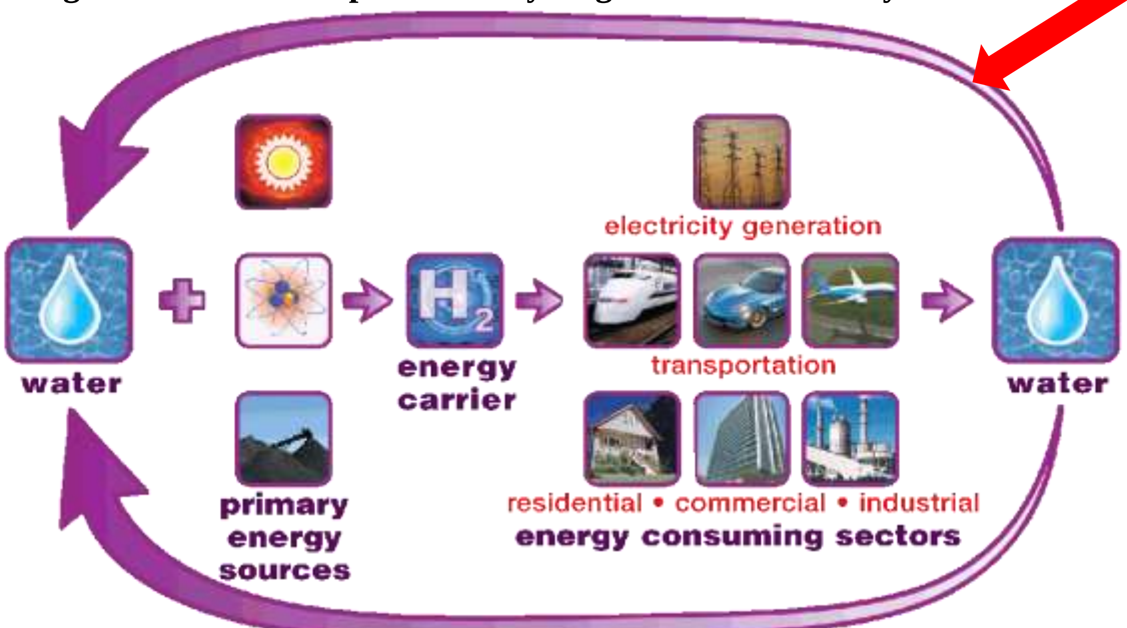


Fig. 7. Economic comparison of hydrogen and fossil fuel systems.



Produced from water Hydrogen burns back to water

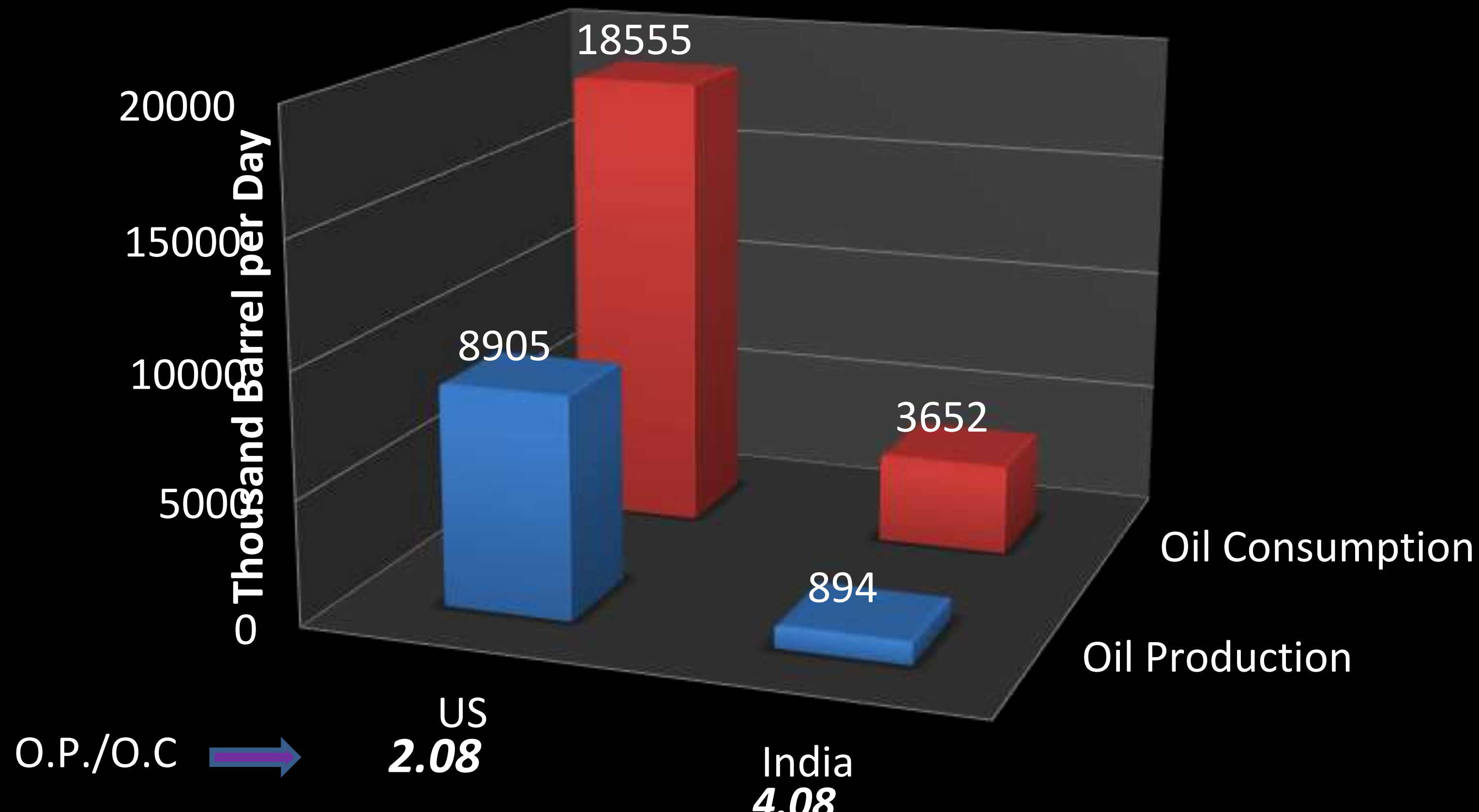
ENERGY OPTIONS FOR INDIA

For Electricity INDIA will cotinue to depend on Coal fired Power Stations because of Huge Coal Reserves that it has..

INDIA..~ 60.6 Bt(Fifth biggest Coal Reserves)
CHINA..~114.58Bt
Russia~157.01Bt

At the same time to reduce the Global Warming..as per PARIS AGREEMENT(not more than2degree C up to2050 Dec.2015..INDIA will keep on increasing the Renewable Contribution..IT has risen from ~10%

Oil Production (O.P.) and Oil Consumption (O.C.)in 2012



	US	India
Oil Production	8905	894
Oil Consumption	18555	3652

WHY HYDROGEN FOR INDIA?

1. HUGE DIFFERENCE BETWEEN OIL PRODUCTION AND ONSUMPTION
2. CLIMATE CHANGE EFFECTS
3. Urban AIR POLLUTION

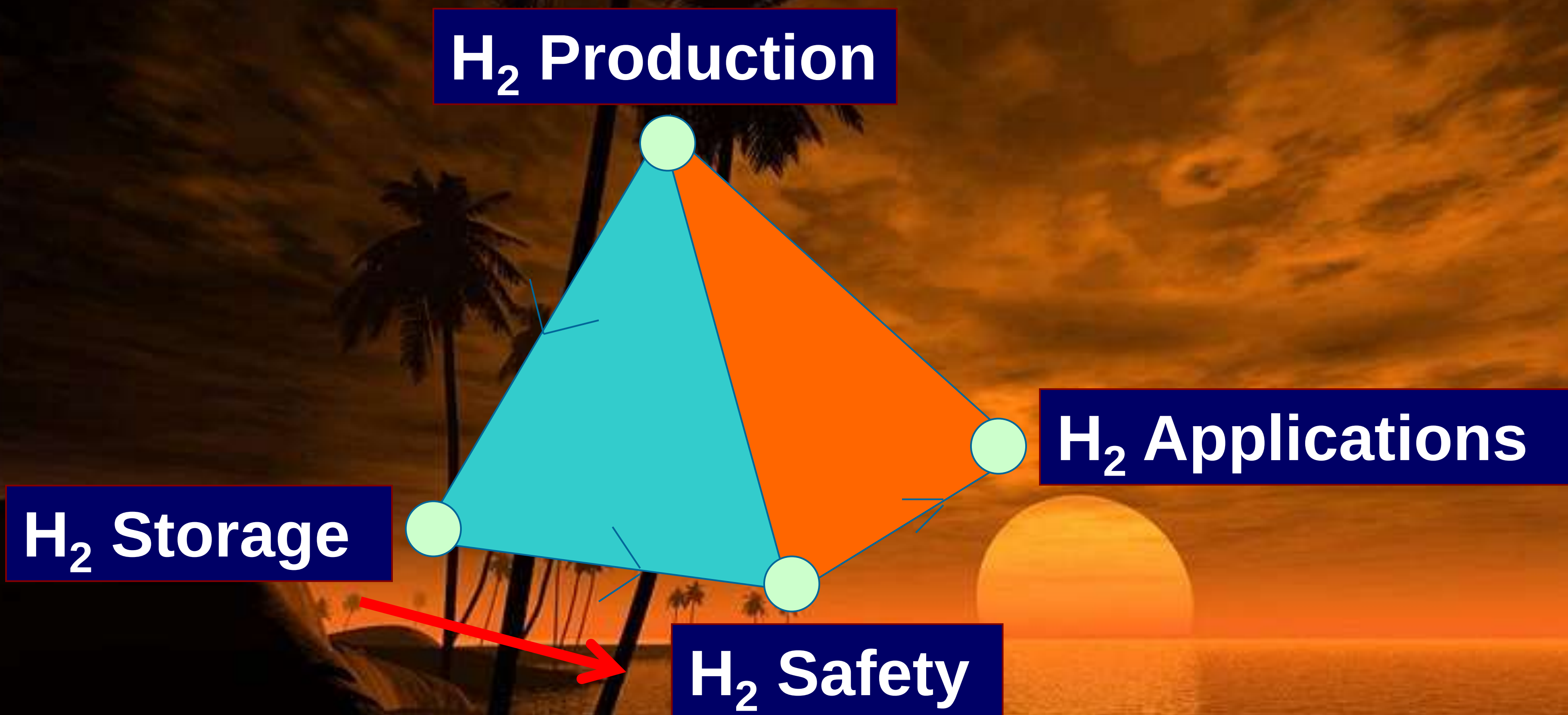
Why Hydrogen for India ?

Various Facets Related with Oil in India(2007)

- 1. EXTREMELY SCANT OIL RESOURCES :Availability of oil ;Depletion Largest difference between demand &supply
- 2. Pollution. (Detoriating urban air quality)
- 3.Global Warming/Climate Change ..(Effect on life of living beings ;Agriculture)
- 4.Energy Security

Why Hydrogen for INDIA? GLOBAL WARMING /

USA	INDIA
Global Warming (Climate Change) say rise of 2^0C will help initially cold countries like USA.	➢Global warming (climate change) (say rise of 2^0C) will start to cause / already causing harmful effects. ➢(Change in monsoon patter, lower agriculture yield etc.) right away. It has in fact already status affecting India.
GLOBAL WARMING / CLIMATE CHANGE	
Glacier melting will affect USA as well.	➢Glacier Melting will affect – India most crucially HIMALAYA
Use of Green i.e. Bio fuels (low carbon fuels) → e.g. synthesized from corn oil) can help USA on a short / mid term basis	➢Use of Green i.e. Bio fuels (low carbon fuels) → e.g. synthesized based on jatropha after initial euphoria has run into problems and is not thought to be quite viable option. ➢"Fuel vs Food Crisis" population
Dependence of GDP on Agriculture ~0.9%	Dependence of GDP on Agriculture ~23% GB affecting Agriculture ~16%



HYDROGEN ENERGY CENTER AT B.H.U. VARANASI (INDIA) CARRIES OUT R&D AND APPLICATIONS ON ALL THESE ASPECTS

4.. Hydrogen as a new renewable, clean and climate friendly fuel: Its production, storage and applications

- Status: Name of BRICS Collaborators with Institution
- 1. Prof. Helton Jose Alves (Universida de Federal do Parana, Brazil)
- 2. Prof . Alexander Yu. Ramenskiy (Vice President International Association of Hydrogen Energy, Moscow, Russia)

- 3. Hydrogen Energy Centre Group (HEC)
- Prof O.N. Srivastava, Prof R.S. Tiwari, Dr M.A. Shaz, Dr T.P. Yadava (Faculty members from Physics Dept): Professor R.K.Asthana and Professor S.P.Singh (Botany): Prof. V.B. Singh Prof. A.S.K. Sinha (Chemical Engineering)

Research Publications in 2017-2018

2017----20 Publications in Peer Reviewed Jornal;

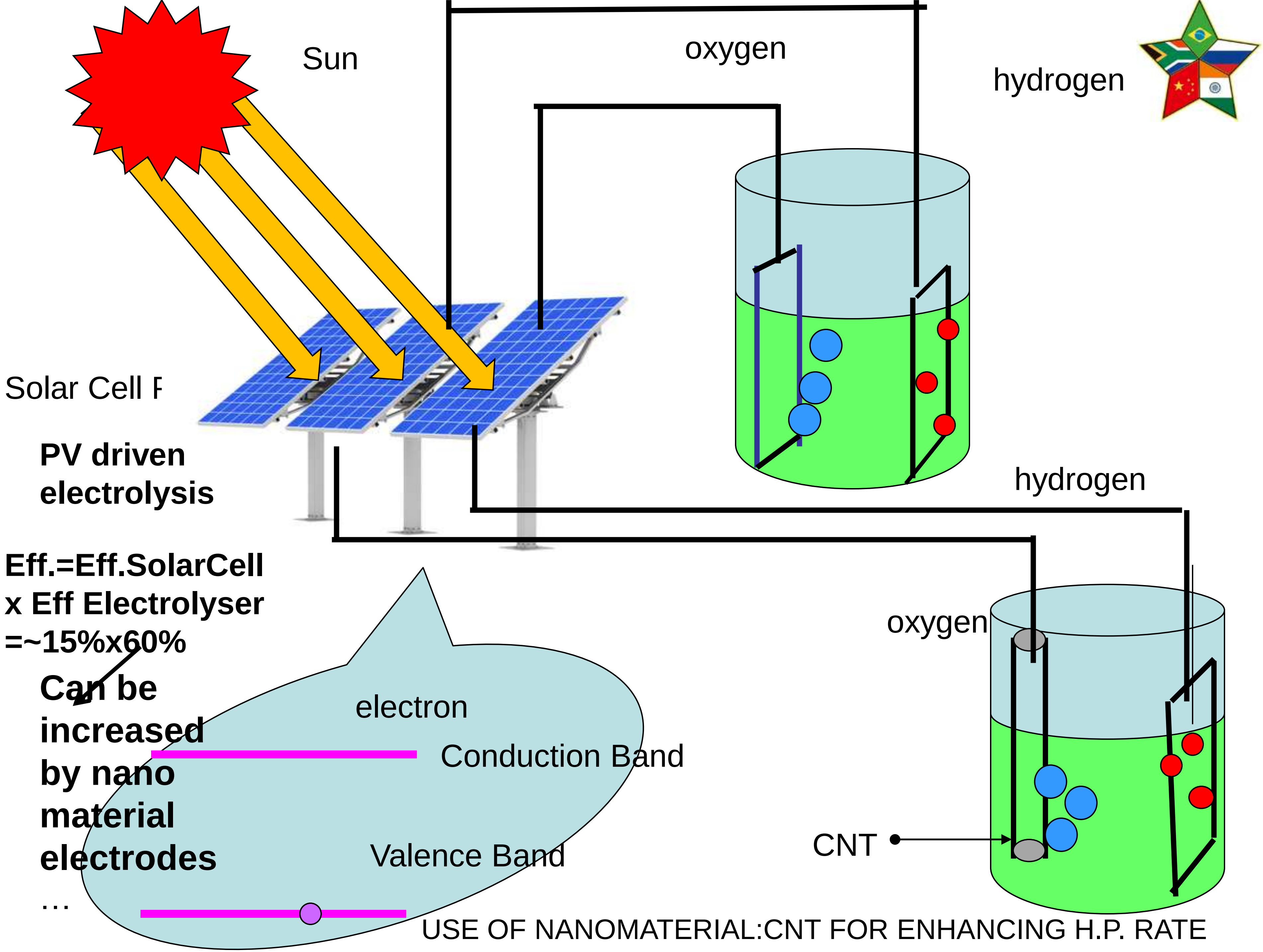
2018-----8+2

Hydrogen production

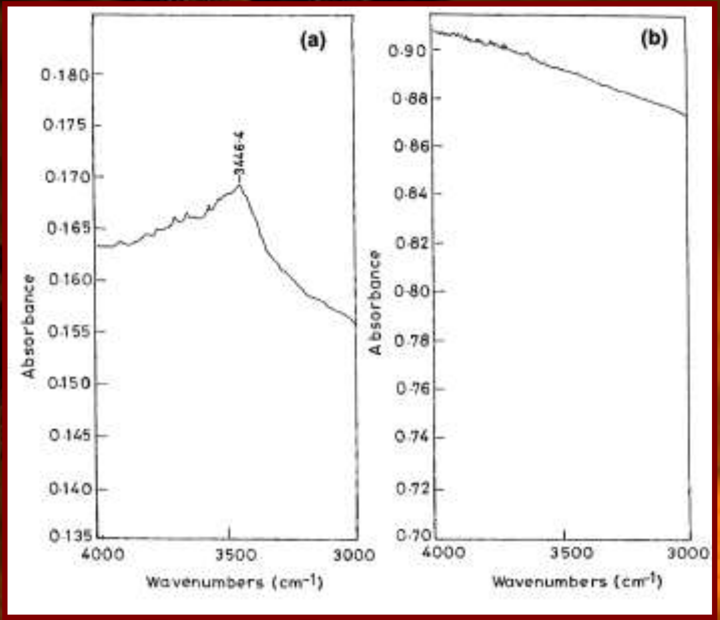
Steam reformation of hydrocarbons → CO_2?

SOLAR HYDROGEN

1. **PV driven electrolysis** ←
2. **Photoelectro chemical electrolysis**
3. **Photocatylytic electrlysis**
4. **Phtobiological route**


Sun
oxygen
hydrogen
Solar Cell F
PV driven electrolysis
Eff.=Eff.SolarCell x Eff Electrolyser =~15%x60%
Can be increased by nano material electrodes …
electron
Conduction Band
Valence Band
hydrogen
oxygen
CNT
USE OF NANOMATERIAL:CNT FOR ENHANCING H.P. RATE

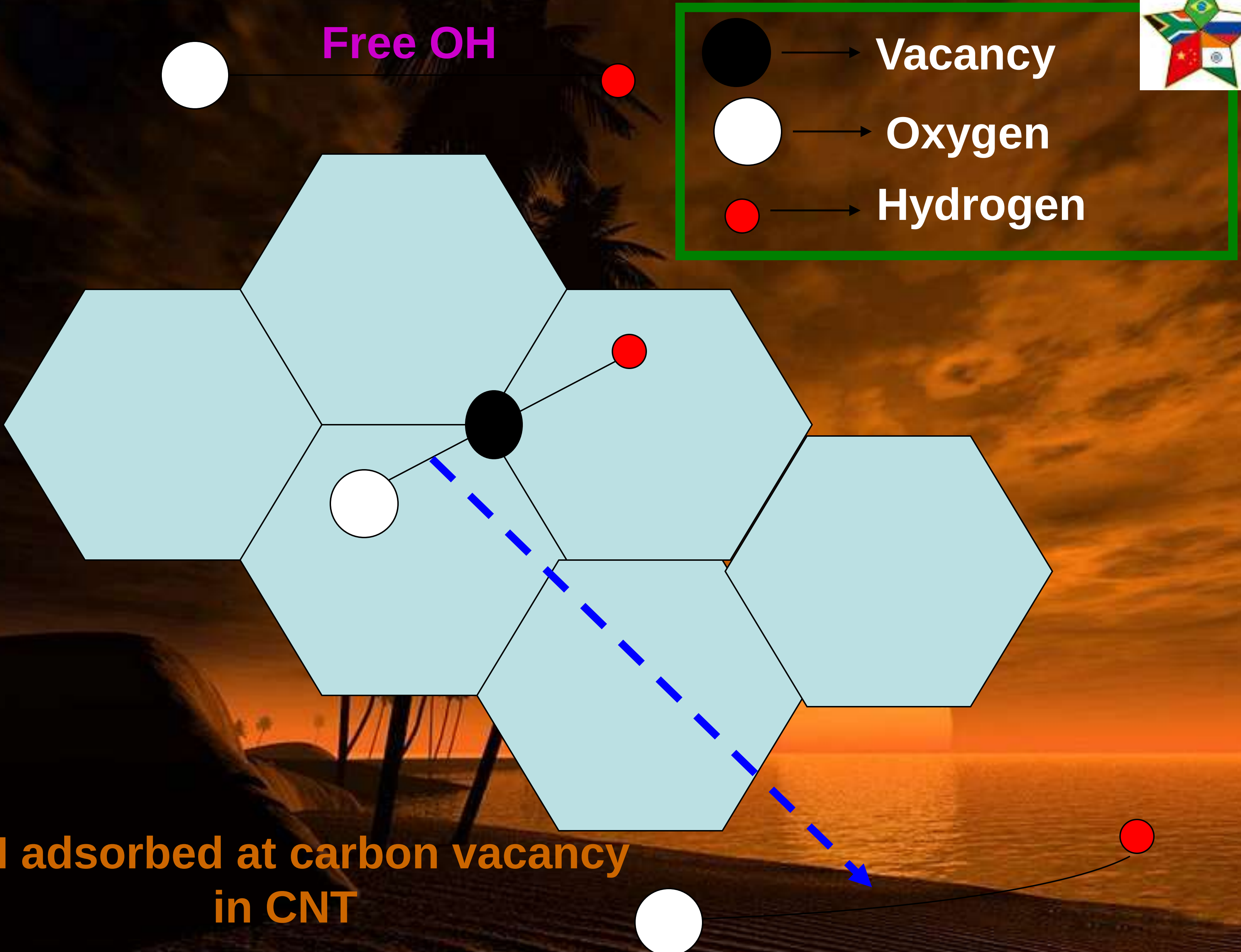
FTIR spectra of CNT electrode



(a) Immersed in the alkaline water and pre-dried and

(b) Bare, without immersion in alkaline water.

Notice the presence of peak at ~3446 cm^{-1} representing the OH radical.



OH adsorbed at carbon vacancy in CNT

- Applications of CNT as Electrode(anode) for electrolysis of water.
- Electrolysis taking place ~1.2V instead of ~2V will imply increasing electrolysis cell efficiency by ~40%.

H.P.----PV Route
Medanta Near New Delhi

500 kW_p SPV Power Plant at Medanta Hospital Car Parking at Gurgaon, Haryana

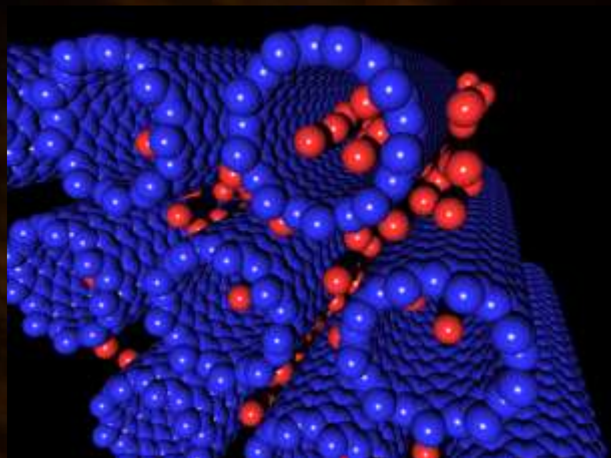
115 kW_p SPV Power Plant at DMRC Anand Vihar metro station, Delhi

100 kW_p SPV Power Plant at Rockwell Industries, Hyderabad, Telangana

500 kW_p SPV Power Plant at Kalinga Institute of Social Sciences

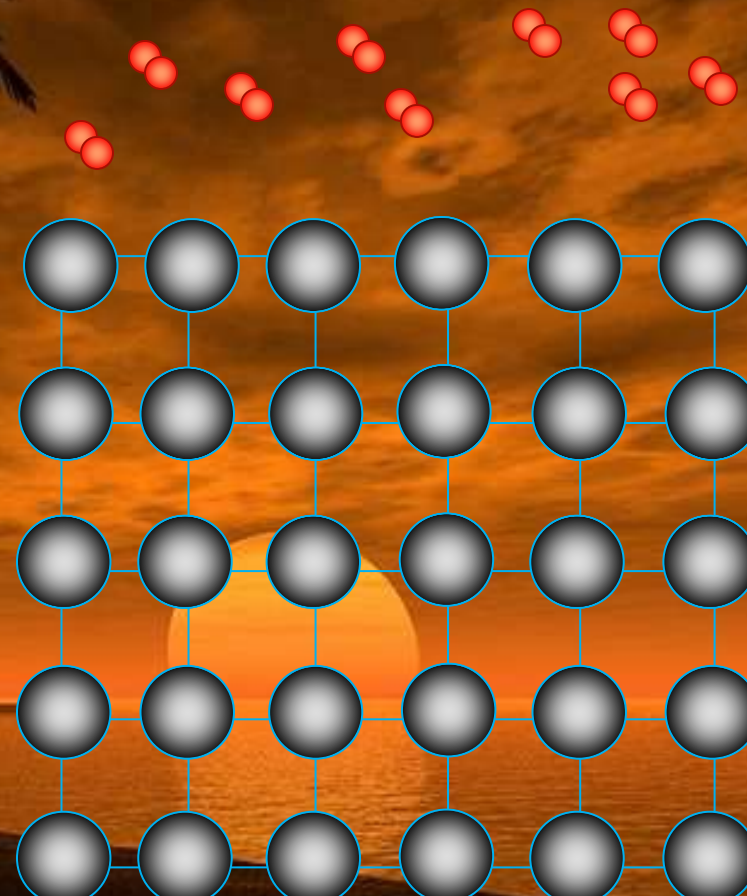
HYDROGEN STORAGE

Types of Hydrogen Storage Materials



Physisorption materials (e.g. CNT, graphene)

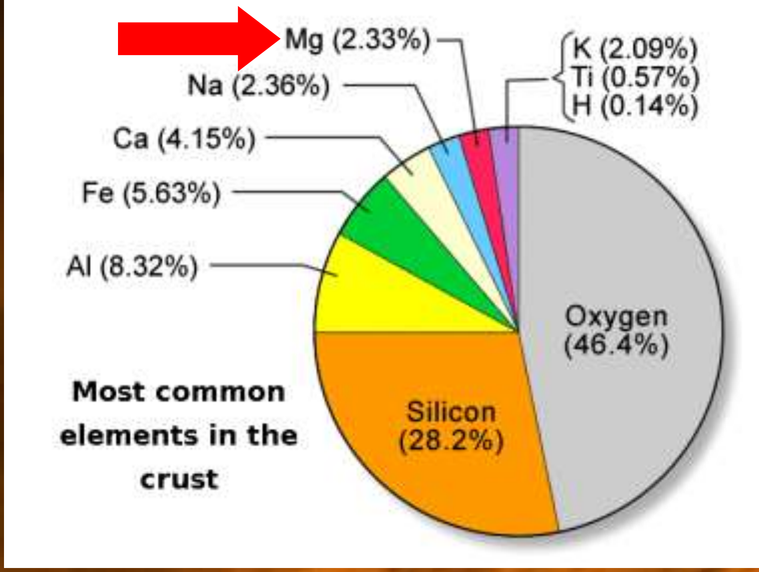
Complex Hydrides (e.g. $NaAlH_4$)



Intermetallic Hydrides (e.g. $LaNi_5$)

Metal Hydride MgH_2 (Pure and Catalysed) This Hydride seems to become State of the Art Hydride

Why MgH_2?



Advantages

- ❖Large deposit of Mg in earth crust.
- ❖Low cost
- ❖A very Light metal hydride
- ❖High gravimetric storage capacity (7.6wt%)
- ❖High Volumetric Storage capacity (110 kg/m^3)

ISSUES

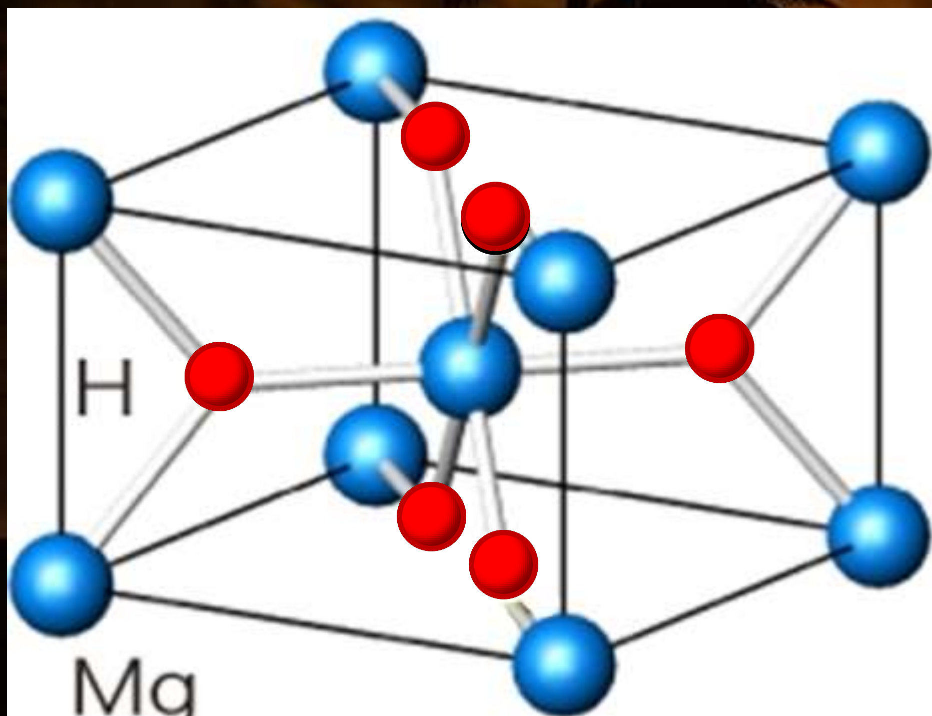
- ❖High desorption Temperature above 400^0C(desired ~$150-200^0C$).
- ❖High desorption activation energy ~97 kJ/mol.
- ❖Slow Kinetics.

Approaches

Tailoring by Ball-milling followed by the deployment of different catalysts such as transition metals/alloys/oxides and carbon based nanostructures. Which reduces the desorption temperature and also enhances the uptake and releasing kinetics of the materials .

Role of Catalysts in Destabilizing and regenerating MgH_2

Nano catalyst

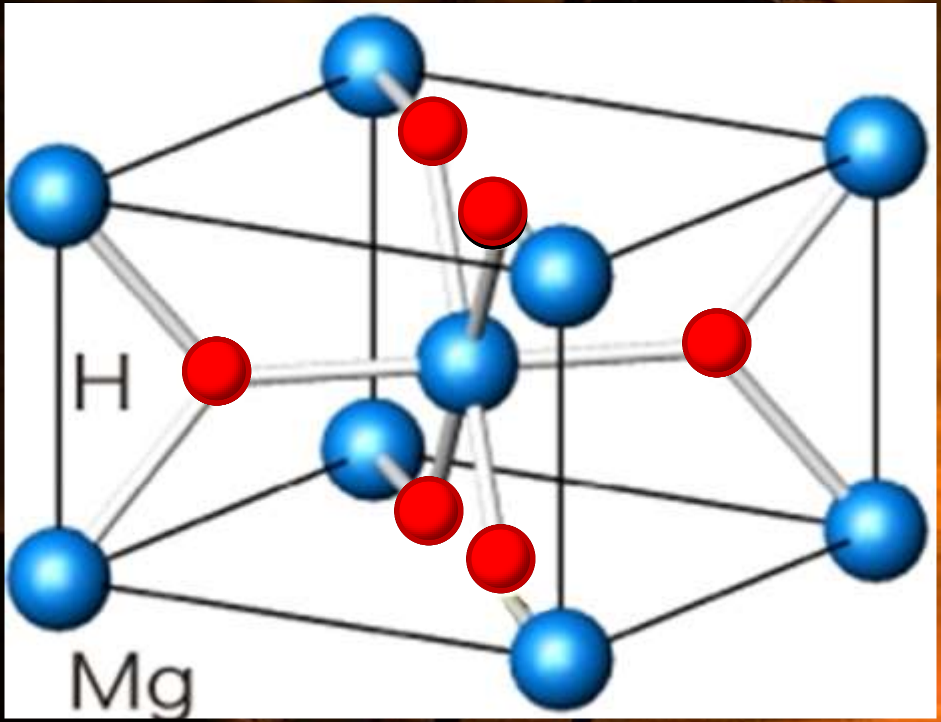


1. Redox reactions
2. Variable oxidation states

NEW CATYLYSTS DEPLOYED FOR MgH2

1. NANO TiO2 Of Different Sizes
2. TiF3
3. TiF3+SWNT
4. Leached Nano Quasicrystal

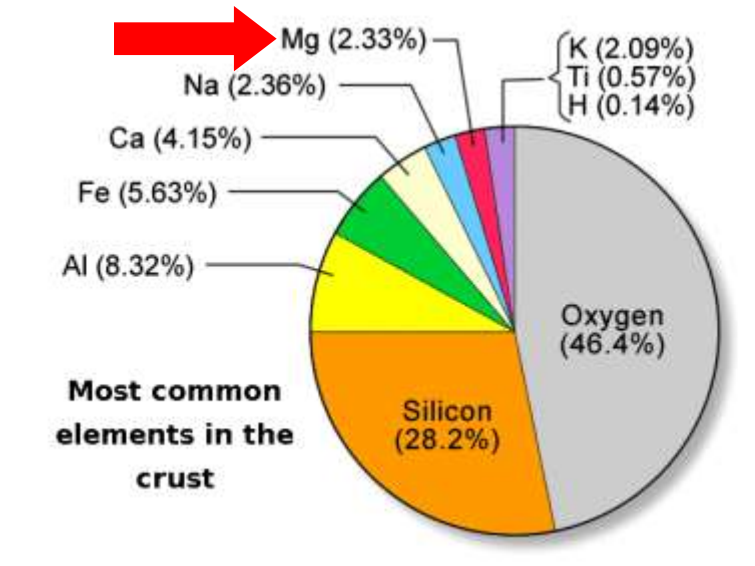
Nano catalyst



Effect of Catalyst on Light Weight Hydride (MgH_2)

Metal Hydride MgH_2 (Pure and Catalysed) This Hydride seems to become State of the Art Hydride

Why MgH_2?



Advantages

- ❖Large deposit of Mg in earth crust.
- ❖Low cost
- ❖A very Light metal hydride
- ❖High gravimetric storage capacity (7.6wt%)
- ❖High Volumetric Storage capacity (110 kg/m^3)

ISSUES

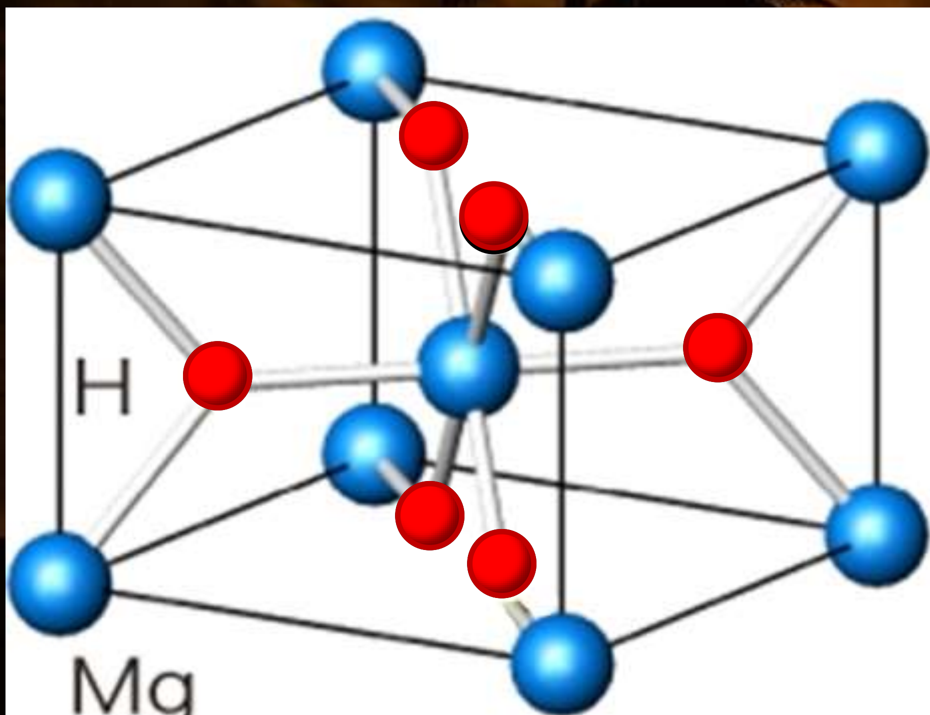
- ❖High desorption Temperature above 400^{0}C(desired ~150-200^{0}C).
- ❖High desorption activation energy ~97 kJ/mol.
- ❖Slow Kinetics.

Approaches

Tailoring by Ball-milling followed by the deployment of different catalysts such as transition metals/alloys/oxides and carbon based nanostructures. Which reduces the desorption temperature and also enhances the uptake and releasing kinetics of the materials .

Role of Catalysts in Destabilizing and regenerating MgH_2

Nano catalyst

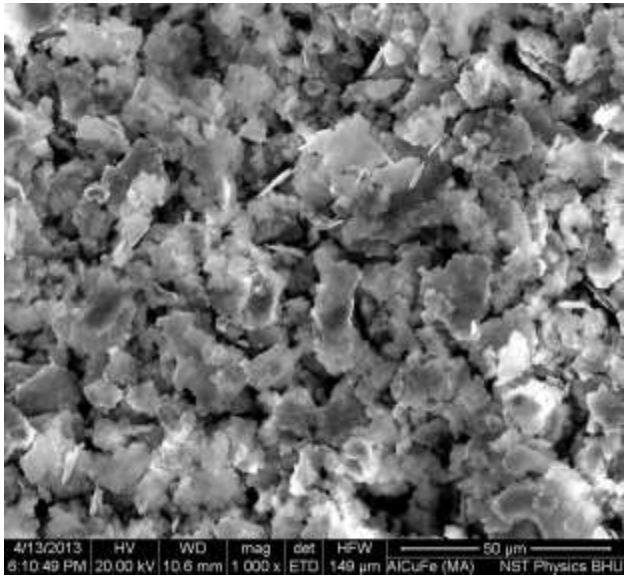


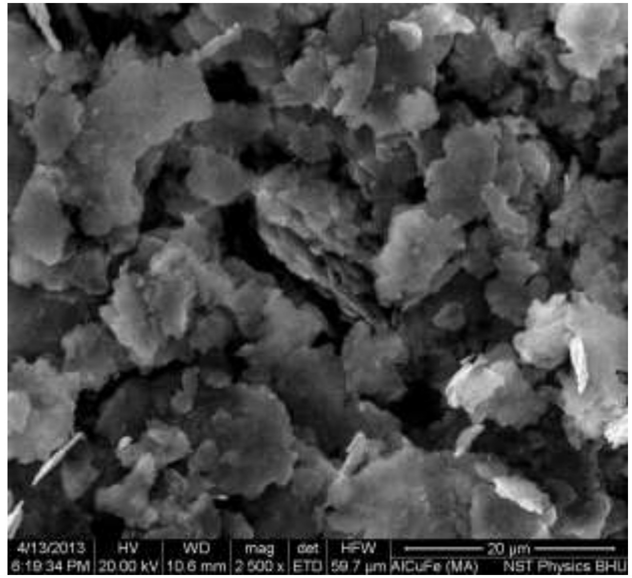
1. Redox reactions
2. Variable oxidation states

New Catylyst found by BHU

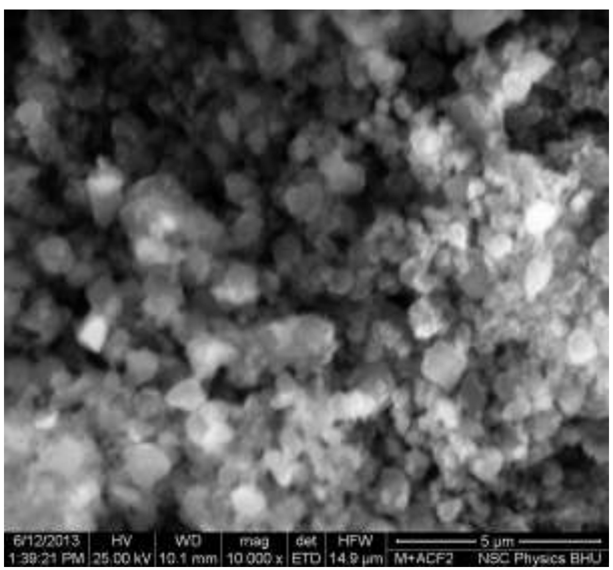
LEACHED QUACRYSTALLINE(AlCuFe) MATERIALS AS NEW EXOTIC CATYLYST FOR HYDROGEN SORPTION IN MgH_2

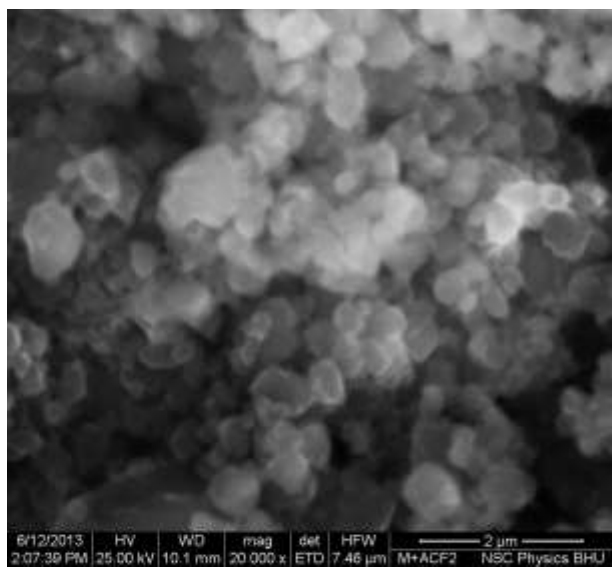
SEM: **MgH_2 catalyzed with Leached ball-milled Al-Cu-Fe**





Leached ball-milled Al-Cu-Fe

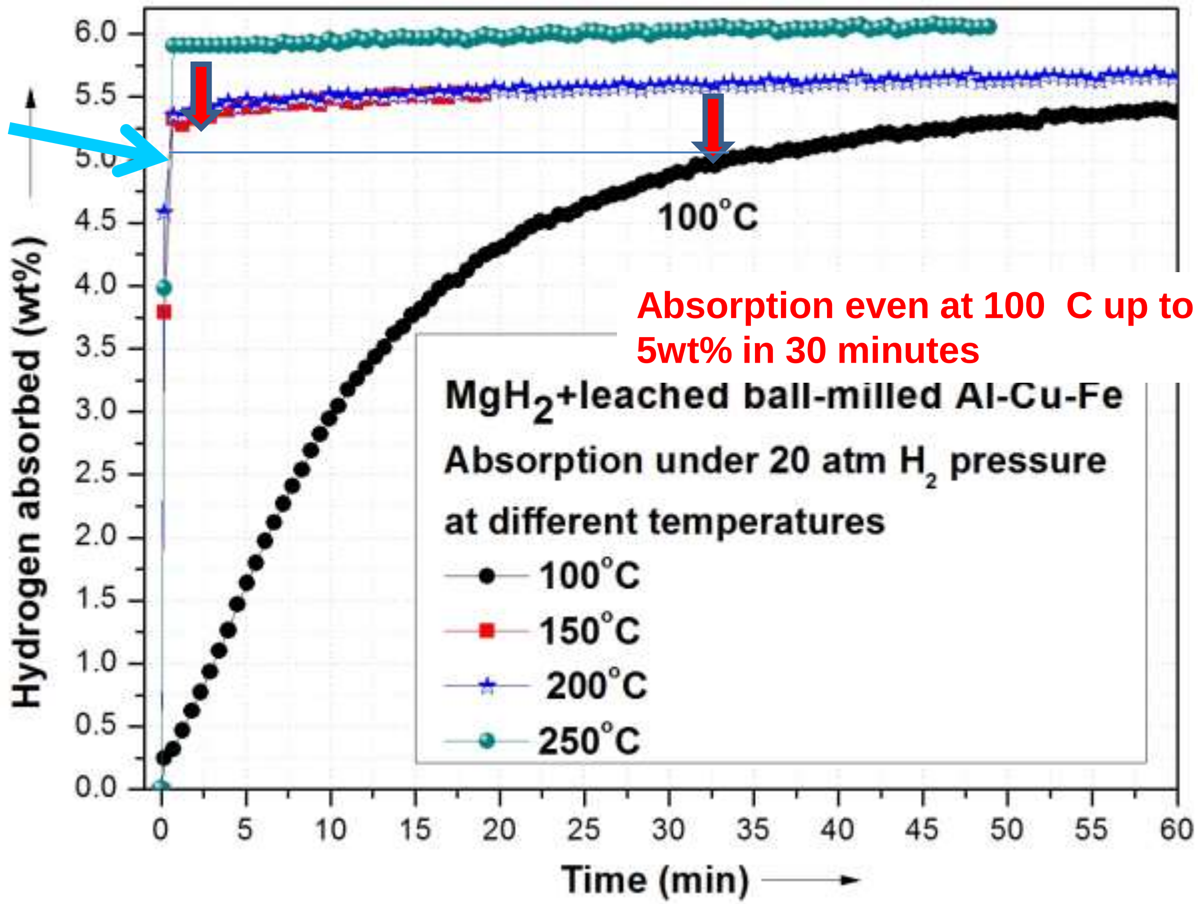




MgH_2 catalyzed with Leached ball-milled Al-Cu-Fe

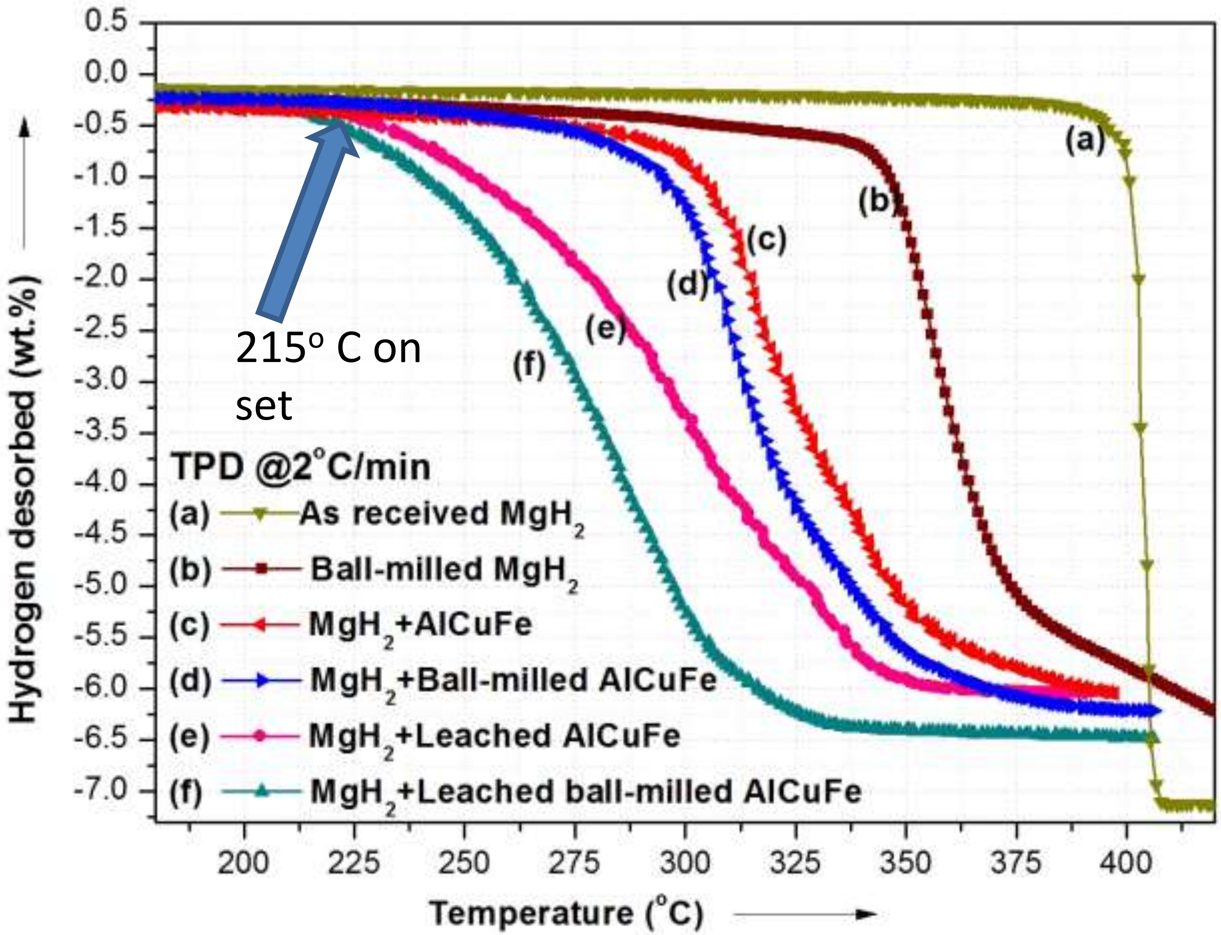
Fig 3: Absorption characteristic curve from 250ºC to 100ºC temperature

Absorption within 1.5 ninutes



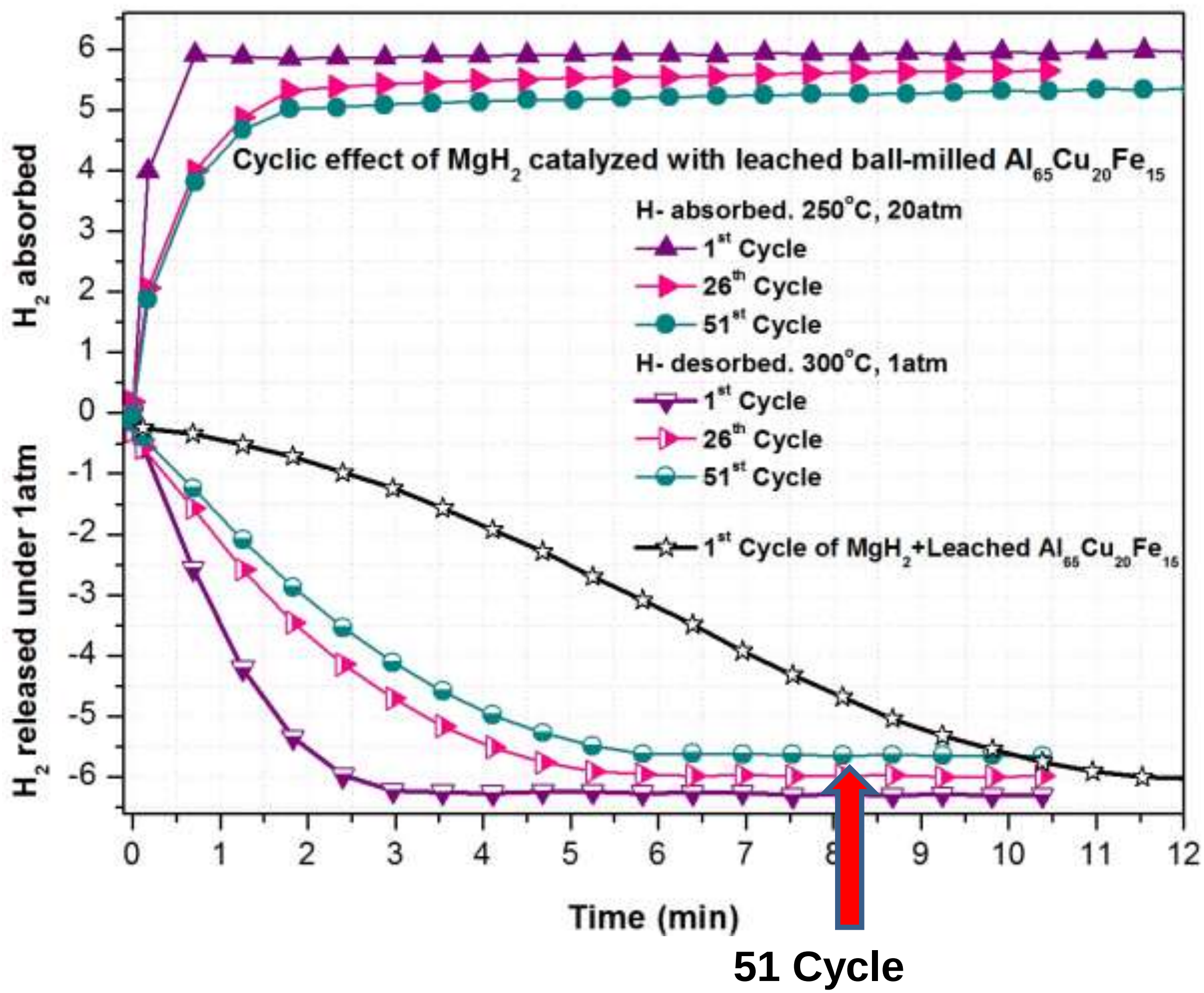
Absorption even at 100 C up to 5wt% in 30 minutes

Fig 1: TPD curves of (a) as received MgH_2 (b) ball-milled MgH_2 and MgH_2 catalyzed with (c) $Al_{65}Cu_{20}Fe_{15}$ (d) Ball-milled $Al_{65}Cu_{20}Fe_{15}$ (e) Leached $Al_{65}Cu_{20}Fe_{15}$ and (f) Leached ball-milled $Al_{65}Cu_{20}Fe_{15}$

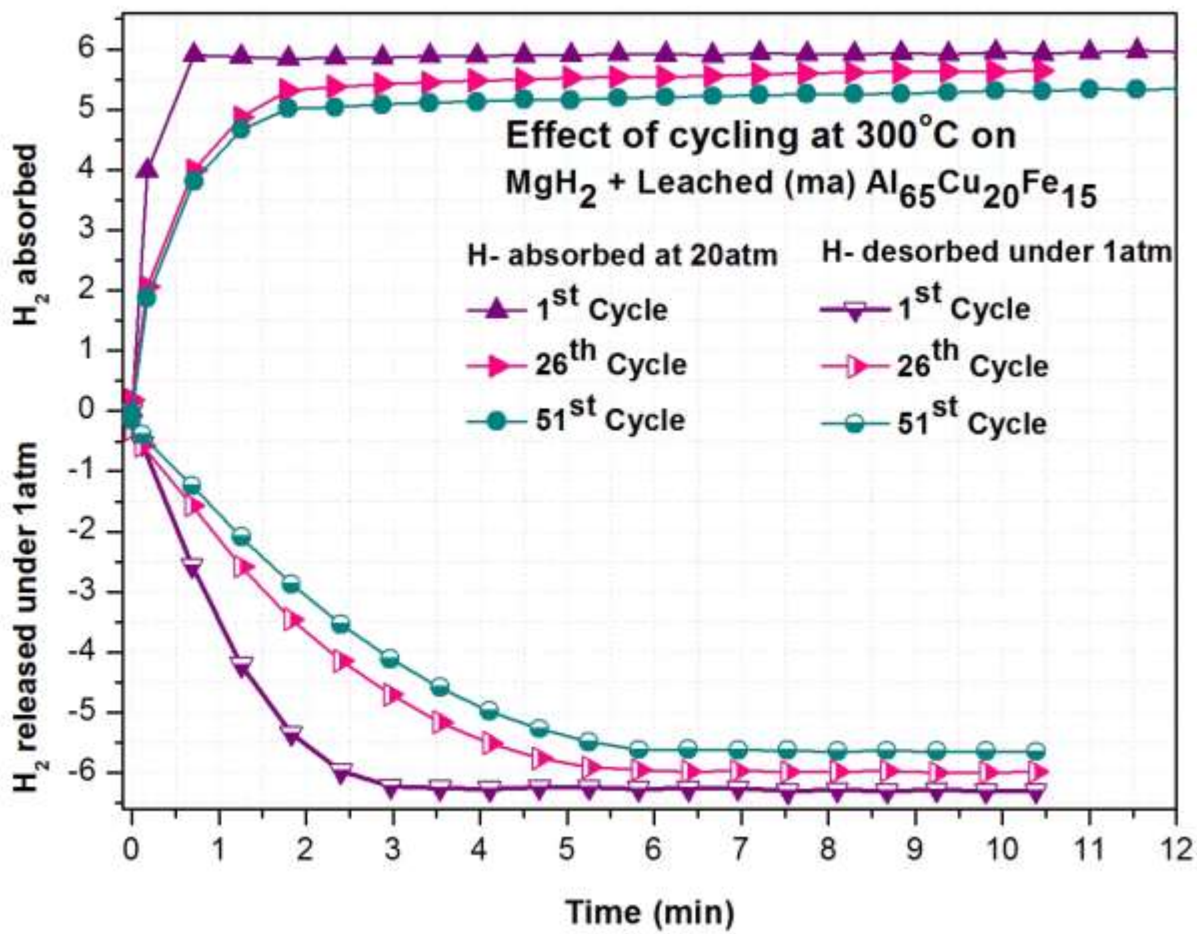


310°C

Fig 5: Cyclic effect of Leached ball-milled $Al_{65}Cu_{20}Fe_{15}$ catalyzed MgH_2

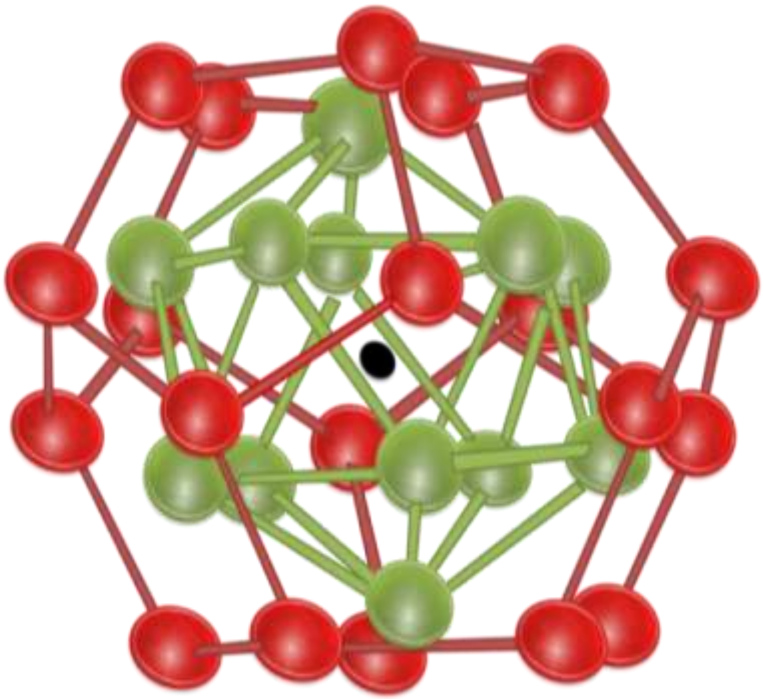


51 Cycles of absorption and desorption

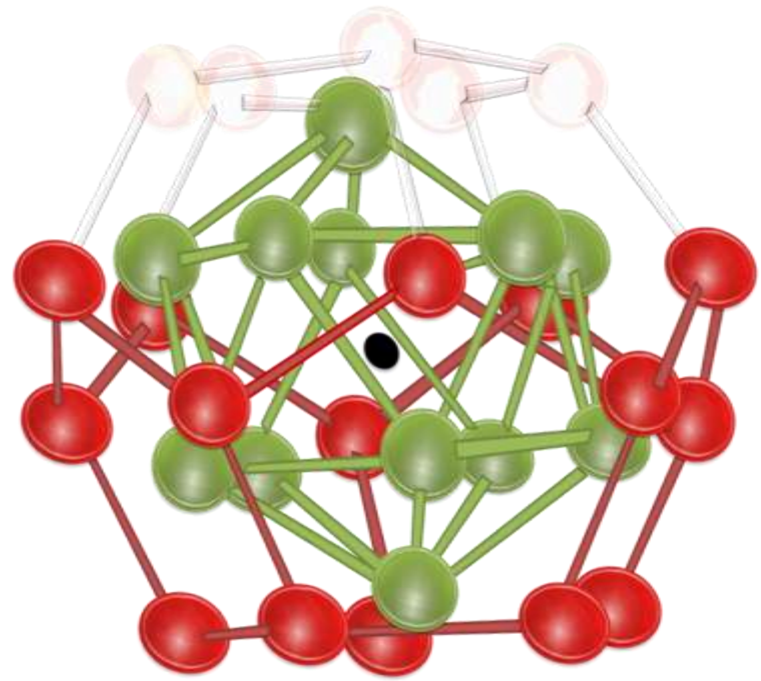


Theme (a) : a1-i Solar energy storage through storage of hydrogen in new exotic hydrides

Al Cu Fe

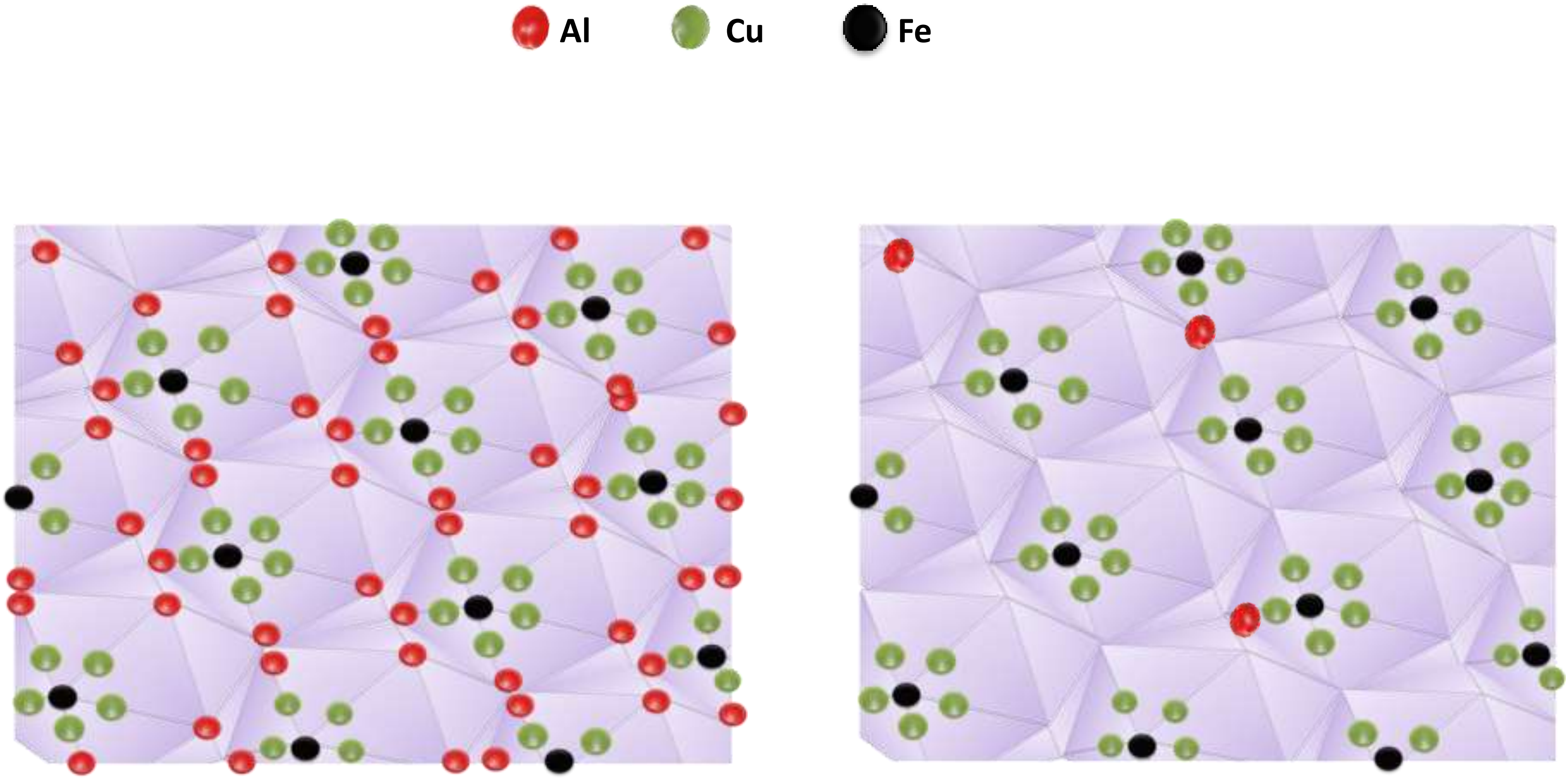


Before Leaching
AlCuFe



After Leaching treatment
AlCuFe

Theme (a) : a1-i Solar energy storage through storage of hydrogen in new exotic hydrides



Before Leaching AlCuFe

After Leaching treatment AlCuFe

Theme (a) : a1-i Solar energy storage through storage of hydrogen in new exotic hydrides

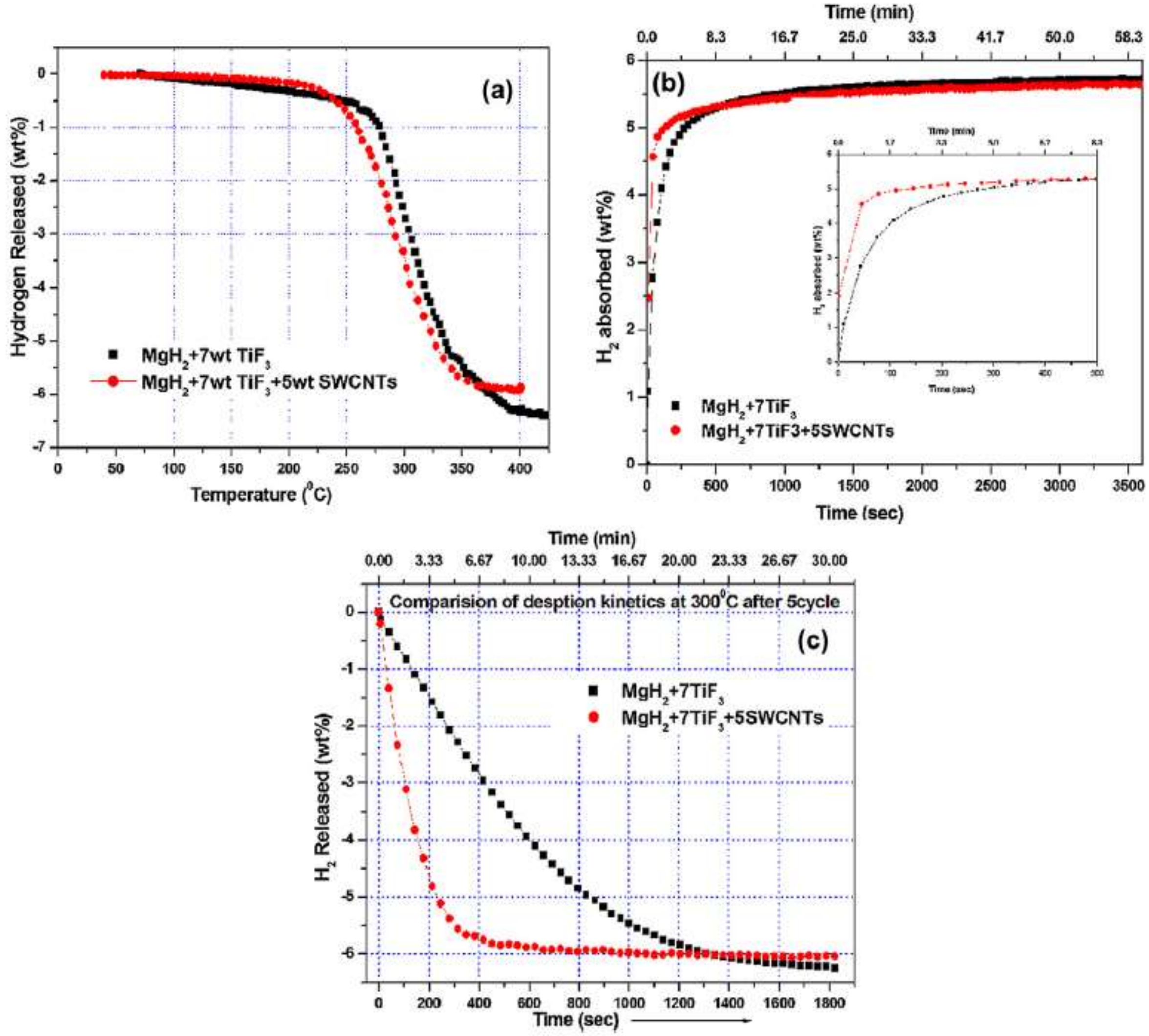
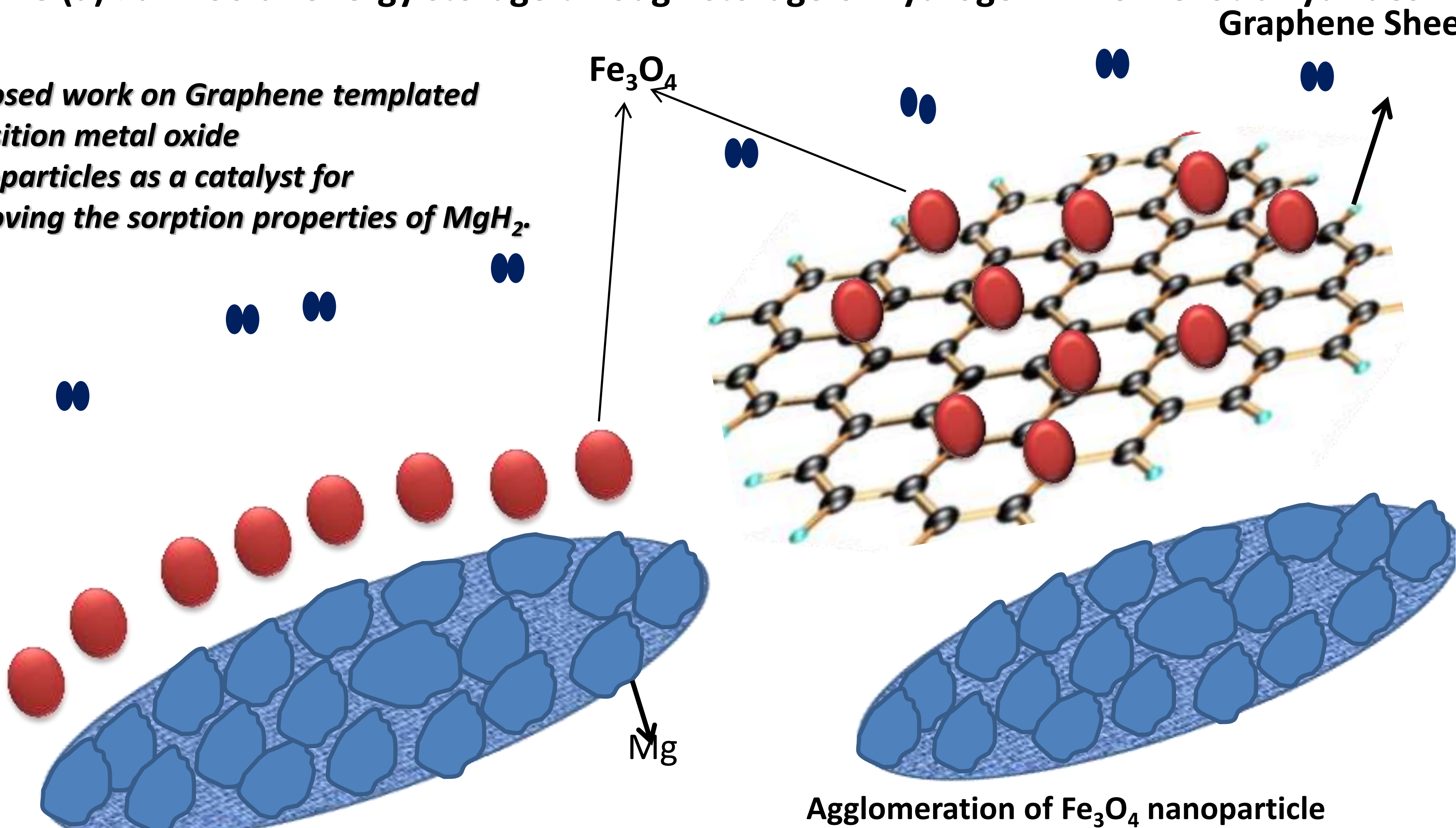


Fig. 4) TPD profile at 5 °C/min, (b) absorption kinetics plot at 27 °C, 1.2 MPa of hydrogen pressure and (c) desorption kinetics plot at 300 °C and 1atm for 5th cycle for MgH_2+TiF_3 with and without SWCNTs.

MgH_2 Catalyzed by TiF_3 and TiF_3 + SWCNT

Theme (a) : a1-i Solar energy storage through storage of hydrogen in new exotic hydrides

Proposed work on Graphene templated transition metal oxide nanoparticles as a catalyst for improving the sorption properties of MgH_2.



Agglomeration of Fe_3O_4 nanoparticle during cycling de/rehydrogenation study MgH_2

Agglomeration of Fe_3O_4 nanoparticle avoided by using Fe_3O_4 templated Graphene (*Fe_3O_4@Graphene*) as catalyst cycling de/rehydrogenation of MgH_2

Cycli rogenation of MgH_2 catalyzed by Fe_3O_4 and Fe_3O_4@Graphene

State of the art AB_5 type hydride (Mm-La-$Ni_{4.5}Fe_{0.5}$

Example of Material Tailoring in AB_5 (Mm-Ni-Fe)

(~1.5 ------- ~2.4wt%)

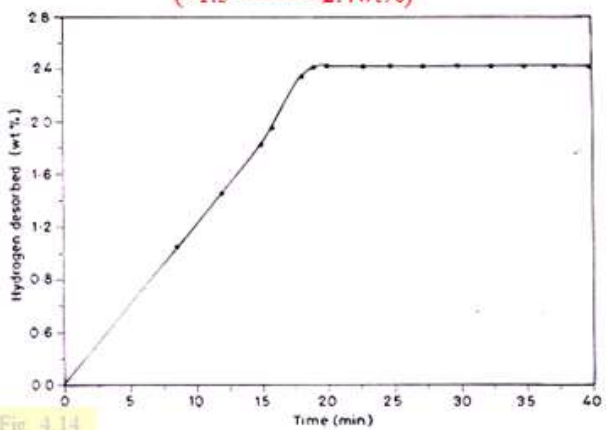
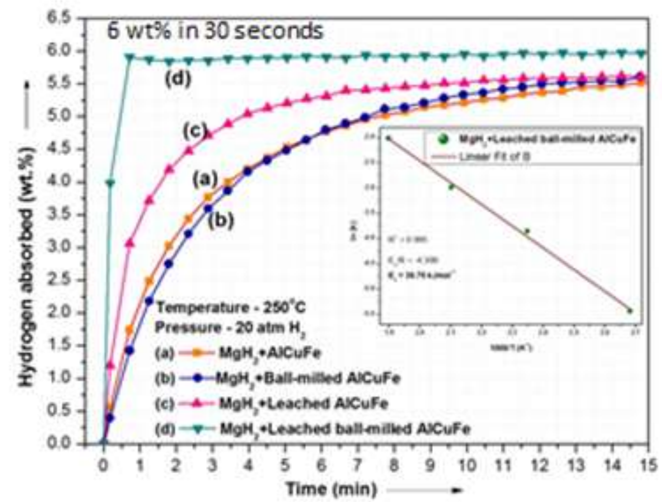


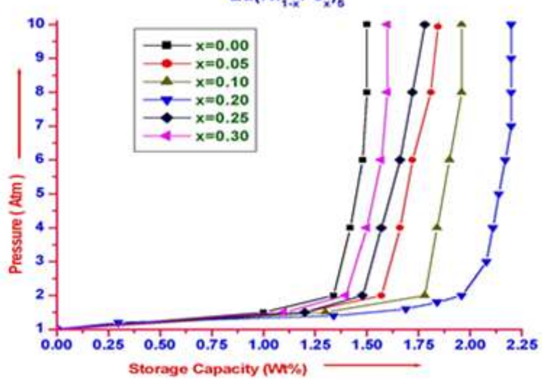
Fig. 4.14

New hydride (upcoming) catalyzed MgH2

Fig 2: Absorption characteristic curve of the completely desorbed MgH_2 i.e. Mg catalysed by (a) $Al_{65}Cu_{20}Fe_{15}$ (b) ball-milled $Al_{65}Cu_{20}Fe_{15}$ (c) Leached $Al_{65}Cu_{20}Fe_{15}$ and (d) Leached ball-milled $Al_{65}Cu_{20}Fe_{15}$

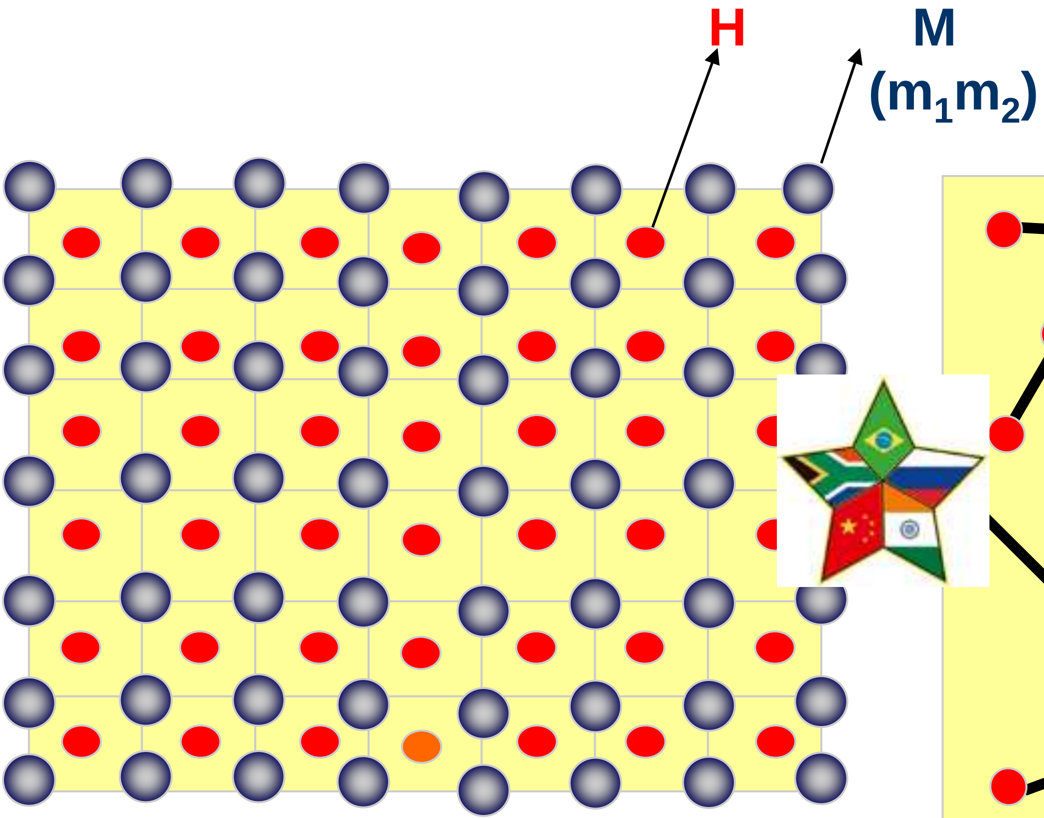


La(Ni1-xFex)5

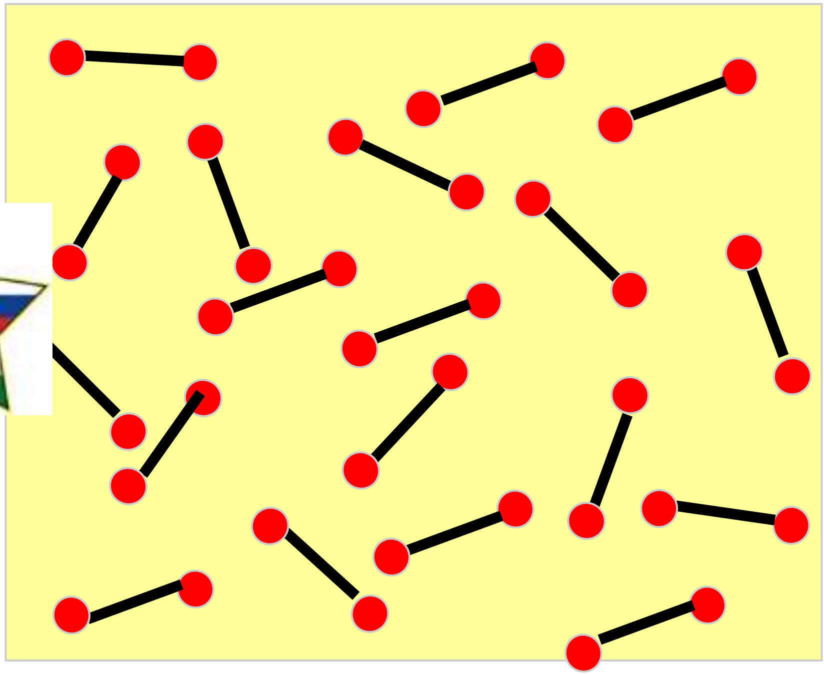


Representative pressure-composition desorption isotherms of the $La(Ni_{1-x}Fe_x)_5$ alloys (x=0,0.05,0.10,0.20,0.25,0.30).

- Why emphasis on solid state storage (Hydrides)?
- They are more efficient.
- They are safest mode of hydrogen storage.
- They generally satisfy the requirement of volumetric efficiency which is very important for vehicular applications.(Gravimetric efficiency?)
- They posses lot of potential for improvement through material tailoring.



Metal Hydrides



Gaseous / Liquid Hydrogen

Required and Obtained Storage Characteristics

	Gravimetric Storage (2014) (2015) Wt%		Volumetric Storage (Kg/m^3)
DOE (USA)	~4.5/ 5.5	At moderate temp ~80 to 100 ^{0} C	60 (45gm/l)
Compressed H_2 (~200 bar%....700 bar..........................5wt	<1		~20
Compressed H_2(~400 bar)(600 bar)	3/4		~30
Liq. H_2	~4		~40
Intermetallic Hydride	1.5--2.4 (3) (can be increased)		80-130 (Already meets the DOE Limit)
			♦ Already meets the
Complex Hydride / (Built in Hydrides)	~5 to ~10		~ 60 &Higher

Other Hydrides such as Mg and Mg Compounds, Alanes, Borohydrides, MOF's, Zeolites, Clatherates, Liquid Hydrides etc. (Potential candidates which can satisfy the required storage capacity/efficiency, Intense R&D required) (Japan)

(Gravimetric Storage Capacity)

Gaseous Hydrogen is not a feasible and safe way of storage of hydrogen ..AT 700 atmosph. Storage capacity is ~5Wt%....

In Hydride ; MgH_2 at 20-50 atmosos. It is~6Wt.

(Volumetric Storage capacity) At 700 atmos for high pressure gaseous VSC is 40 Kg/m3…

For MgH_2 at 20-50 atmosos VSC is~ 110Kg/m3

Why Hydrogen Storage in Hydrides for Small Vehicles like Two and Three Wheelers?

1. Volumeric Storage Capacity
2. Safety

THANK YOU FOR YOUR ATTENTION

Queries

Or

questions

are welcome

- **3. Methodology and Plan of work (5 years)**
- **3.1 Hydrogen Production: Methodology and Plan of work (5 years)**
- **3.1.1. Use of carbon nano structures (CNT and Graphene) for increasing the efficiency of production of Solar Hydrogen**
- **3.1.2. Use of graphene Templated TiO_2 for efficient Solar Hydrogen Production**

- **3.2 Hydrogen Storage: Methodology and Plan of work (5 years)**
- **3.2.1. Hydrogen Storage in light weight hydrides**
- **3.2 Hydrogen Storage:**
- **Methodology and Plan of work (5 years) 3.2**
- **3.2.2. Hydrogen Storage in Carbon / Graphene Aerogel**

- **3.3 Hydrogen Applications and Plan of work (5 years)**