Design/Practical Experience [EEN1010]
Department of Electrical Engineering
Final Report

Academic Year: 2021-22

Semester: 4

Date of Submission of Report: 30/04/22

1. **Name of the Student:** Mitarth Arora

2. **Roll Number:** B20EE096

3. **Title of the Project:** Designing Mg-Li binary alloys for hydrogen storage applications

4. **Project Category: 3**
   Summer/Winter/Semester projects with Institute faculty within or outside the department

5. Targeted Deliverables:

a.) Knowing the importance of hydrogen storage at industrial level
b.) Study of various materials that are currently used for hydrogen storage applications along with their specific characteristics
c.) Why Mg-Li alloys as hydrogen storage material?
d.) Theoretical prediction of different Mg-Li alloys for hydrogenation and dehydrogenation kinetics
e.) Problems and Solutions of different Mg-Li alloys for Hydrogenation and DeHydrogenation Kinetics Principles
f.) Classification based on crystal structure, Role of vacancies and interstitials to improve the hydrogen storage.
g.) Explaining hydrogenation and dehydrogenation process with help of flowchart.
h.) Hydrogenation and Dehydrogenation aspects on the Mg based alloys
i.) Viewing out the Macrostructures of Mg AZ31

6. Work Done:

a.) Motivation of the Project :

The main aim behind this project is to design a material made up of Mg-Li Binary alloy which would be used out for the storage of Hydrogen gas and we would look upon its various applications in real aspects.

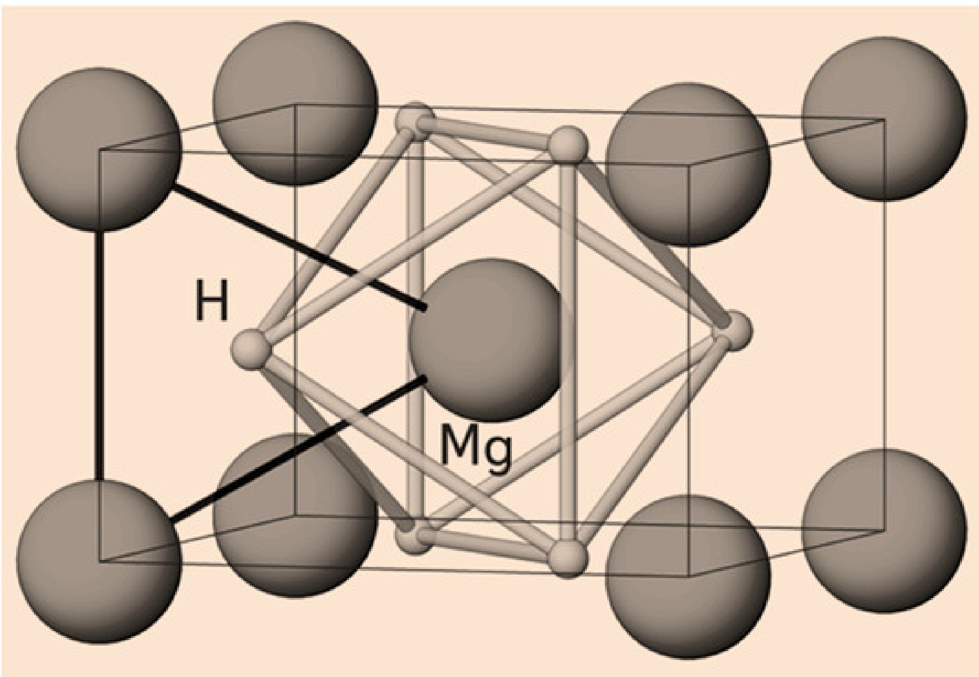


Fig (1.a) Depiction of How Hydrogen is being stored among the lattices

b.) Importance of Hydrogen Storage at Industrial Level :

Population growth and increasing demand for energy have prompted us to explore more sustainable energy resources. Reducing vehicle dependence on fossil fuel is vital to reducing greenhouse gas emissions.

This has made hydrogen a preferred fuel because it is light, contains high energy density, and emits no harmful chemical by-products during combustion. Furthermore, hydrogen is considered a green energy because it can be generated from renewable sources and is non-polluting.

Industrial Hydrogen Use has been greatly influenced by the fact that its use and dependence towards economic growth have increased dramatically by 300%.

Some of the applications of Hydrogen at Industrial Level include:

a.) 55% of the world's hydrogen is used to produce Ammonia, which is the main component of chemical fertilizer production for any country.

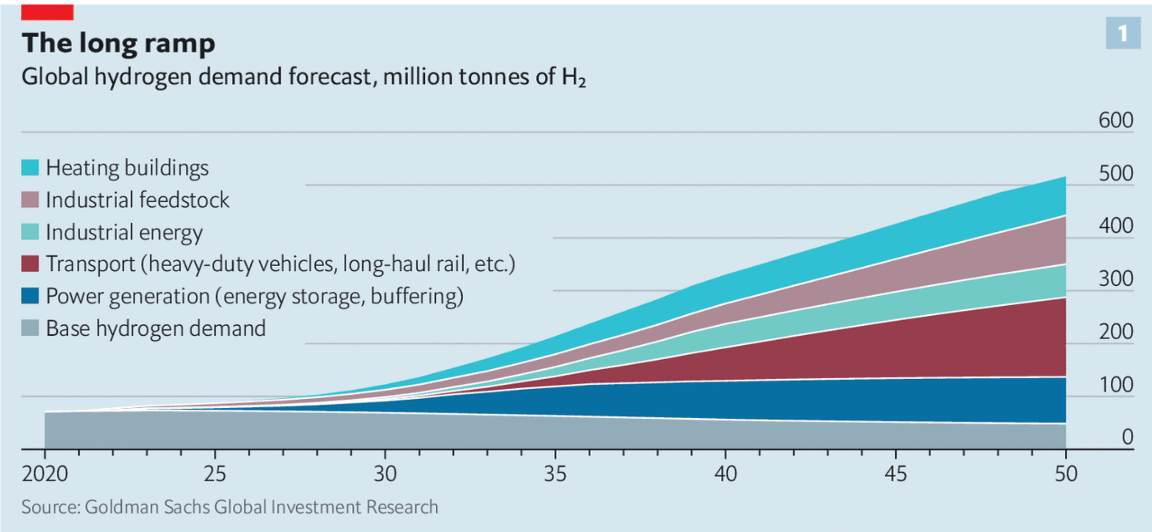
b.) 25% of the world's hydrogen is used for the petroleum refinery and its co-substitute products.

c.) Methanol, an important industrial by-product, consumes 10% of all global hydrogen.

d.) Around 10% of the global hydrogen supply goes to other important industrial uses such as Welding , Electronic Manufacturing , Aviation , Space Exploration, and Power Generation, and there are countless other uses whose list is inexhaustible.

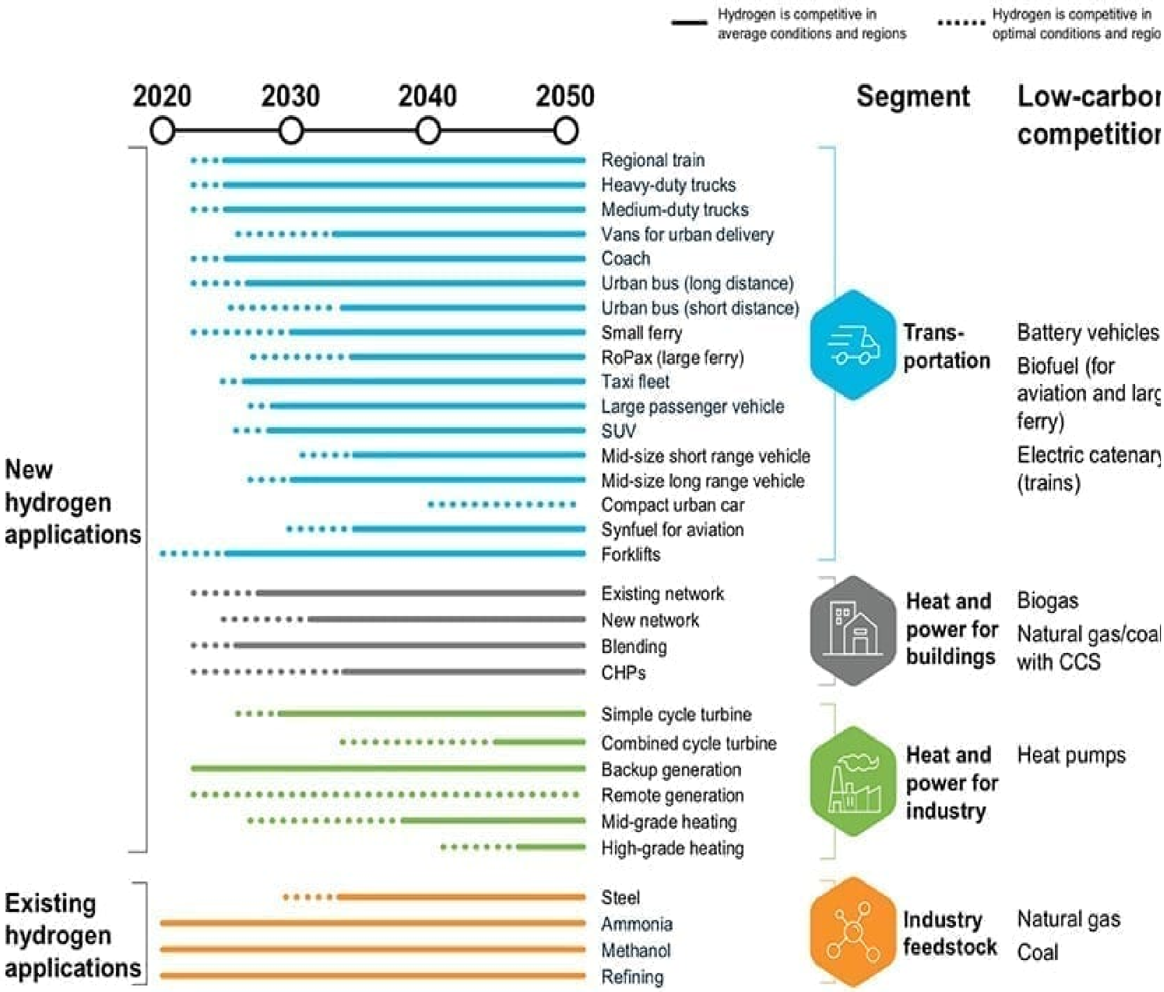
Hydrogen stationary storage has the purpose of either minimizing hydrogen delivery costs by balancing supply and demand, or serving as a backup fuel source. The demands of a particular application may have a substantial influence on the capital and operating costs of the storage.

Hydrogen storage is a key enabling technology for the advancement of hydrogen and fuel cell technologies in applications including stationary power, portable power, and transportation. Hydrogen has the highest energy per mass of any fuel; however, its low ambient temperature density results in a low energy per unit volume, therefore requiring the development of advanced storage methods that have potential for higher energy density.



The Economist

<u>Fig (1.b) Current Global Hydrogen Demand</u>



<u>Fig (2.b) Future Industrial Hydrogen Applications</u>

c.) A description of the materials which are used in Hydrogen storage and their special properties :

a.) It has been estimated that gas cylinders with a mass of 110 kg, and a pressure of 70 MPa can store hydrogen with a gravimetric density >5 -6 mass% along with the volumetric density of 30 kg/m3 (3.9 kgH2/100 L inner volume).

b.) Since hydrogen has a very low critical temperature of 33 K, liquid hydrogen is stored at very low temperatures in cryogenic containers under ambient pressure. The volumetric density of liquid hydrogen is 71 kg/m3, which is higher than gaseous hydrogen.

c.) In comparison to gaseous hydrogen and liquid hydrogen storage systems, hydrogen can be safely stored in materials with a higher density.

d.) The following properties of various types of materials have recently been researched:
1.High gravimetric and volumetric density of hydrogen.
2.Suitable thermodynamic properties, including hydrogen sorption and desorption at moderate temperatures and pressures.
3.Rapid kinetics.
4.Easy handling.
5.Resources that are abundant and low in cost.

e.) There are several new and novel materials available for hydrogen storage that have the potential to store hydrogen depending on their structure and type of interaction with hydrogen.

f.) Hydrogen storage in solid form can be categorized into the following categories:
1.metal hydride storage;
2.light metal hydride storage;
3.chemical hydride storage (complex hydride storage);
4. nanostructured materials storage (adsorption of molecular hydrogen).

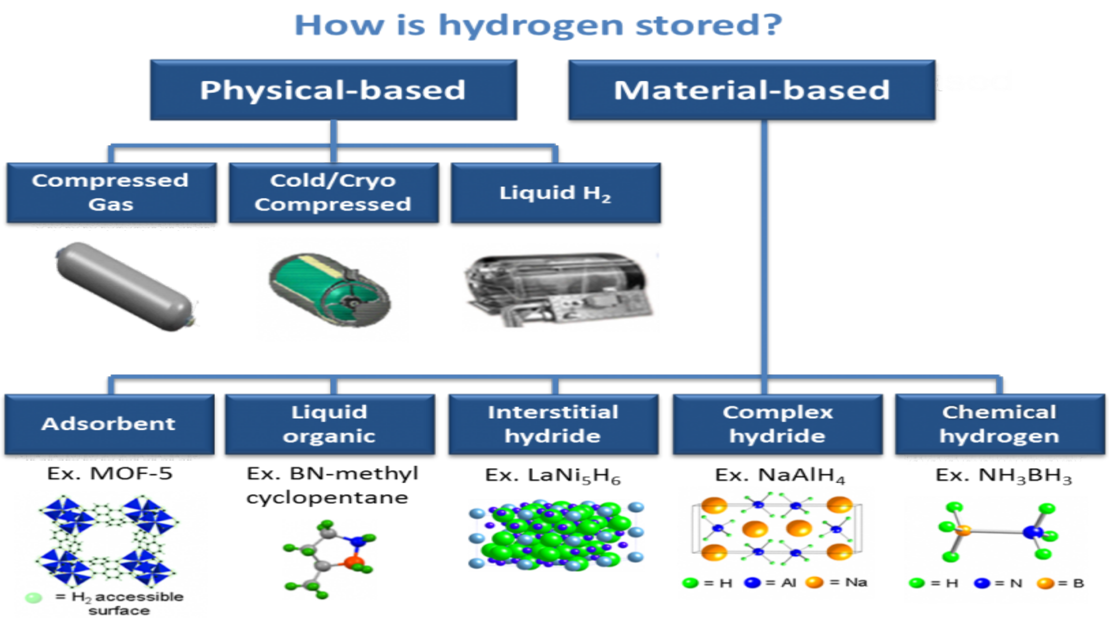


Fig (1.c) Different Modes of Hydrogen Storage

With so many possible hydrogen storage options, it is logical to categorize them. However, finding an optimal categorization system is not an easy task, and every case appears to utilize slightly different categorization systems.

g.) It breaks down hydrogen storage technologies into three main categories:

(1) hydrogen can be stored as a liquid or a gas in pure, molecular form without significant physical or chemical bonds with other materials;

(2)There is the possibility that molecular hydrogen can be adsorbate on or into a material by relatively weak physical van der Waals bonds;

(3) atomic hydrogen may be chemically bonded (absorbed).

Also, it is helpful to separate chemical bonding storage technologies into two subcategories: the metal hydrides and the chemical hydrides.

d.) Why Mg-Li alloys as Hydrogen Storage Material ? :

a.) Due to their abundance and availability, as well as their extraordinary level of gravimetric and volumetric density storage properties , magnesium and lithium compounds have been extensively investigated as potential hydrogen storage and thermal energy storage materials in recent years.

b.) In this paper, there is a special focus on discussing the efforts made by the scientific community to improve the thermodynamic and kinetic properties of magnesium and lithium alloys while maintaining a high hydrogen storage capacity.

c.)The occurrence of α-Mg(Li) and β-Li(Mg) phases in the Mg-Li binary system is characterized by the presence of ordered and disordered forms of magnesium, which may impact the hydrogenation characteristics of magnesium.

d.) As a result, the hydrogenation characteristics of Mg-Li alloys changed by the addition of 4.0 wt. percent, 7.5 wt. percent, and 15.0 wt. percent lithium were investigated, with findings made in each instance.

e.) It was discovered that when the lithium level of the powders increased, the grinding conditions altered, affecting the morphology and particle size of the powders. The capacity of magnesium to adopt a disordered position in α-Li(Mg) solid solutions was clearly higher than the hydrogenation of magnesium in the form of β-Mg(Li).

f.) Magnesium hydride produced by hydrogenation of this lithium-modified alloy (4.0, 7.5, and 15.0 wt%) has a high hydrogen desorption activation energy.

g.) The flow diagram shown depicts out the complete summarized picture of how Mg-Li alloys help out in Hydrogen Storage .

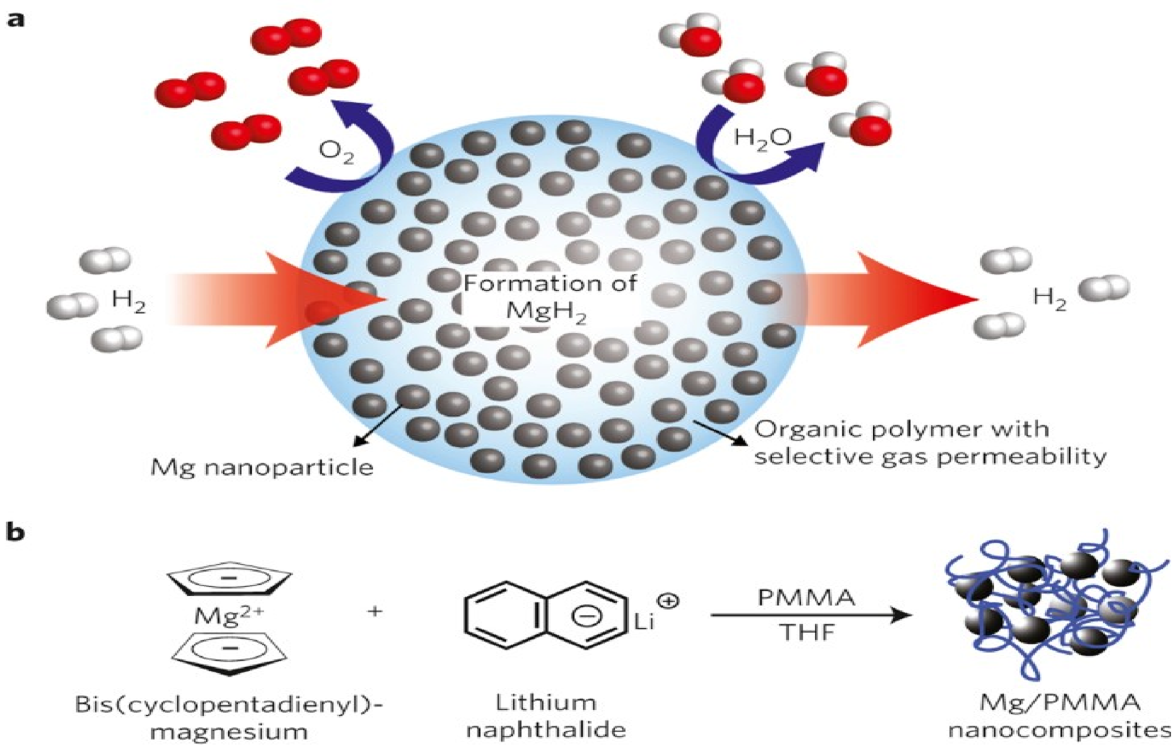
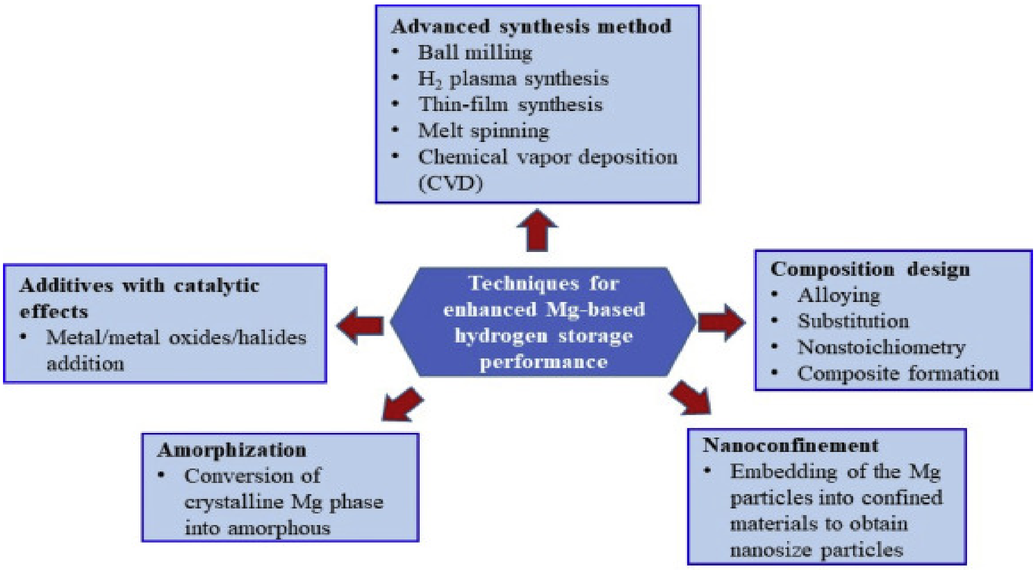


Fig (1.d) How Mg-LI alloys help in Hydrogen Storage

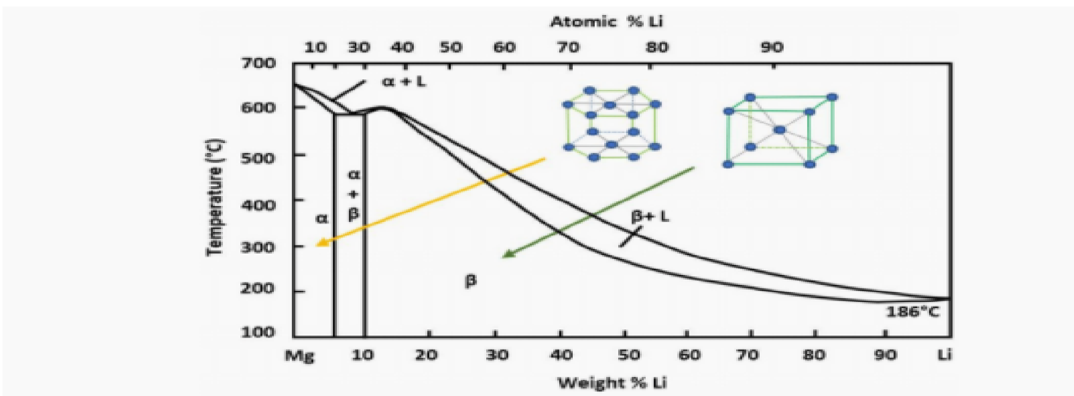


Fig(2.d) Techniques for enhanced Hydrogen Storage

e.) Theoretical Predictions of different Mg-Li alloys for Hydrogenation and DeHydrogenation Kinetics :

a.) Magnesium hydride was produced by hydrogenation of the Mg-Li alloy, which had been modified with 4.0, 7.5, and 15.0 wt. percent lithium additions, and had high hydrogen desorption activation energies of 250, 187, and 224 kJ/mol, respectively.

b.) To assess how the phase structure of the Mg-Li alloy affected its hydrogenation properties, alloys with different lithium contents between 4.0 and 15.0 wt.% were tested. The graphs and results will follow :

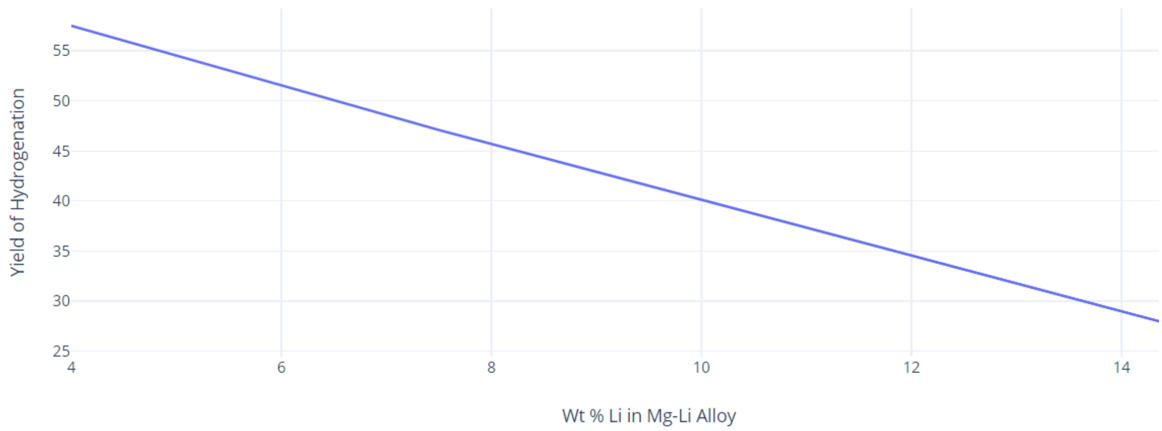


Magnesium-lithium phase diagram (made on the basis of data contained

Fig (1.e) Phase Structure and Morphology of the Materials Before and After Hydrogenation

Sample	Theoretical Hydrogen Capacity in MgH_2 (wt.%)	Measured Hydrogen Capacity in MgH_2 (wt.%)	Yield of Mg Hydrogenation Reaction (%)
Mg 4.0 wt.% Li	7.3	4.2	57.5
Mg 7.5 wt.% Li	7.0	3.3	47.1
Mg 15.0 wt.% Li	6.5	1.7	26.2

Fig (2.e) The hydrogenation properties of alloys with various Lithium contents



Graph (3.e) To Depict Hydrogenation Capacity with the increase in Wt% of Li in Mg-Li Alloy

f.) Problems and Solutions of different Mg-Li alloys for Hydrogenation and DeHydrogenation Kinetics Principles :

a.) The use of highly light-weight materials in hydrogen storage materials is recommended. Magnesium Lithium-based molecules have this capability. As a result, a lot of effort has gone into this study topic for a long time. The exceedingly poor (de)-hydrogenation kinetics of magnesium alloys, however, looked to be a significant disadvantage.

b.) There has been renewed interest in nanostructured materials since it was discovered that they could enhance these properties.

c.) Indeed, electrochemical studies of particular fluorite-type magnesium-based alloys alloyed with scandium with compositions ranging from 50 to 100 percent have been conducted. The favorable discharge kinetics were found to be preserved up to 80 percent magnesium. The more open fluorite structure of scandium hydride, rather than the more compact rutile structure of ordinary magnesium hydrides, has been linked to the improved (de)hydriding kinetics when compared to pure magnesium.

d.) Due to the high cost of scandium, efforts to develop cheaper replacements have lately been made. Titanium and lithium also make dihydrides with the same fluorite structure as scandium hydride, making them likely possibilities. When compared to pure magnesium hydride, experiments using $Mg_{80}Ti_{20}$ and $Mg_{80}Li_{20}$ thin film electrodes demonstrated a comparable substantial improvement in discharge (dehydrogenation) kinetics (MgH_2). A more detailed investigation of the Mg–Li system indicated that the hydrogen storage capacity was composition dependent in a manner similar to the Mg–Sc system, with a maximum around 80% magnesium.

e.) Despite the fact that a number of issues, such as degradation and material cost, must be addressed, this new class of magnesium materials is not only interesting for future applications, but it also has the potential to provide interesting storage properties for applications that require hydrogen to be stored in the gas phase.

g.) Classification based on crystal structure, Role of vacancies and interstitials to improve the hydrogen storage :

a.) Metal hydrides occur when the hydrogen content in an alloy reaches a specific level. As a result, hydrogen takes up residence in particular metal lattices.

b.) The interaction of hydrogen with metal atoms at the interstitial site determines the properties of hydrogen storage in an alloy, hence the hydrogen storage qualities are primarily governed by the alloy's crystal structure.

c.) A variety of hydrogen-storing alloys have been created to date, and they may be divided into five categories based on the crystal structure of the alloy and the similarity of their hydriding properties.

d.) All of the alloys, however, include magnesium, and their hydrogenation properties are extremely similar. These alloys have a larger hydrogen storage capacity, but the hydride's stability is so high that hydrogen can only be desorbed at higher temperatures.

e.) A number of transition-metal impurities and vacancies were discovered to be useful in changing the Fermi level and boosting hydrogen storage capacity. However, various contaminants in different combinations cause shifts of varying magnitudes (or do not shift the Fermi level at all).

f.)They do exhibit a predicted increase in kinetics for several contaminants that have been demonstrated to be effective in the lab. The absence of impurity enhancement may also be explained in terms of our findings. Furthermore, we have given alternative reasons for the unrecoverable loss during the dehydrogenation process and the increased hydrogen storage capacity observed experimentally based on our research of the lattice relaxations generated by hydrogen-related defects and impurities.

g.)The contaminants can be located on the Li and Mg sites, as well as at interstitial sites, among the available places. Calculations can be performed in multiple configurations for each type of substitutional or interstitial impurity to ensure that the lowest-energy configurations are attained. To ensure that the global minimum is established, a significant amount of work must be expended.

h.) Significant Amount of research and work is being continued and done on this part in finding out that global minima and hence we studied out so much of the classification based on crystal structure, Role of vacancies and interstitials so as in conclusion to improve the hydrogen storage capacity in total .

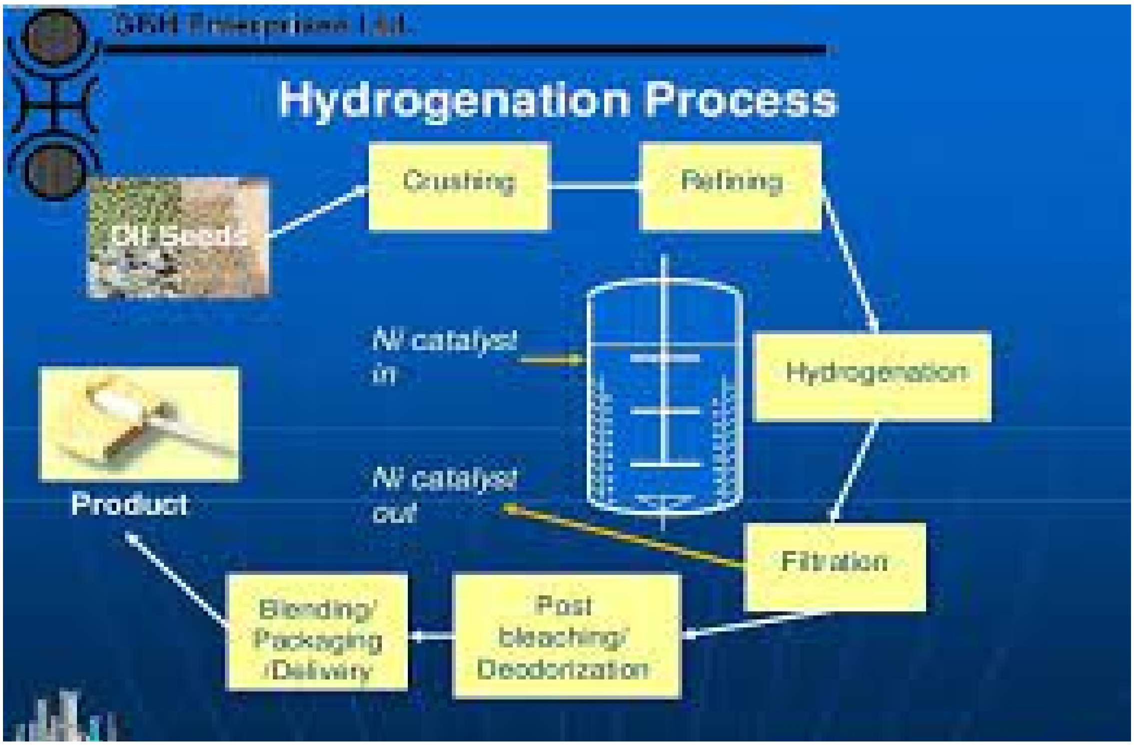
Type	**Alloy**	**Crystal structure**
A_2B	Mg_2Ni	(P6222)
	Mg_2Cu	(Fddd)
AB	TiFe	B2(CsCl)
	TiCo	B2 (CsCl)
	ZrCo	B2 (CsCl)
	ZrNi	(CrB)
AB_2	$TiCr_{1.8}$	C15
		C14
	$TiMn_{1.5}$	C14
	$ZrCr_2$	C15
		C14
AB_5	$CaNi_5$	($CaCu_5$)
Solid Solution	Ti-V	BCC
	V-Nb	BCC

Table (1.g) Different types of Alloy along with their possible crystal structure

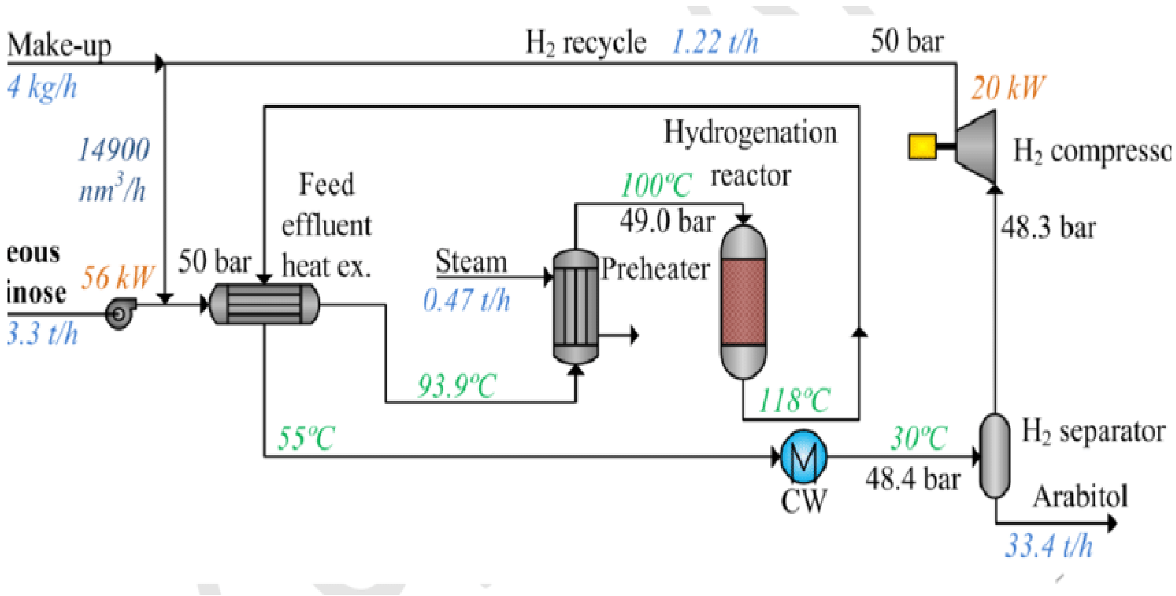
h.) Explaining hydrogenation and dehydrogenation process with help of flowcharts :

a.) Hydrogenation is a chemical process that occurs when molecular hydrogen (H2) reacts with another substance or element in the presence of a catalyst, such as nickel, palladium, or platinum. Organic molecules are routinely reduced or saturated using this method. Hydrogenation is the process of adding two hydrogen atoms to a molecule, most often an alkene. The process requires catalysts to be useful; non-catalytic hydrogenation occurs only at extremely high temperatures. Hydrogenation breaks down hydrocarbons' double and triple bonds.

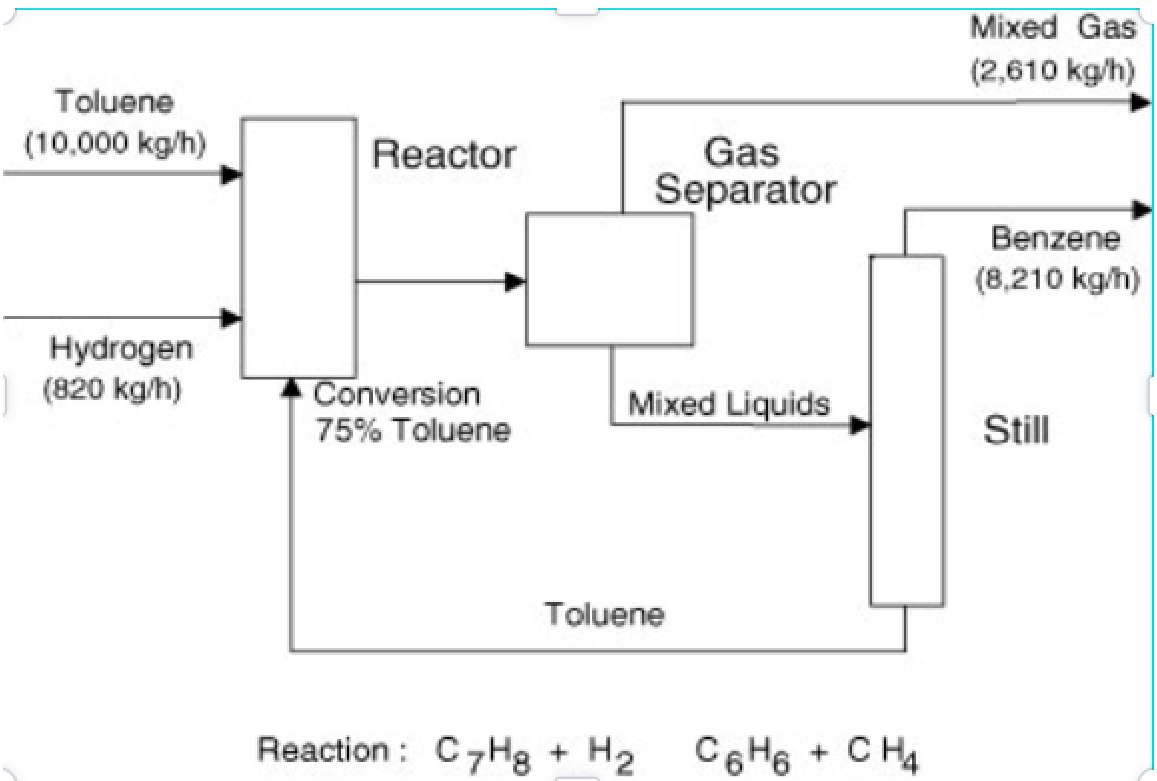
b.) Dehydrogenation is the process of removing hydrogen from an organic molecule in order to create a new chemical (e.g., to convert saturated and unsaturated compounds). Dehydrogenation of alcohols is used to make aldehydes and ketones. Acetone, cyclohexanone, methyl ethyl ketone, and styrene are all important products.



Flowchart (1.h) Hydrogenation Industrial Example

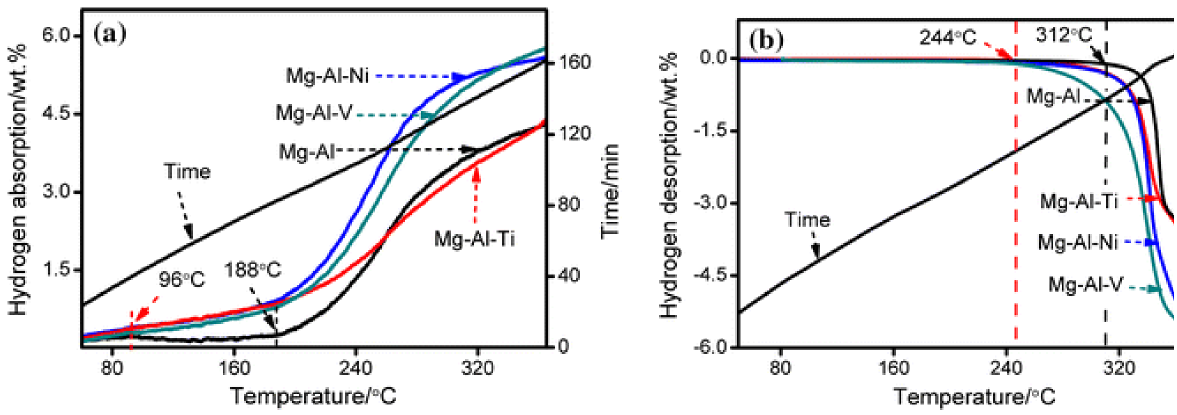


Flowchart (2.h) De Hydrogenation Industrial Example



Flowchart(3.h) Another Dehydrogenation Industrial Example

i.) Hydrogenation and Dehydrogenation graphical aspects on the Mg based alloys:



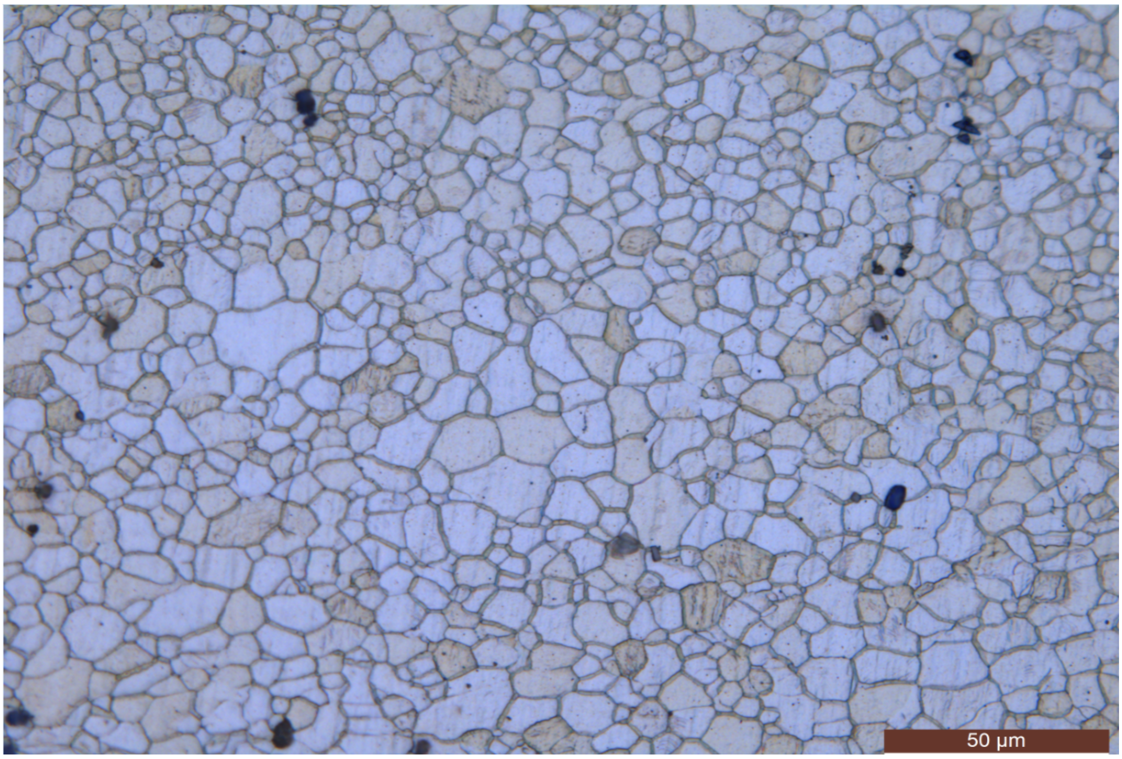
j.) Practical Aspects of the Project and Viewing out the Macrostructures of Mg AZ31

1.) **Paper Polishing:** 400-2000 grit emery paper was being used out and this will generate a reflective finish on most common non-hardened metals and is the preferred technique for polishing metals prior to Lapping.

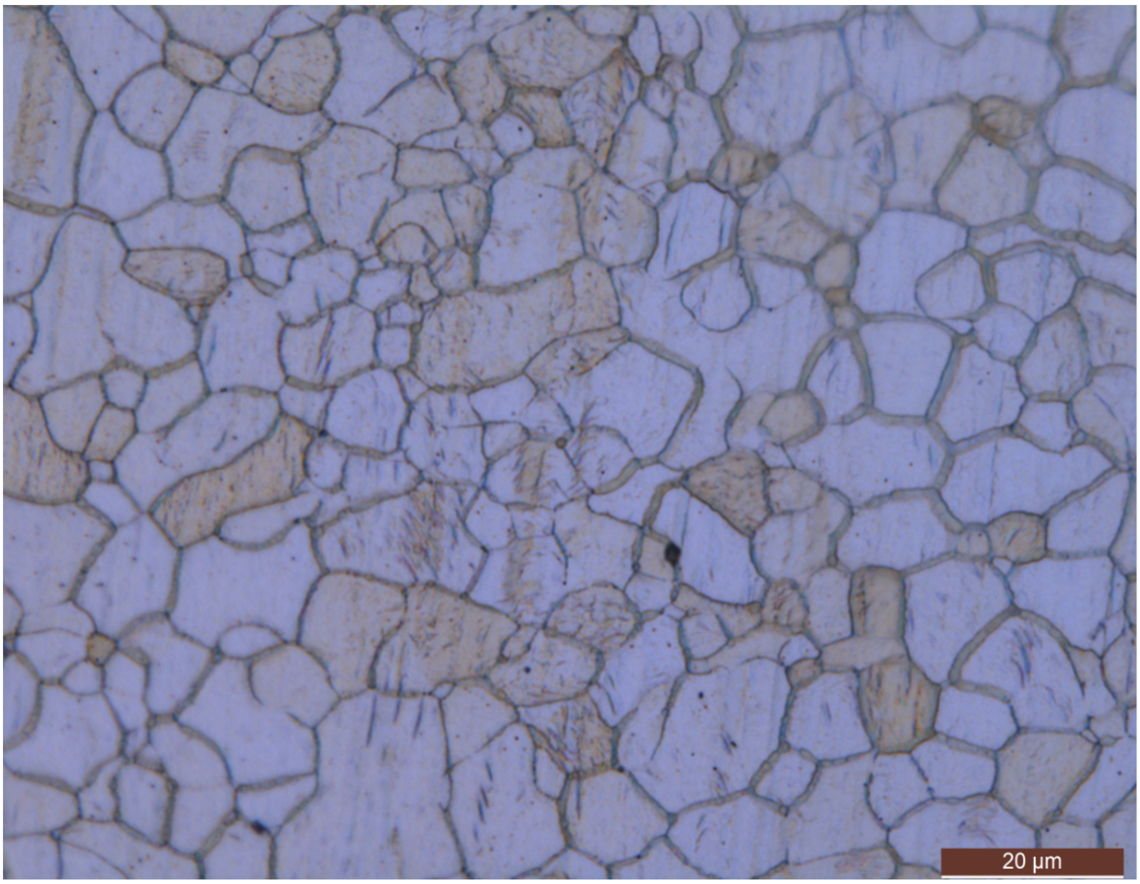
2.) **Cloth Lapping:** Lapping is a machining process in which two surfaces are rubbed together with an abrasive between them, by hand movement or using a machine. In this whole process Kerosene was being used out during the time of lapping.

3.) Etching: Etching is used to reveal the macrostructure of the metal through selective chemical attack. It gives out the grain boundaries which have higher energy than grains which corrodes out and gives us the macrostructures.

4.) The given extracted images of the Magnesium AZ31 macrostructures obtained during the practical work are being attached below:



Fig(1.j) Extracted Macrostructures of Mg AZ31 at 50 µm



Fig(2.j) Extracted Macrostructures of Mg AZ31 at 20 µm

7. Concluding Remarks:

a.) While working on this project, I came to a conclusion that there is such a vast field of research in which things can be explored more and more, and some great research could be done, as hydrogen and its storage applications will have a huge use in the future.

b.) After studying and writing this paper, I gained an incredible understanding of how much effort and focus our scientific community is putting forth to improve the thermodynamic, kinetic, Hydrogenation, Dehydrogenation, and Interstitial storage properties of magnesium and lithium alloys while maintaining a high hydrogen storage capacity.

c.) In this paper and project report, we examine materials made up of Mg-Li binary alloy that are suitable for storing hydrogen and their various applications.

d.)We began the article by discussing the real-world applications and industrial uses of hydrogen before moving on to the section where we examined in depth the particular materials and their unique qualities that must be considered anytime hydrogen storage is considered.

e.) We discussed why only Mg-Li alloys should be considered as the best options and what can be done better while considering all scientific factors such as theoretical predictions along the lines of Hydrogenation - Dehydrogenation Principles while also focusing on their problems and solutions while also considering factors based on crystal structure, role of vacancies and interstitials to improve the hydrogenation efficiency.

f.) I would like to conclude by saying that I have tried my best to cover all the major key points of the report in such a way that we have been able to achieve our primary objective .

8. Acknowledgment :

I want to thank and acknowledge the following links and papers that have helped me to gain some knowledge for this report. Without the assistance of **Dr. Saurabh Sanjay Nene** sir, this report would have been an indefinite task for me.

I have listed all links from which educational pictures and data were used. In case of missing links, I would like to thank the owner and promise to abide by the fact that educational content is in fair use without violating the copyright rules.

9. References(Bibliography):

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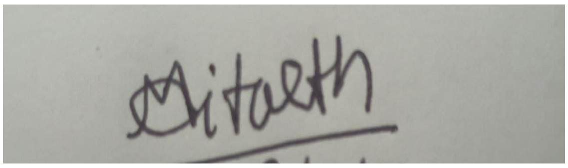

Signature of the Student

Signature of the Supervisor

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END OF THE REPORT

Supervisor's Recommendation for the Evaluation

Please tick any one of the following

1. The work done is satisfactory, and sufficient time has been spent by the student. The submission by the student should be evaluated in this term.
2. The work is not complete. Continuity Grade should be given to the student. The student would need to be evaluated in the next semester for the same Design Project with me.
3. The work is not satisfactory. There is no need for evaluation. The students should look for another Design Credit Project for the next semester.
4. [Other Comment, if 1-3 are not valid] ____________________

Signature of the Supervisor