GH2THON

Green Hydrogen Innovation Challenges

"Optimist"

A Data Driven Framework to Accelerate and Innovate R&D Processes

Ashwini Verma, Piyush Maharana, and Kavita Joshi
CSIR - National Chemical Laboratory, Pune

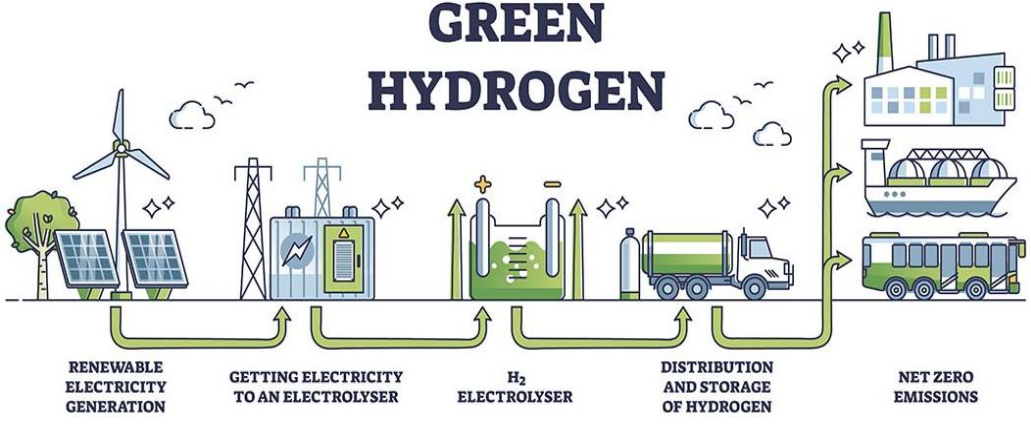
12th September 2024

2nd INTERNATIONAL CONFERENCE ON GREEN HYDROGEN

Optimization!

https://oworkers.com/8-process-optimization-techniques-how-to-get-started/

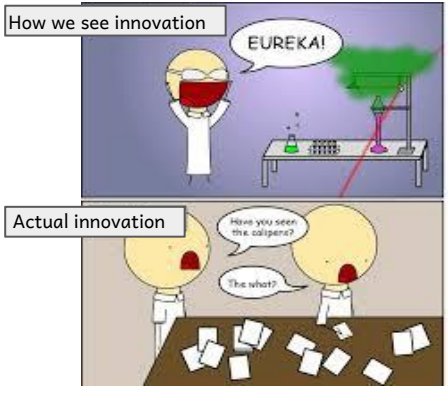
Need of the Hour: Accelerated Process Optimization!

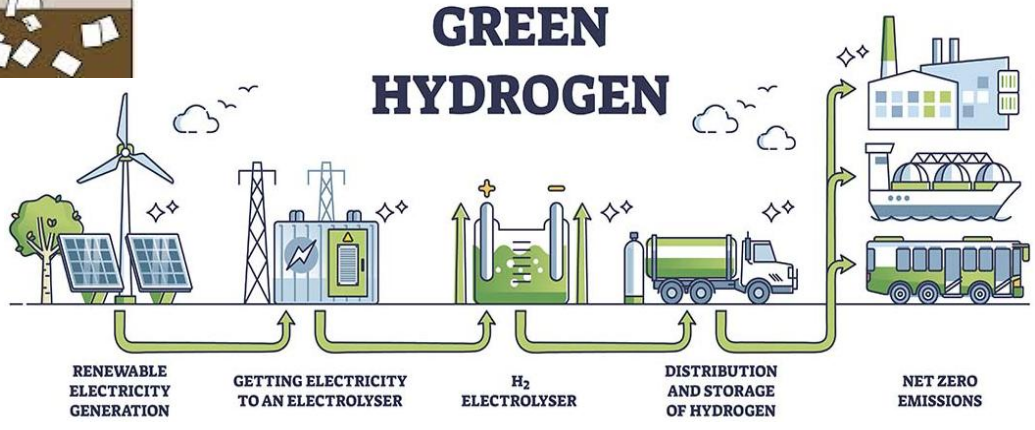


https://aibe.uq.edu.au/article/2023/03/economics-of-green-hydrogen-in-australia-part-1

Need of the Hour: Accelerated Process Optimization!

Finding the solution through trial and error is challenging :)





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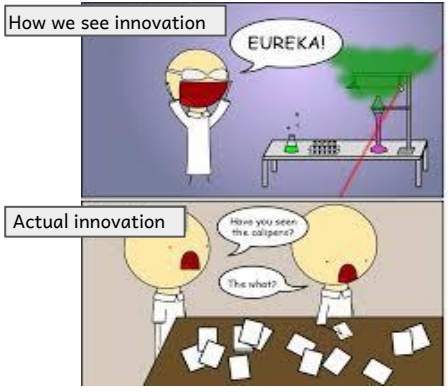
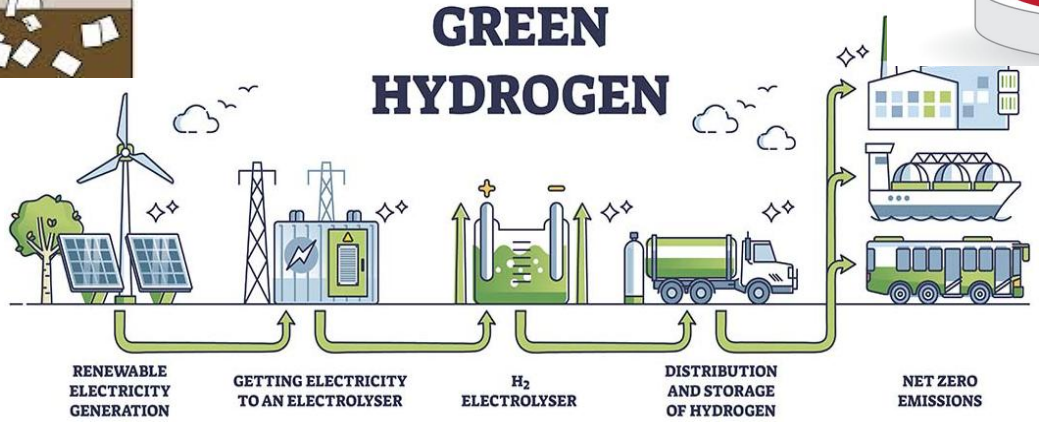


To accelerate the induction of technologies to market



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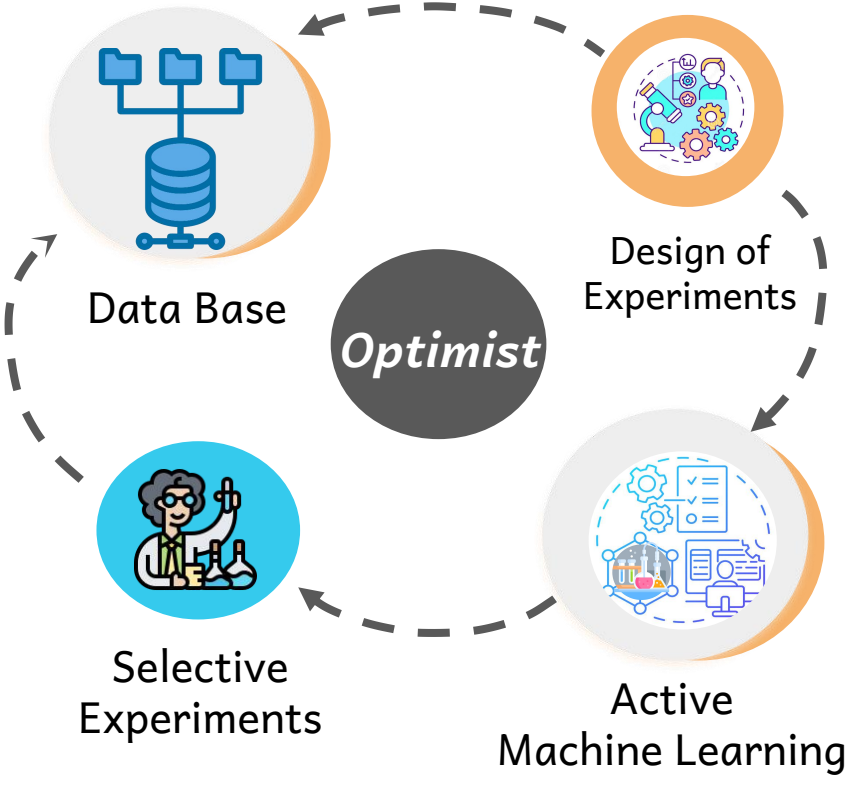
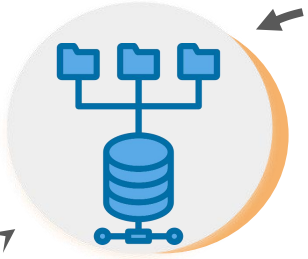
Data Driven Process Optimization



Data Driven Process Optimization

Problem Identification



Data Base

Optimist

Design of Experiments

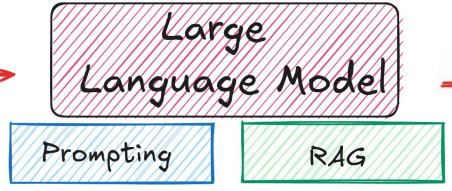
Selective Experiments

Active Machine Learning

- Data acquisition and analysis
- Improve decision-making
- Speed up innovation
- Cost Reduction

Data Building Using LLM

Unstructured Data



	A	B	C	D
1	Composition	T (K)	P(bar)	Target
2	Ga0.29Mg0.71	647	7.67	-0.27
3	Ga0.29Mg0.71	623	4.48	-0.80
4	Mg0.95Sn0.03Zn0.02	573	2.26	-1.49
5	Ce0.05Mg0.9Sm0.05	652	6.15	-0.49
6	Ce0.05Mg0.9Sm0.05	632	3.72	-0.99
7	.....	.....	.....	.....

Structured Data

1. *P.R. Maharana and K. Joshi, Retrieval Augmented generation for building databases from the scientific literature. (Manuscript under preparation)*
2. *N Wilson, AD Verma, PR Maharana, AB Sahoo And K Joshi,* HyStor: An Experimental Database of Hydrogen Storage Properties for Various Metal Alloy Classes, ChemRxiv, (2024), DOI:https://doi.org/10.26434/chemrxiv-2024-6.

Design of Experiments

Describe

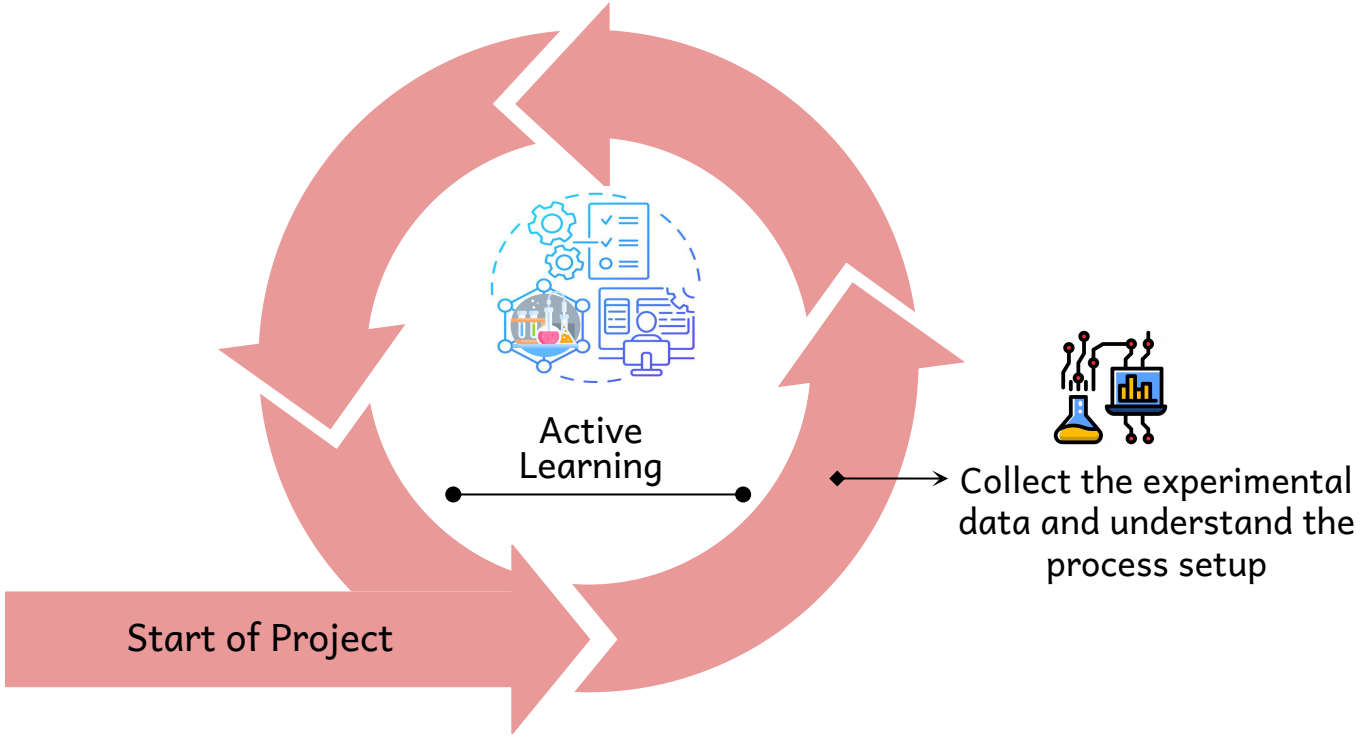
Specify

Design experiments and collect data

Fit the model

Predict

Integrating ML with Experiments



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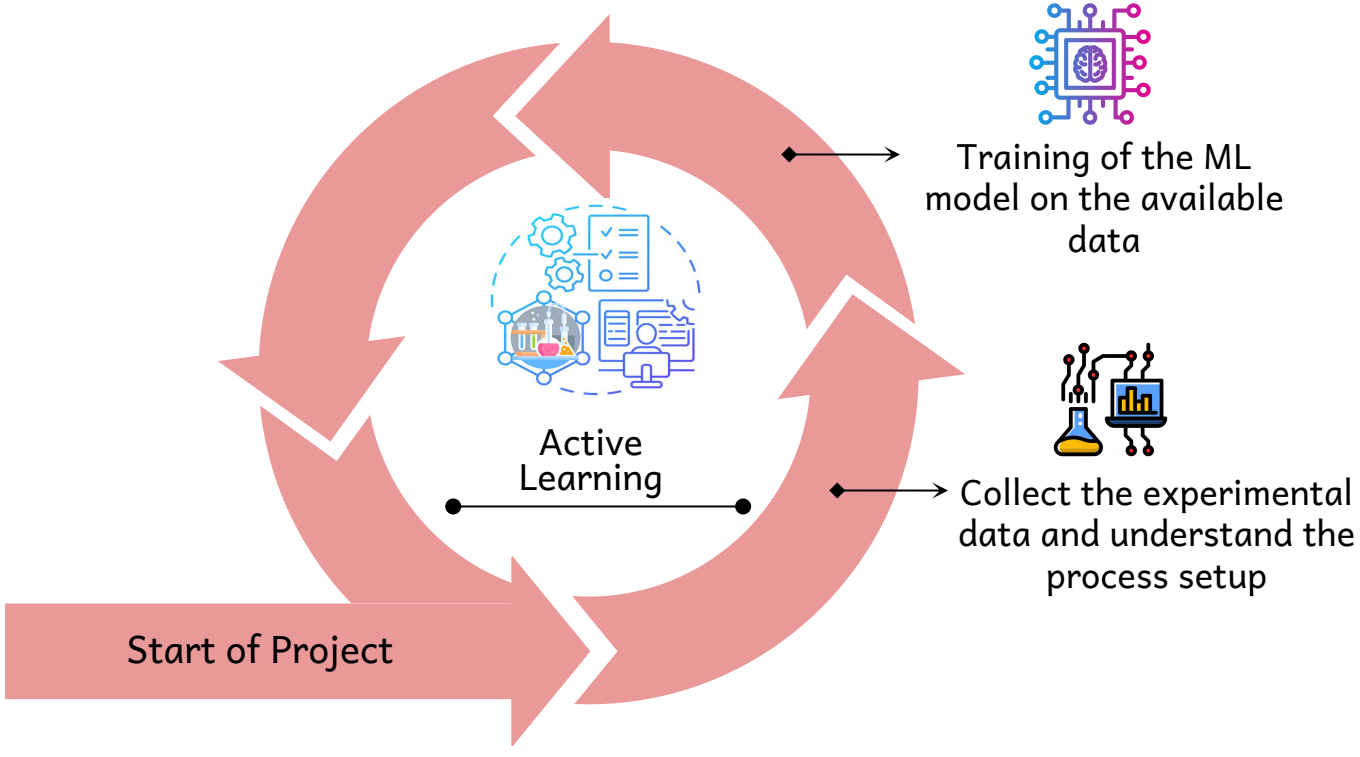

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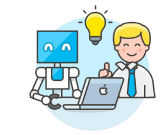
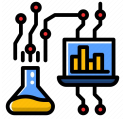


The trained model will be employed to predict the output and suggest the next experiment

Training of the ML model on the available data

Active Learning



Collect the experimental data and understand the process setup

Start of Project

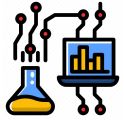
Integrating ML with Experiments

The trained model will be employed to predict the output and suggest the next experiment

Training of the ML model on the available data

Experiments should be carried out to validate the predictions

Active Learning



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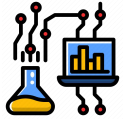


Feedback data + Collected data

Start of Project

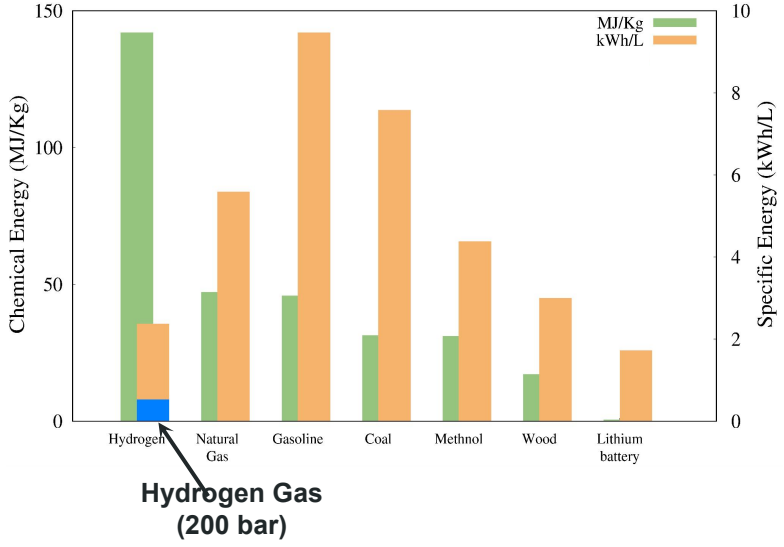
Requirements met?

NO

YES

Better Material

Use-Case: Materials Discovery for Solid-State Hydrogen Storage



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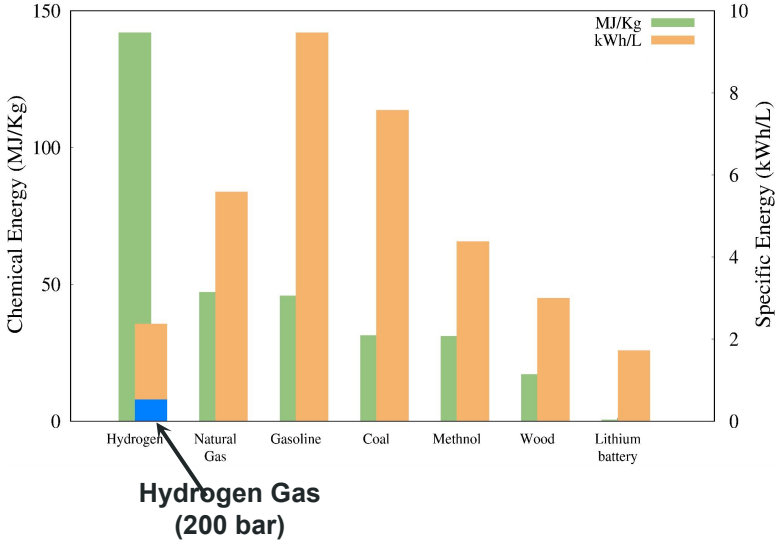

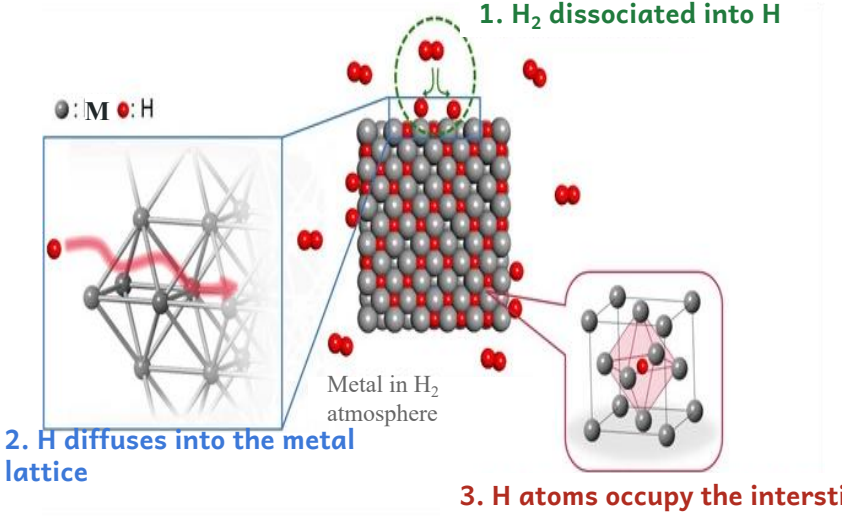

Dekura et.al ChemPhysChem 2019, 20, 1158.

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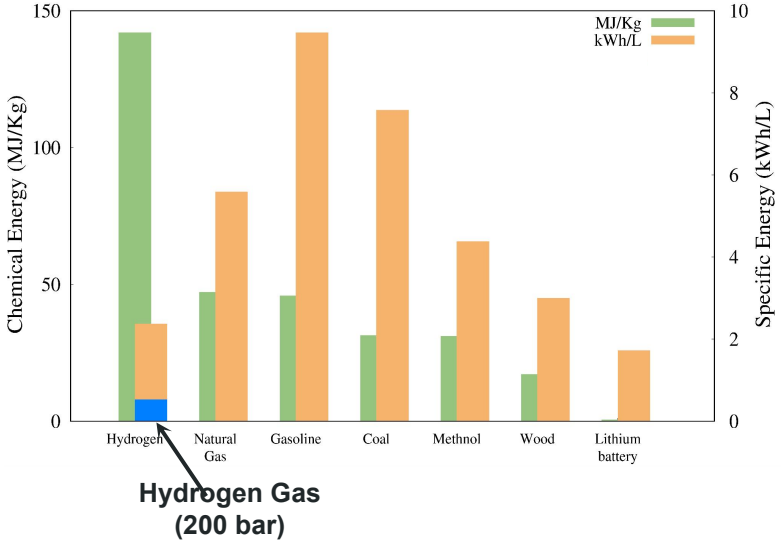
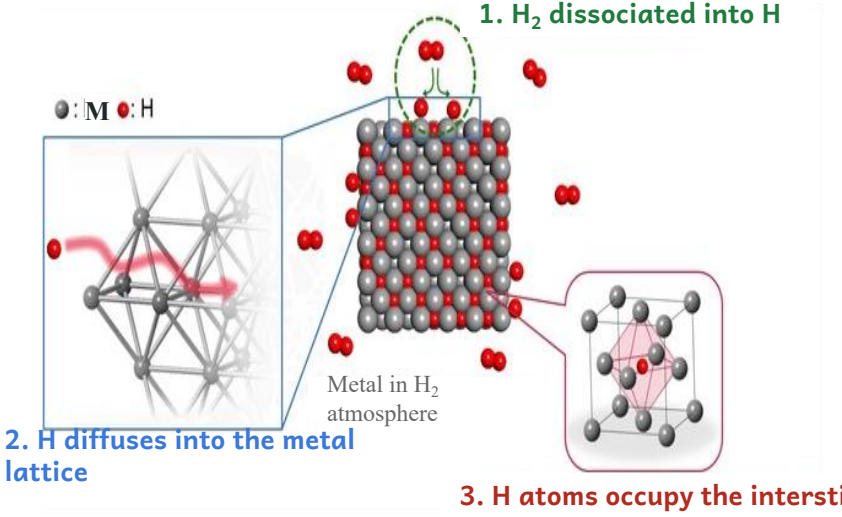
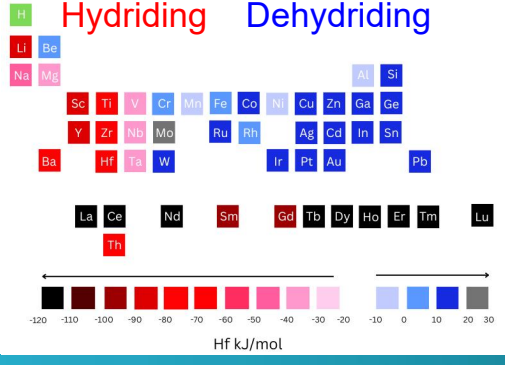




Dekura et.al ChemPhysChem 2019, 20, 1158.

High H2wt% Capacity | Low Hydriding Enthalpy | Ambient Conditions | Reversible & Durability

Infinite possibilities



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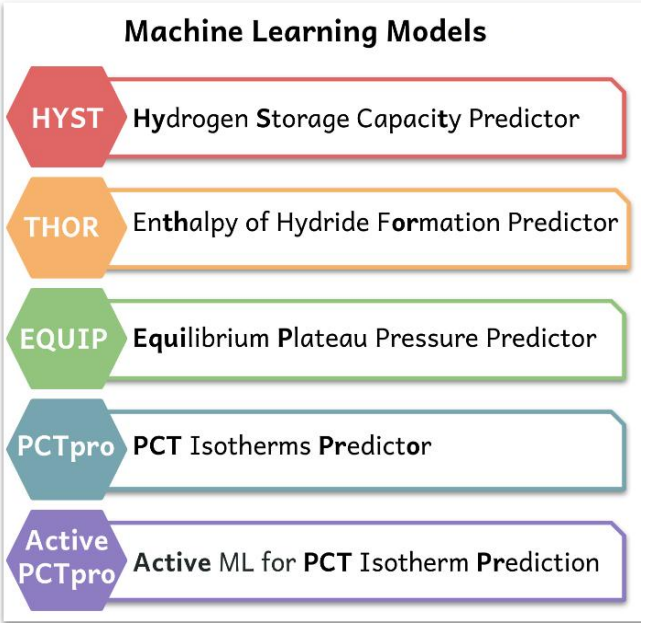

3. Kavita Joshi and Ashwini Verma; Provisional Patent No. 202211028454 [2022]

4. Kavita Joshi and Ashwini Verma, Provisional Patent No. 202311064135 [2023]

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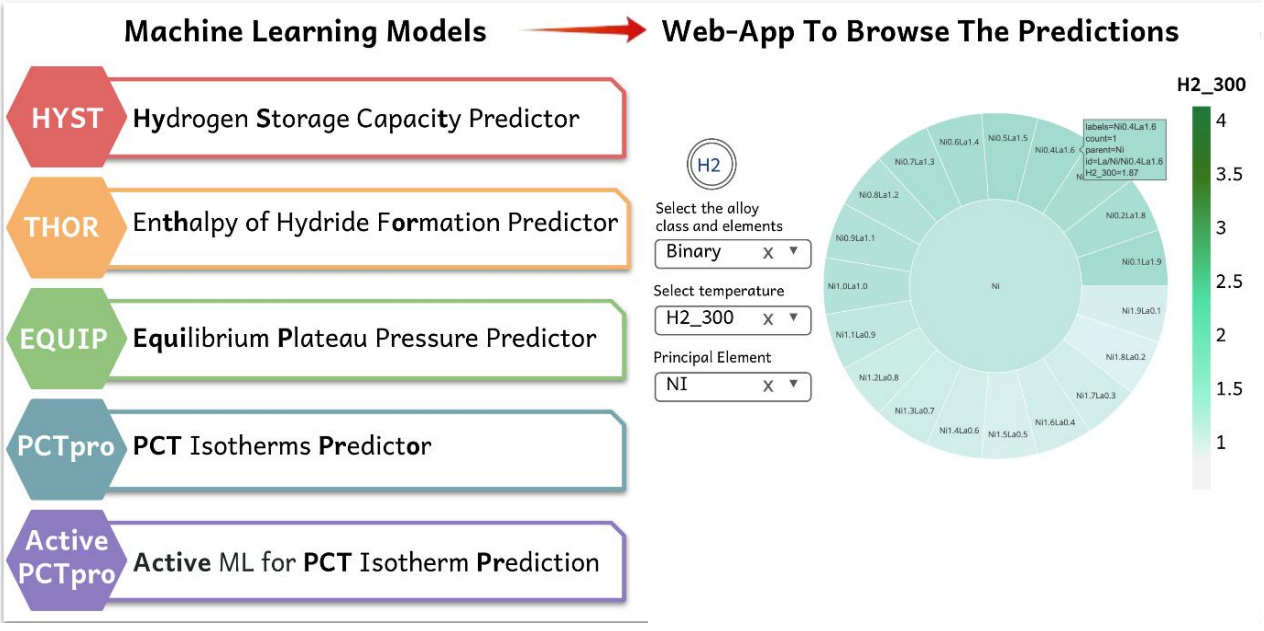

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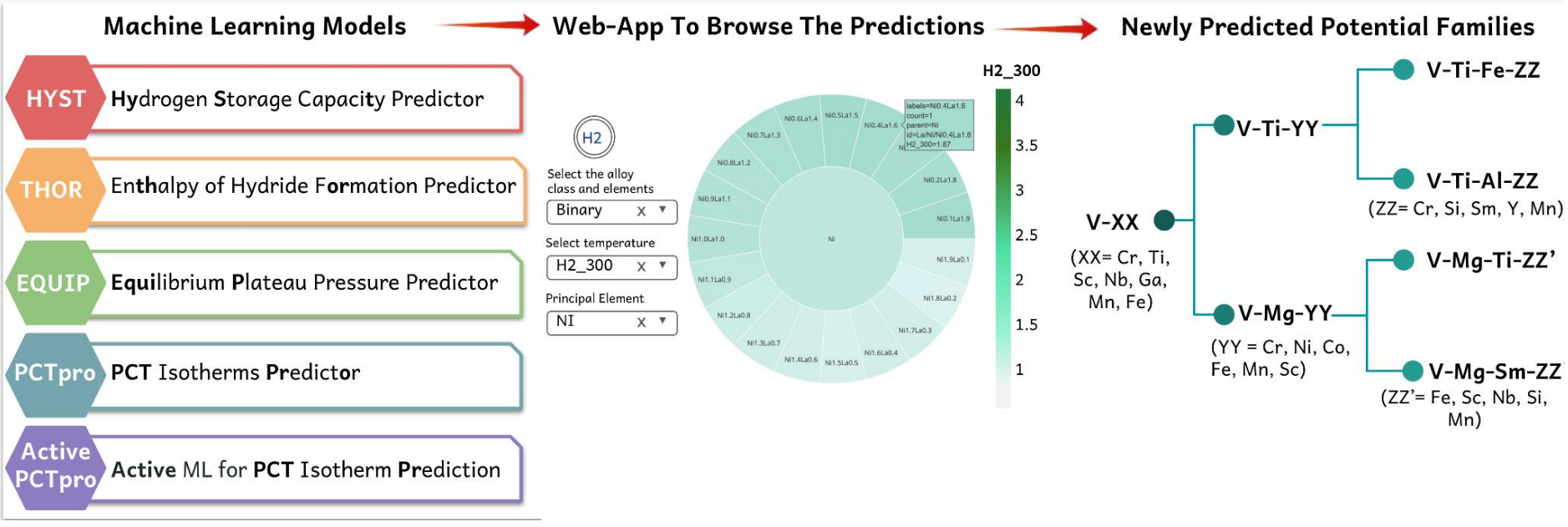

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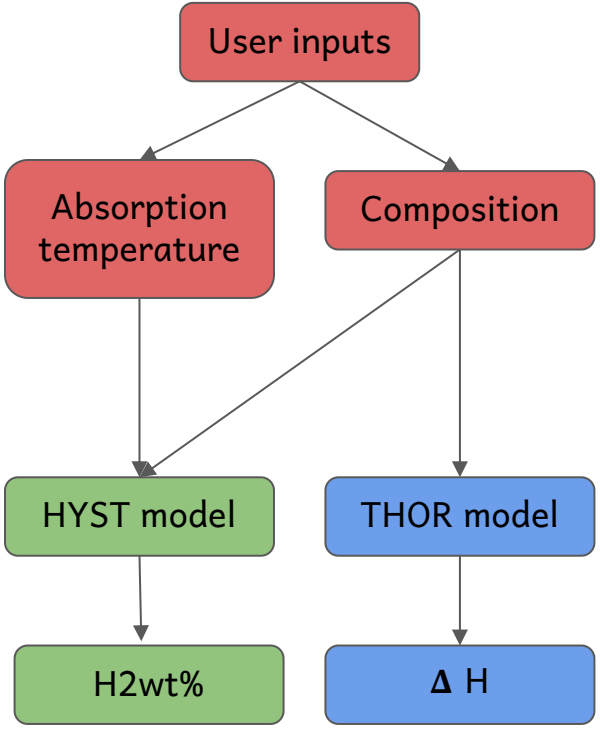
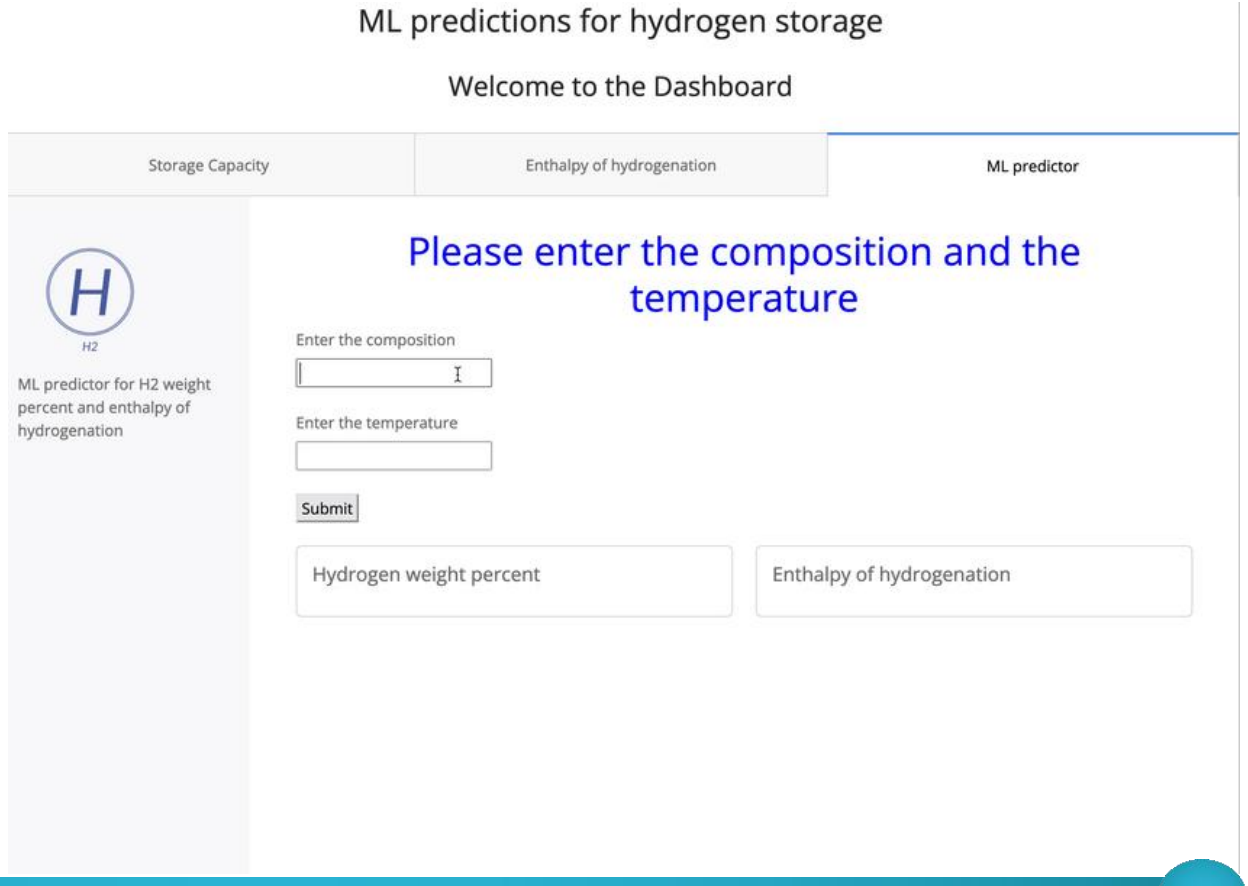
5. Ashwini Verma, Nikhil Wilson And Kavita Joshi, Solid state hydrogen storage: decoding the path through machine learning, Inter. Journal of Hydrogen Energy., 50, 1518 - 1528 (2024)

6. *Ashwini Verma And Kavita Joshi,* PCTpro: A Machine learning model for rapid prediction of Pressure-Composition-Temperature (PCT) isotherms, ChemRxiv. , (2024), DOI:https://doi.org/10.26434/chemrxiv-2024-g33f9

Web Application for Real Time Prediction

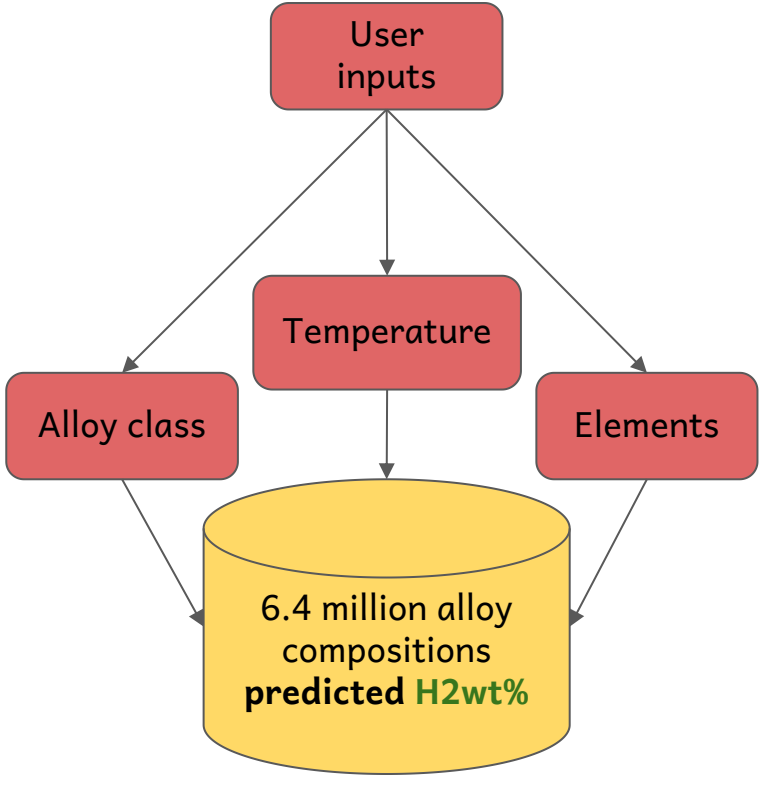
ML predictor module

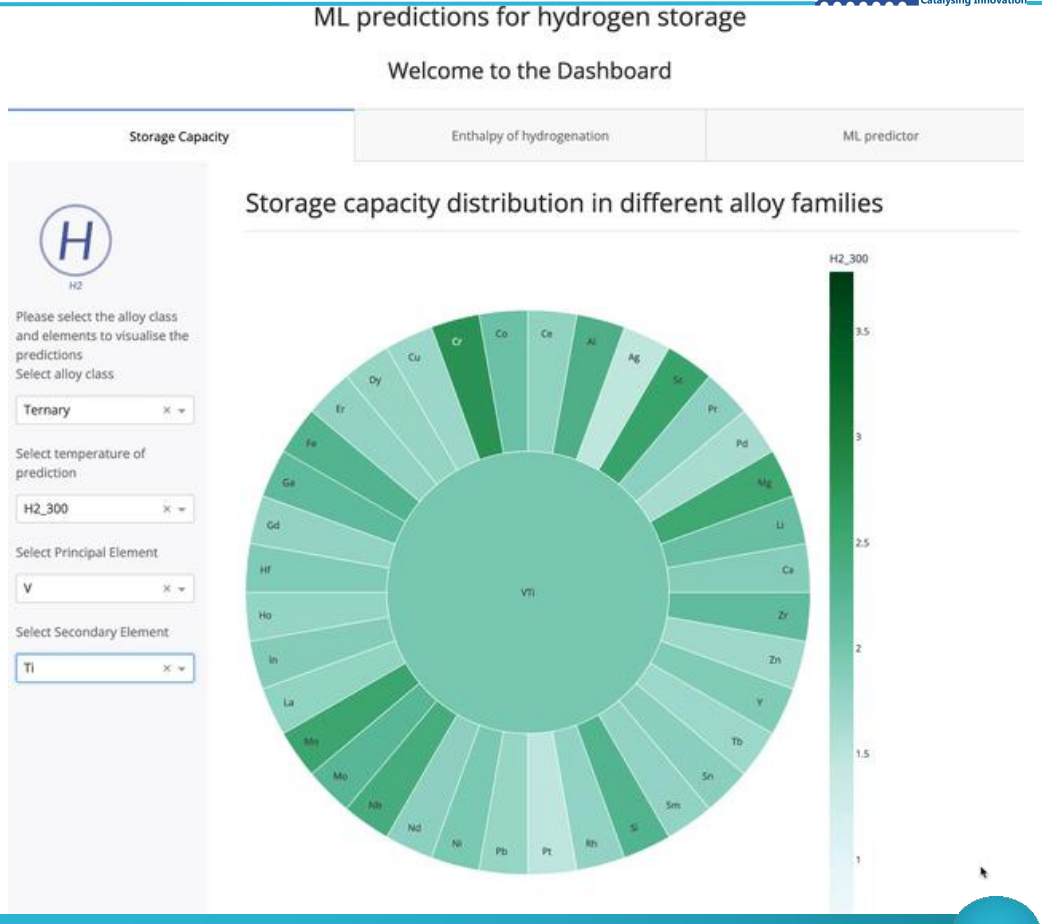




Web Application: Visualization Module

H2wt% visualize module





Use-Case: Materials Discovery for Solid-State Hydrogen Storage

H2wt% > 2.5 at room temperature and ΔH < 60 kJ/mol H2

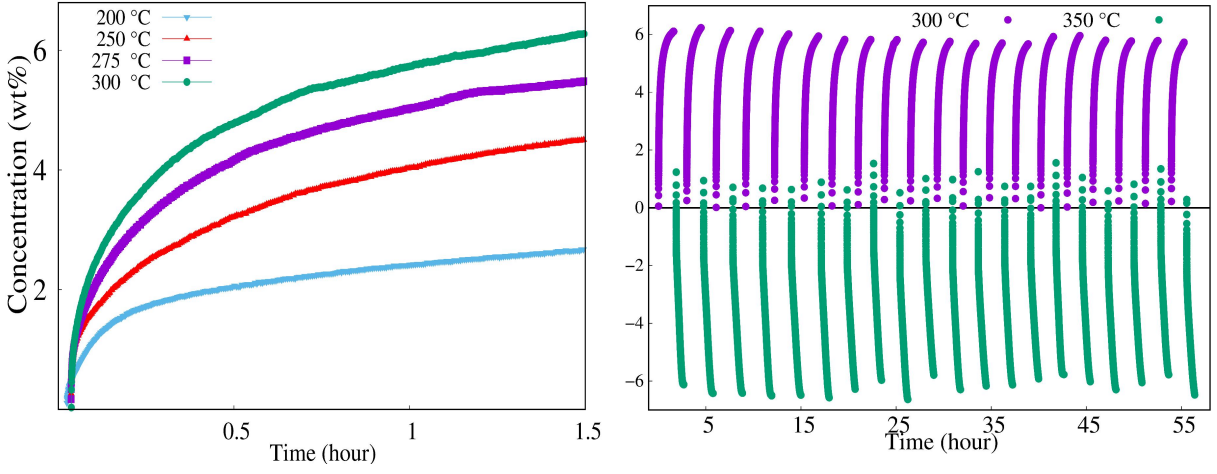
Temperature	300K		400K		500K		600K	
Alloy class	Total number	Unique compositions	Total number	Unique compositions	Total number	Unique compositions	Total number	Unique compositions
Binary	271	122	325	134	499	197	1487	326
Ternary	761	289	1099	391	1808	610	23950	3429
Quaternary	5304	2211	8233	2981	16734	4973	363855	31510

No. of metal alloys reported so far with their H2 storage properties ~3000

Using our models we predicted H2wt% and ΔH of 6.4 million compositions in a day.

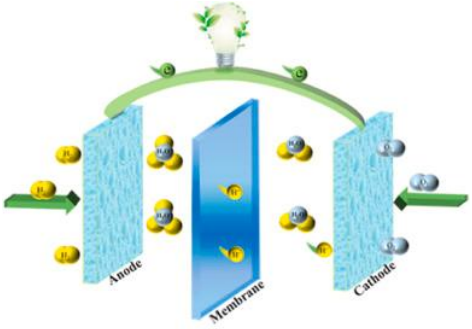
Use-Case: Materials Discovery for Solid-State Hydrogen Storage

Material	Temperature (K)	ML H2_wt%	Expt. H2_wt%
AxxByyCzz	523	5.53	5.15
	548	5.66	5.73
	573	5.82	6.65



7. A. Verma, P. Kumar, S. Kumar and K. Joshi, Hydrogen Storage Performance in Mg-Based Composites. (Manuscript under preparation)

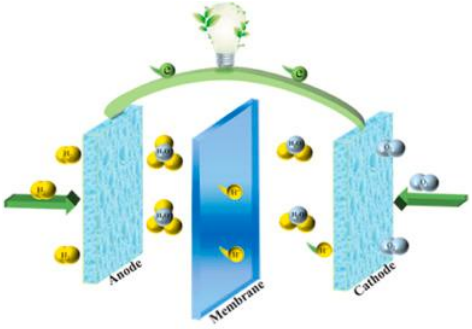
Ongoing Work



Screening of ionomers with enhanced proton conductivity in collaboration with Dr. Sreekumar Kurungot, CSIR-NCL.

https://www.sciencedirect.com/science/article/pii/S0378775322003974 ;

Ongoing Work



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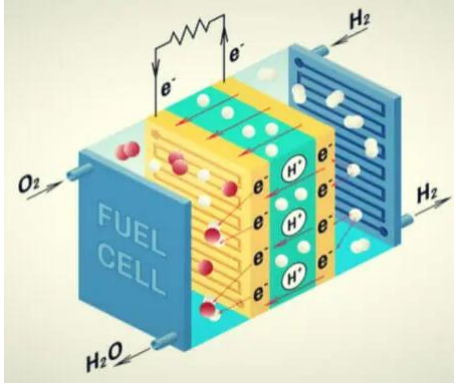
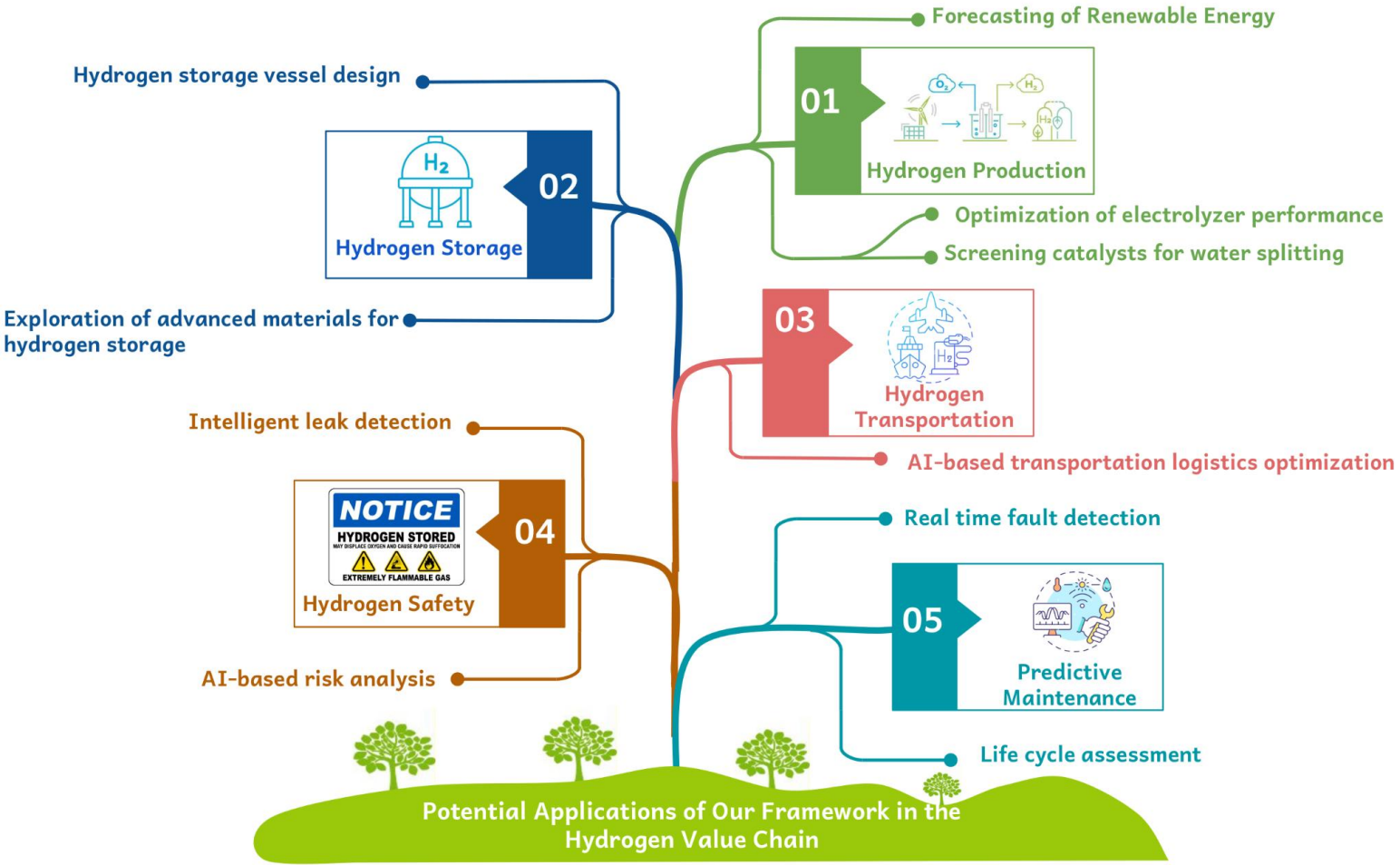


Collaborating with Dr. Pol and the fuel cell team at CSIR-NCL and CSIR-CECRI on fuel cell stack optimization.

https://www.sciencedirect.com/science/article/pii/S0378775322003974 ; https://www.quarktwin.com/blogs/battery/differences-between-hydrogen-fuel-cell-and-lithium-battery/51

Proposed Way Forward



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THANK YOU!!

Group Website: http://academic.ncl.res.in/k.joshi