Structure and dynamics in hydrogen-rich alloys for hydrogen storage

Abhishek Banerjee - *PhD-student at UiS*

Renewable energy solutions that could potentially replace fossil fuels in near future is at global interest. Hydrogen as the storage media for renewable energy have increasingly come into industrial focus due to its abundance, high energy efficiency and potential fossil free production. But due to its extremely light weight and low density at normal conditions, storage and transportation is a challenge. Henceforth, search for new storage technologies is of an immense importance to reduce the overall expense of H2 usage.

This PhD project will focus on the study of new combinations of metal alloys to capture and retrieve H2, which could generate optimal solutions for the above stated problems. The starting phase of the work will involve the use of different synthesis techniques of metal alloys (e.g., mechanochemical, arc melting) followed by in-depth study of fundamental material properties such as chemical bonding, crystallographic and electronic configurations, elemental coordination environments and oxidation states together with characterization of hydrogen dynamics using a selection of advanced characterization techniques.

University of Stavanger

Structure and Dynamics in Hydrogen-Rich Alloys for Hydrogen Storage

ABHISHEK BANERJEE

Supervisor: Assoc.Prof Olena Zavorotynska

Institute of Physics and Mathematics

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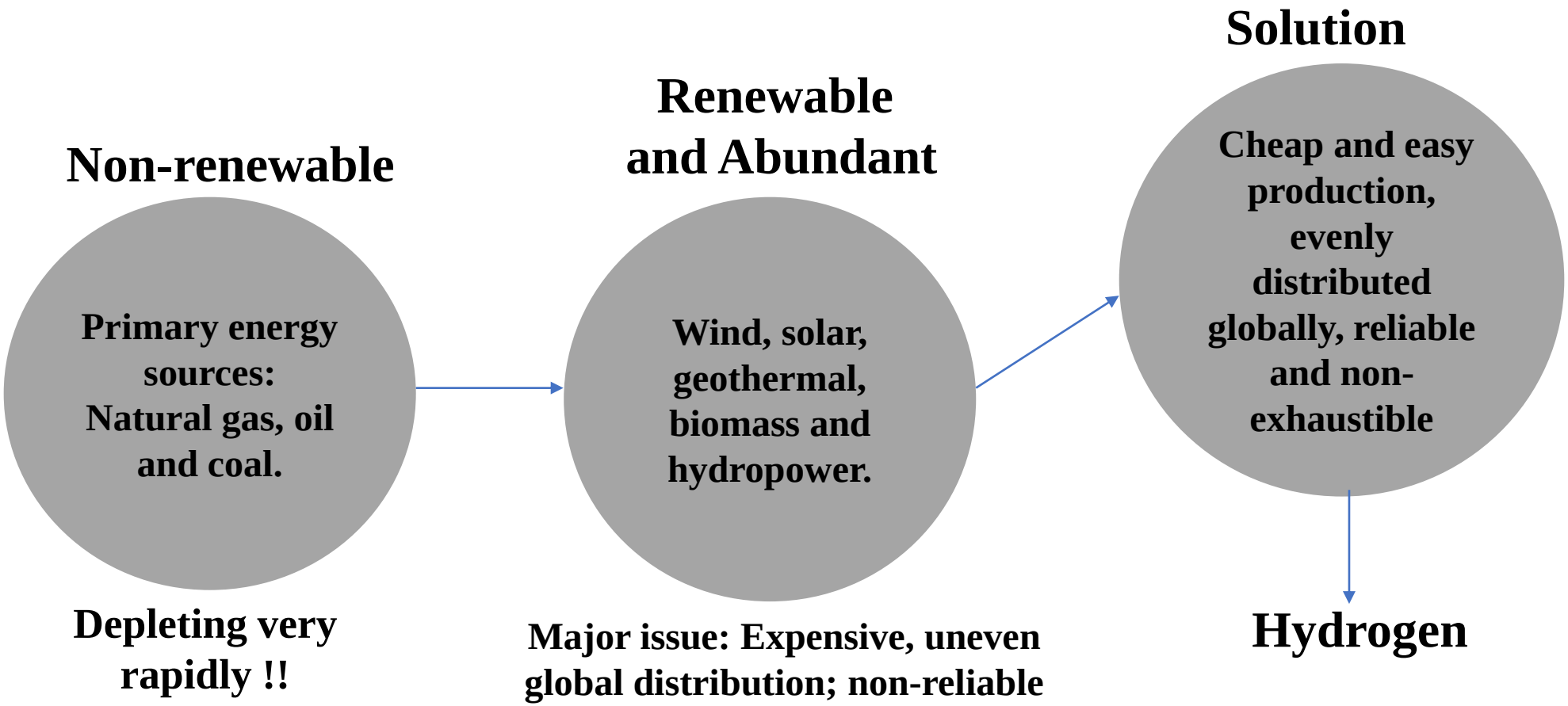
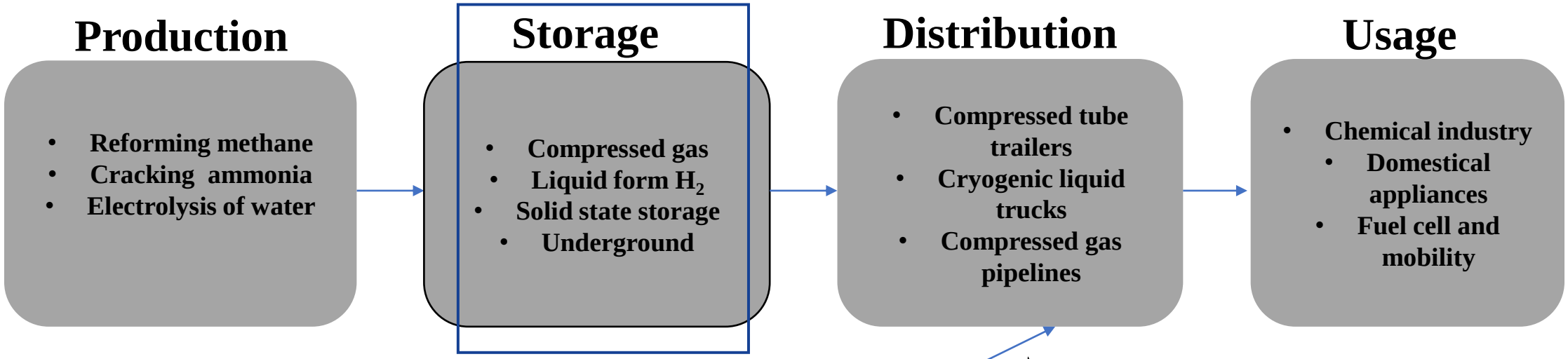
What/bigger picture ?



Hierarchy of Hydrogen Economy

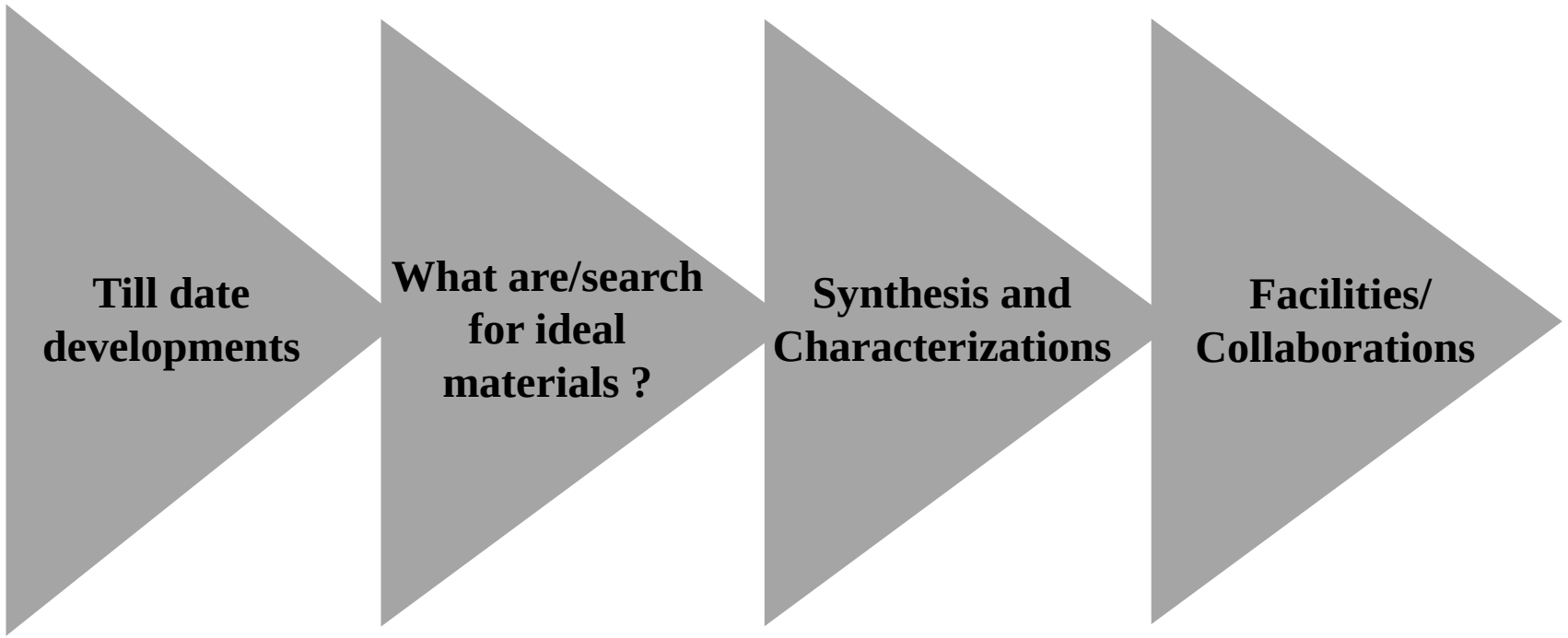


- **Storage is a big problem !!!**

As H_2 is the lightest element (~ 16 times lighter than O_2)

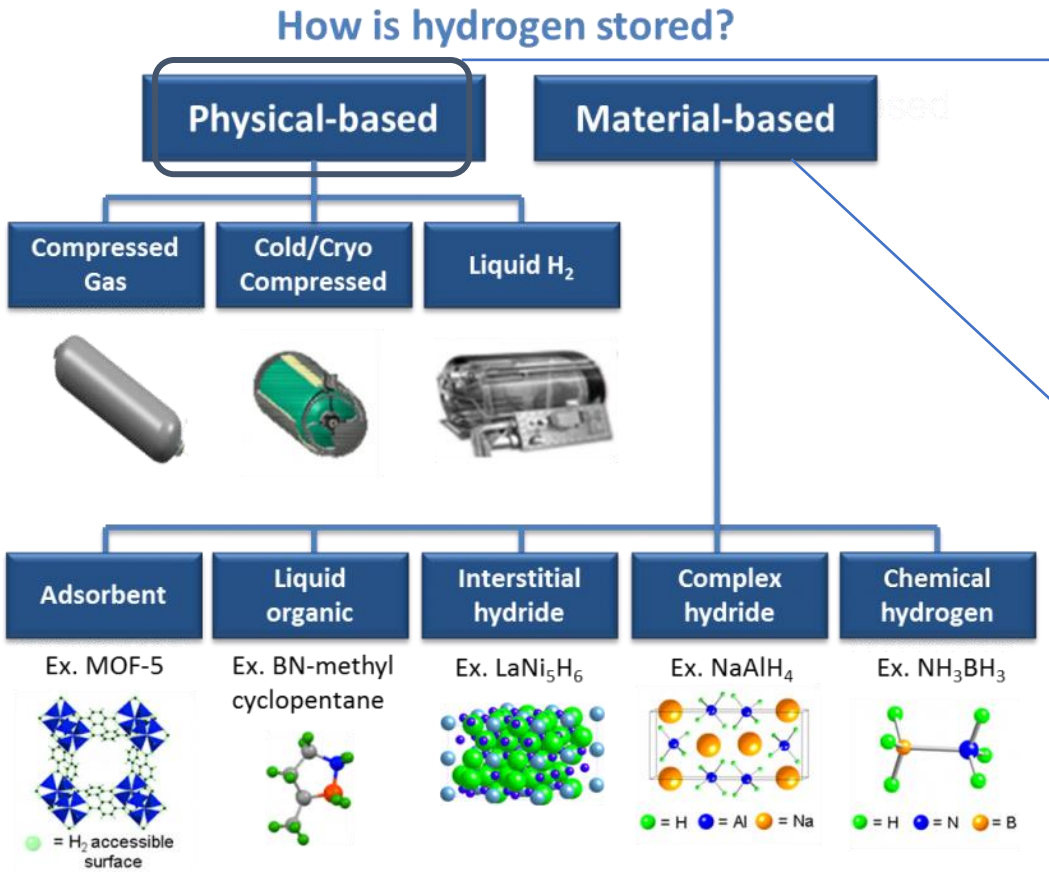
Direct impact

Breakdown of Project Components



Till Date Developments

- **Materials**

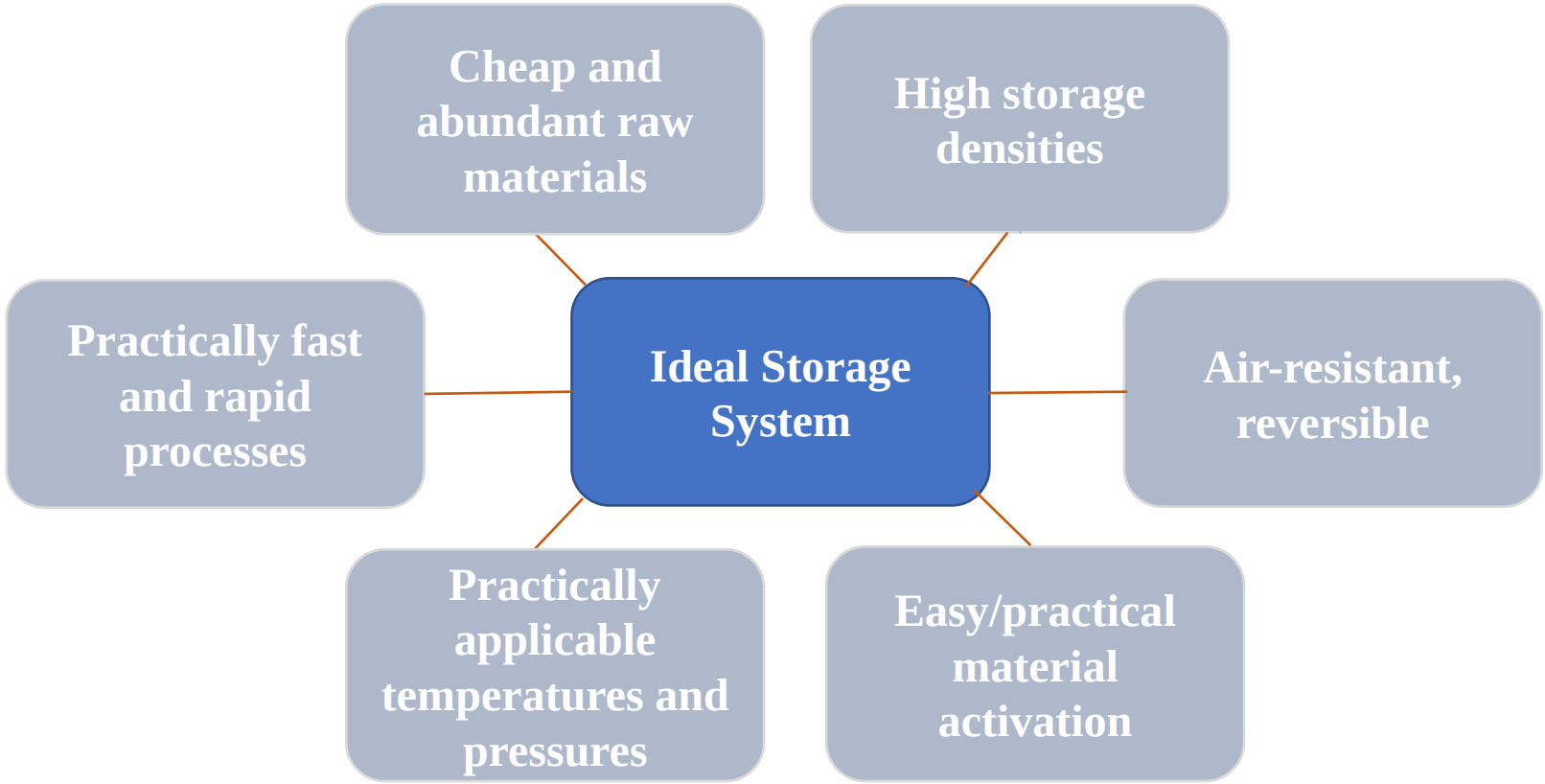


- Expensive to liquify hydrogen.
- Unsafe for transport in liquid and compressed form; risk of explosion.
- Not feasible working conditions.

Main focus!

https://www.energy.gov/eere/fuelcells/hydrogen-storage

What are/search for ideal materials ?



An overview on TiFe intermetallic for solid-state hydrogen storage: microstructure, hydrogenation and fabrication processes G. K. Sujan, Zengxi Pan, Huijun Li, Daniel Liang & Nazmul Alam

Why Titanium-Iron (TiFe) alloy ? According to criteria required by US Dept of Energy

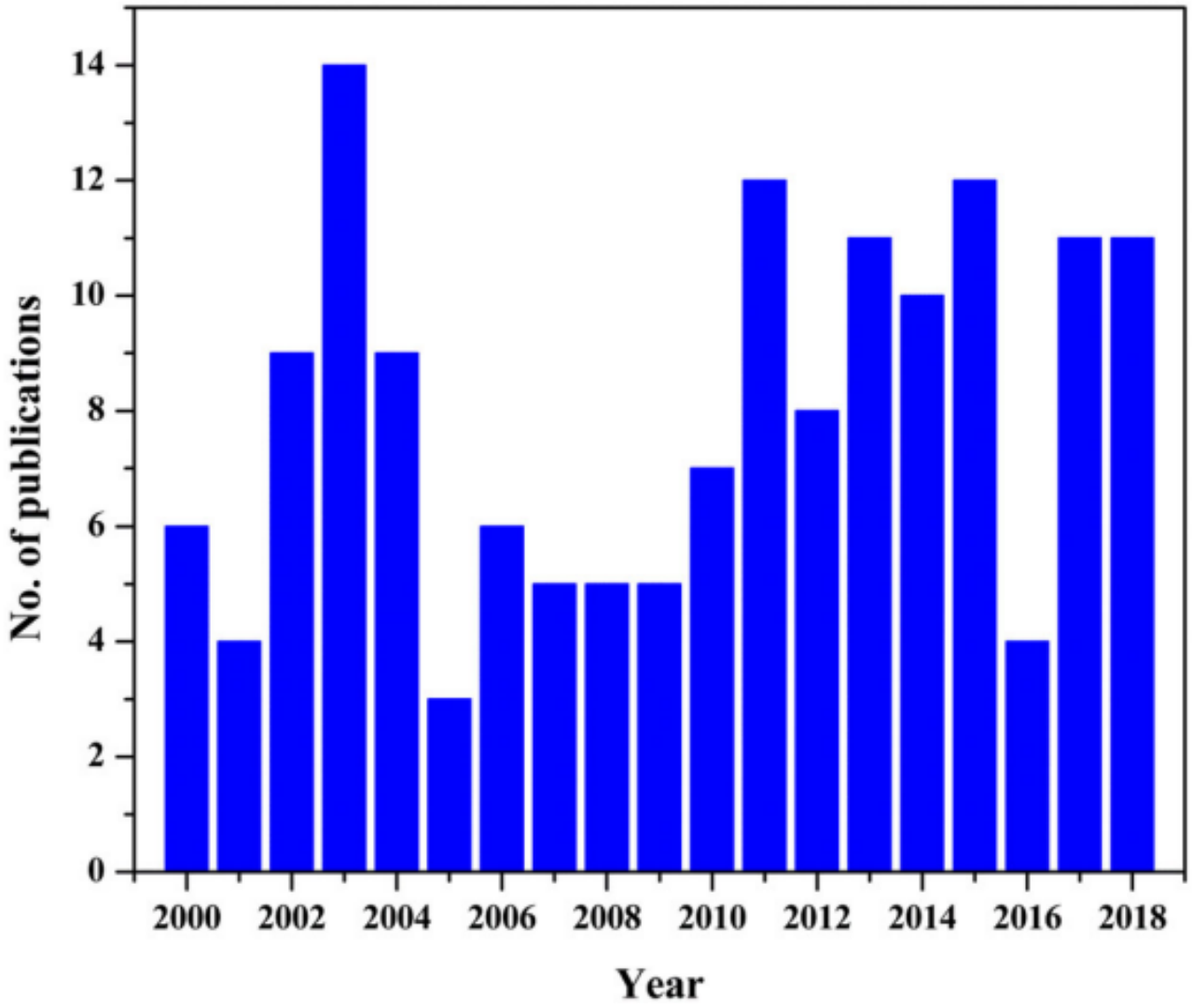
Materials or groups	Volumetric capacity	Gravimetric capacity	Hydrogen charge/ discharge temperature	Hydrogen charge/ discharge rate	Reversible ability
Metallic hydrides					
Intermetallic hydrides (AB_5, AB_2, A_2B, AB_3)	+/0	−	+	+	+
TiFe and its alloys (AB)	+ **96 gm/cm^3**	−	+	+	+
Elemental hydrides (MgH_2)	0	+	−	0	−
Chemical hydrides (ammonia borane)	0	+	0	0	0
Complex hydrides (Alanates, borohydrides)	+/0	+	0/−	0	−
Porous materials (C, MOFs, zeolites)	0	+/0	−	0	0

Challenges

- Gravimetric density (for portable apps).
- Activation conditions.
- Air resistance.

Potential Solutions

- Optimizing synthesis techniques – primarily effects alloy activation
- Alloying – activation/kinetics



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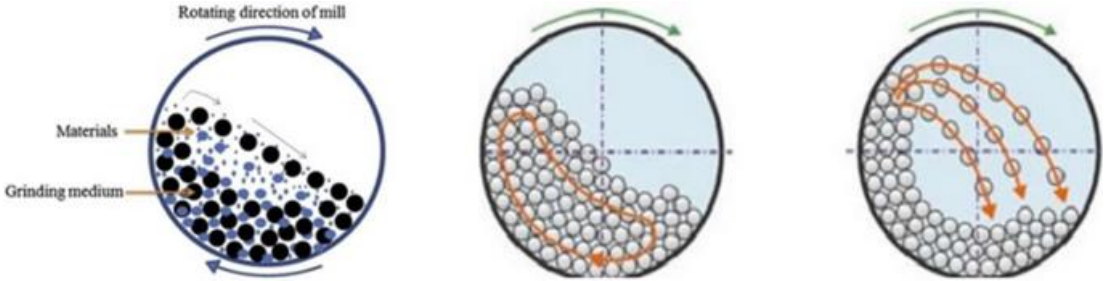
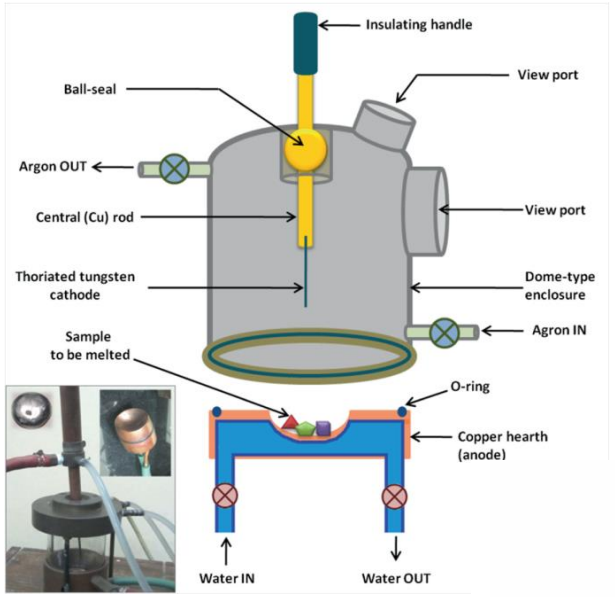
Synthesis and Characterizations

- *Comparative Study on Improving the Ball Mill Process Parameters Influencing on the Synthesis of Ultrafine Silica Sand: A Taguchi Coupled Optimization Technique Zahid Hussain International Journal of Precision Engineering and Manufacturing volume 22, pages679–688 (2021) Cite this article 446 Accesses 2 Citations Metrics*
- *Planetary Micro Mill PULVERISETTE 7 classic line / Description - fritsch.de (fritsch-international.com)*
- *Rubber Bellows for Mini Arc Melter MAM-1, Part 8258– MSE Supplies LLC*
- *Handbook on Synthesis Strategies for Advanced Materials pp 197–213Cite as*
- *Synthesis of Metallic Materials by Arc Melting Technique Dheeraj Jain, V. Sudarsan & A. K. Tyagi*

Ball Milling



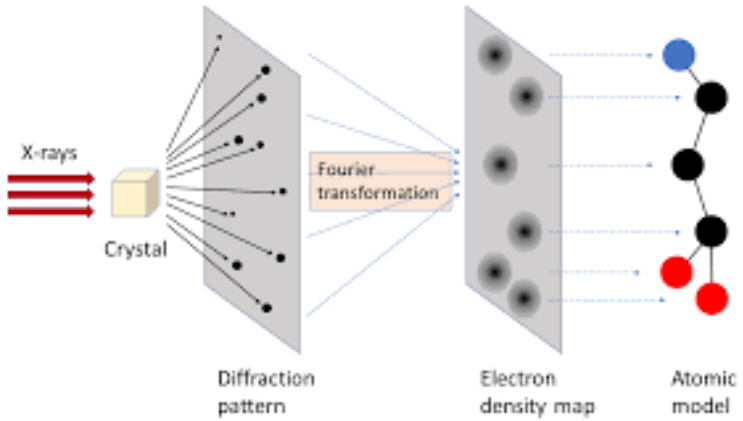
Arc-Melting



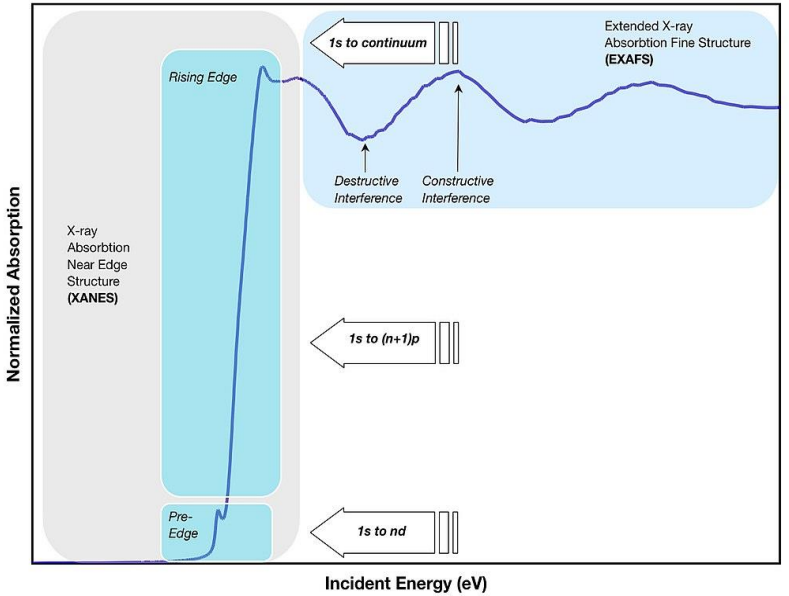
Synthesis and Characterizations

Tracing Crystallographic Structure with X-rays and neutrons

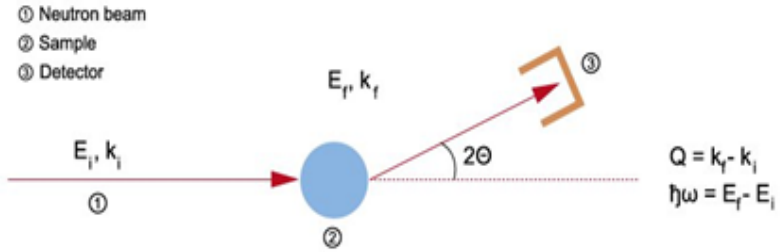
XRD (X-ray Diffraction)



X-ray Absorption Spectroscopy



Neutron Diffraction



- *XAS - Theory - Chemistry LibreTexts*
- *Single crystal X-Ray Diffraction (XRD) - Solid State Chemistry @Aalto - Aalto University Wiki*
- *Diffraction - Structural research - Techniques for ... - Neutron research - The NMI3 information portal*

Facilities/Collaborations

Synthesis

Characterization

Conclusion

- Current primary energy sources in the world are non-renewable and exhausting at a rapid rate.
- Search for alternative renewable, reliable and abundant energy sources are need of the society.
- H_2 is a big player for the past three decades but storage at practical environments and cost is challenging as H_2 is extremely light.
- H_2 storage in atomic form in metal-alloys have shown promise in the last decade.
- Problems like materials activation for H_2 absorption and air-resistance need to be solved.
- Main focus of this work: optimizing synthesis techniques of Titanium-iron (TiFe) metal-alloys and understanding its fundamental properties through different spectroscopic techniques.

THANKS