

Ab initio guided materials designing to enable hydrogen economy

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**Materials Science
and Engineering**



Process and Energy

Sustainable life cycle of materials



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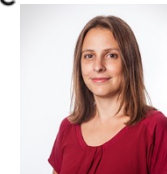
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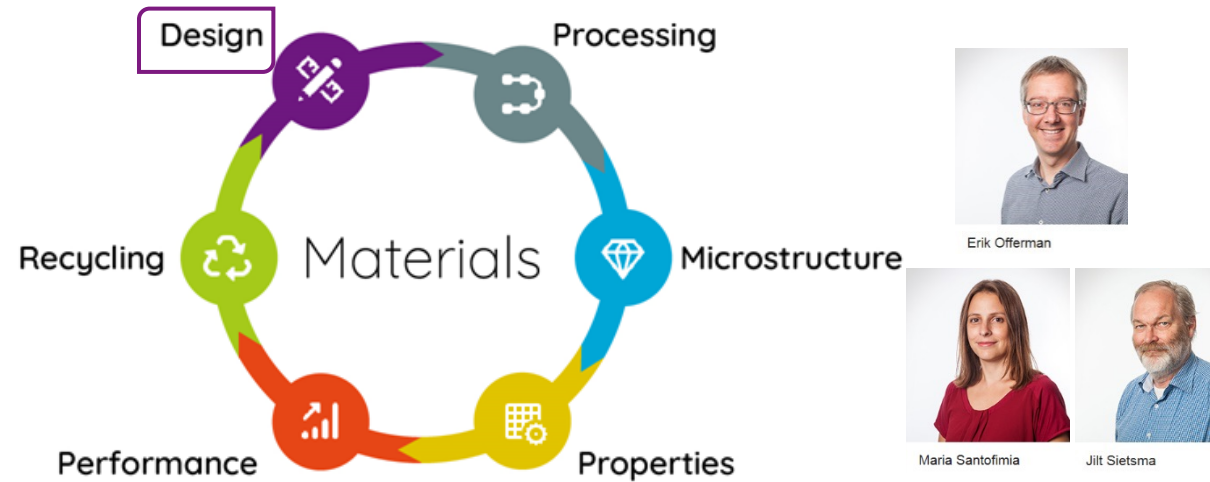
Matthias Alfeld



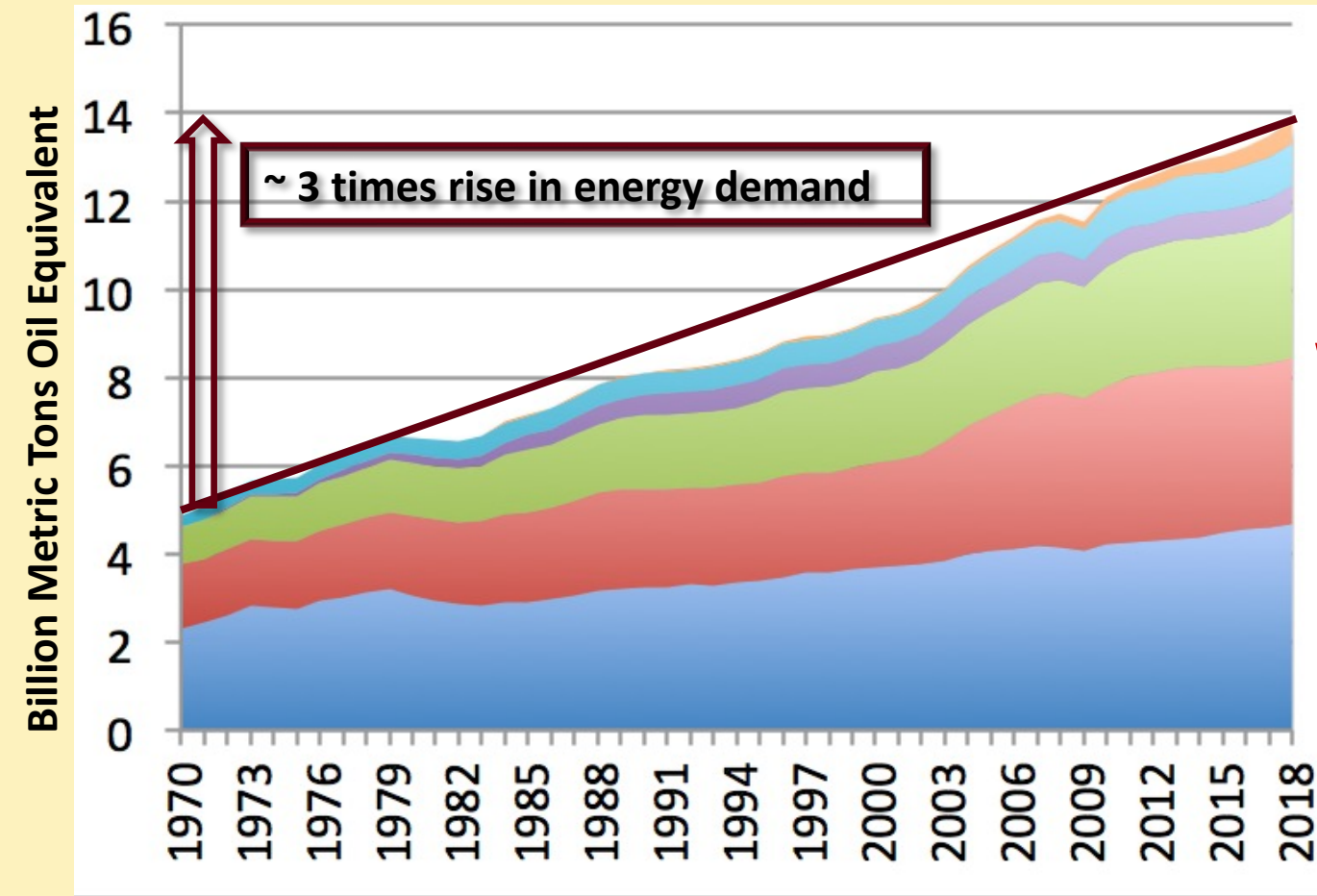
Vera Popovich



Amarante Böttger



World Energy Consumption (BP Statistical Review of World Energy)



What is the need of the hour?

Transition to sustainable sources of energy



Hydrogen Energy

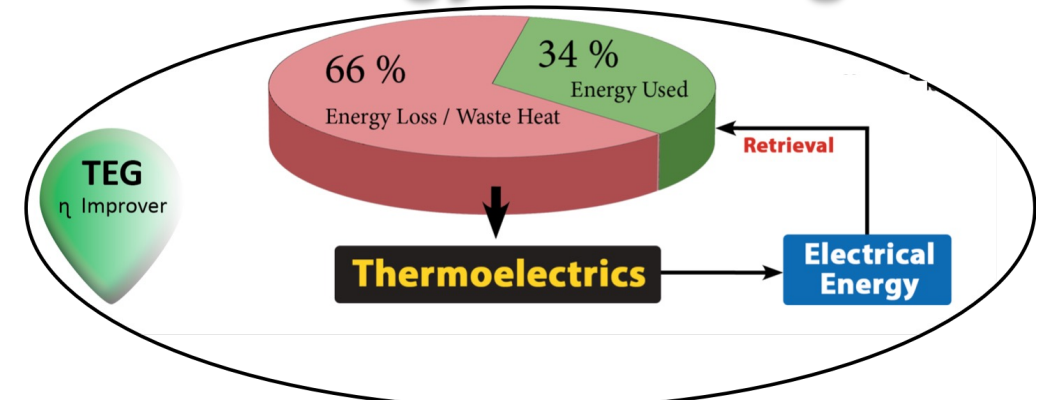


Storage & Transport

Research challenges?



Thermoelectricity – energy & cooling



<https://prometeon.it/advanced-clean-technologies-tech-chip/>

Heat to energy conversion

Hydrogen Embrittlement (HE)....

West Berlin Congress Hall, 1980



Hydrogen intake causing collapse of roof

San Francisco-Oakland Bay Bridge, 2013



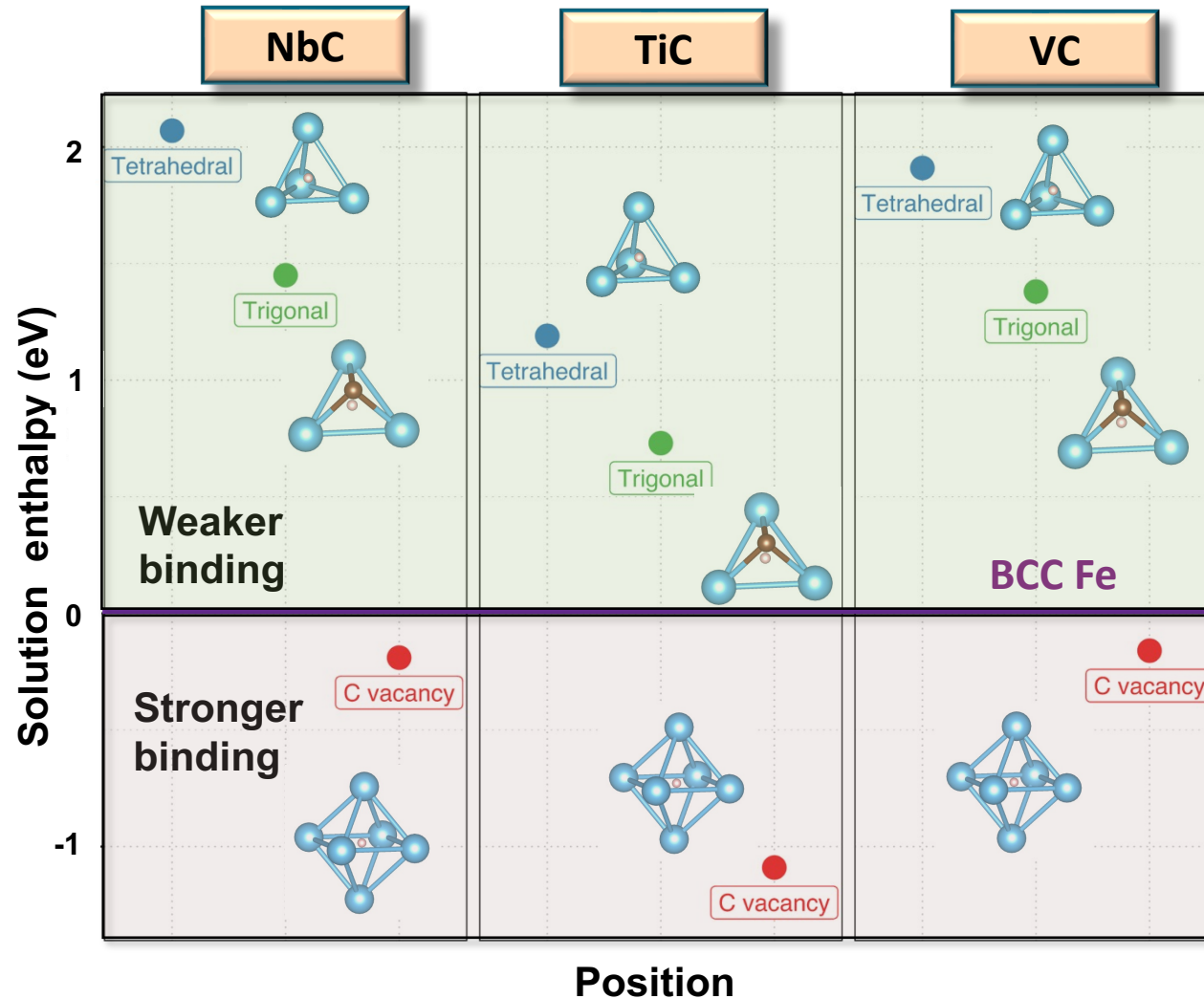
Brittle bolts and cracking due to hydrogen contamination

....big threat!

COMPARATIVE DFT STUDY: H TRAPPING



Mr. Saurabh Sagar



➤ Negative solution enthalpy means H dissolution from Fe into carbide is exothermic

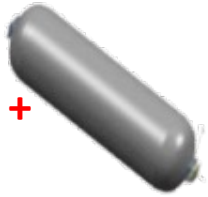
➤ Dissolution in interstitial sites endothermic - trigonal site favoured over tetrahedral site

➤ Strong binding at C vacancy sites - Comparable solution enthalpies for NbC and VC and exceptionally high for TiC

H STORAGE

Physical-based

Compressed Gas



High cost +
Low VD

Cold/Cryo Compressed



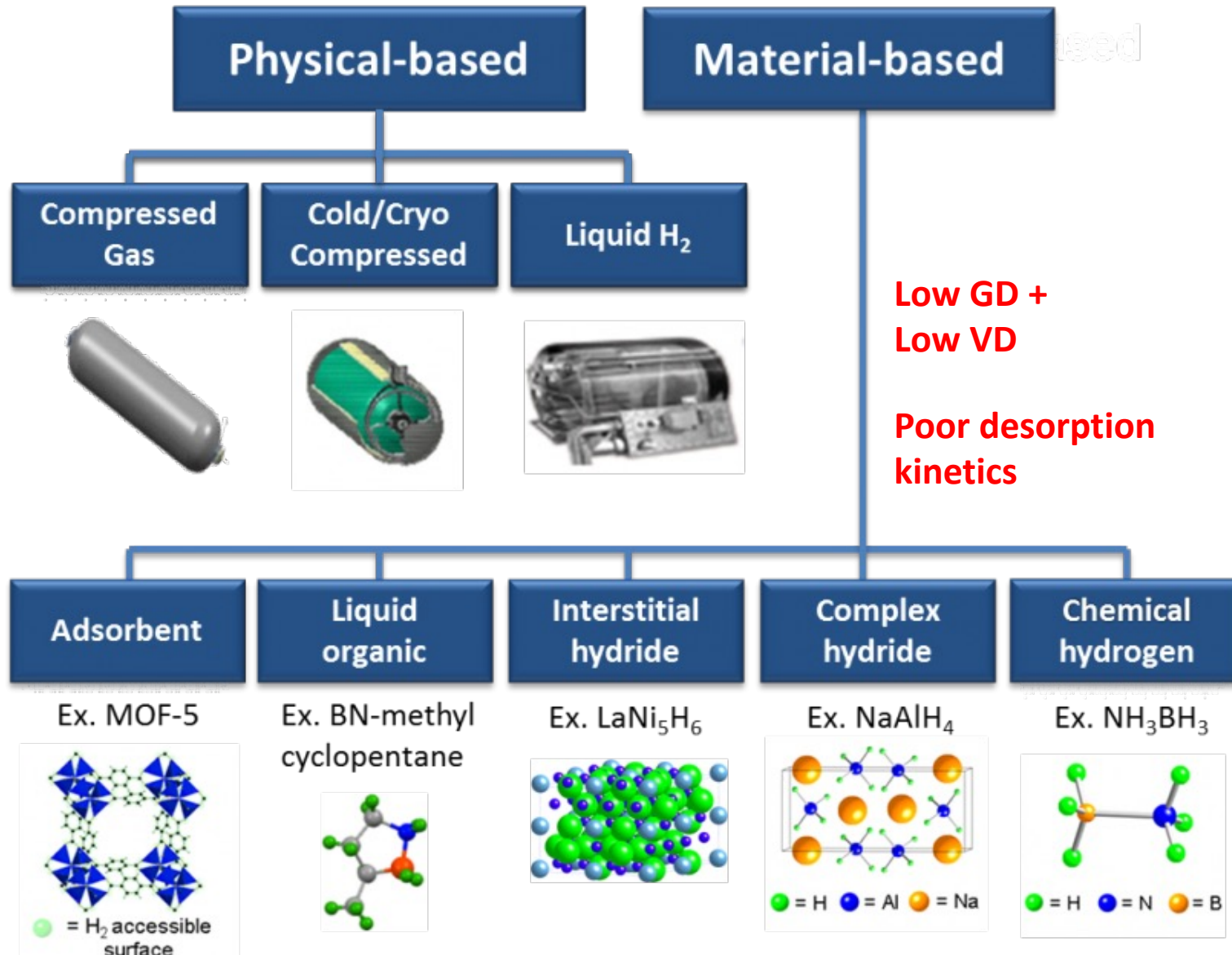
High cost +
boiling off

Liquid H₂

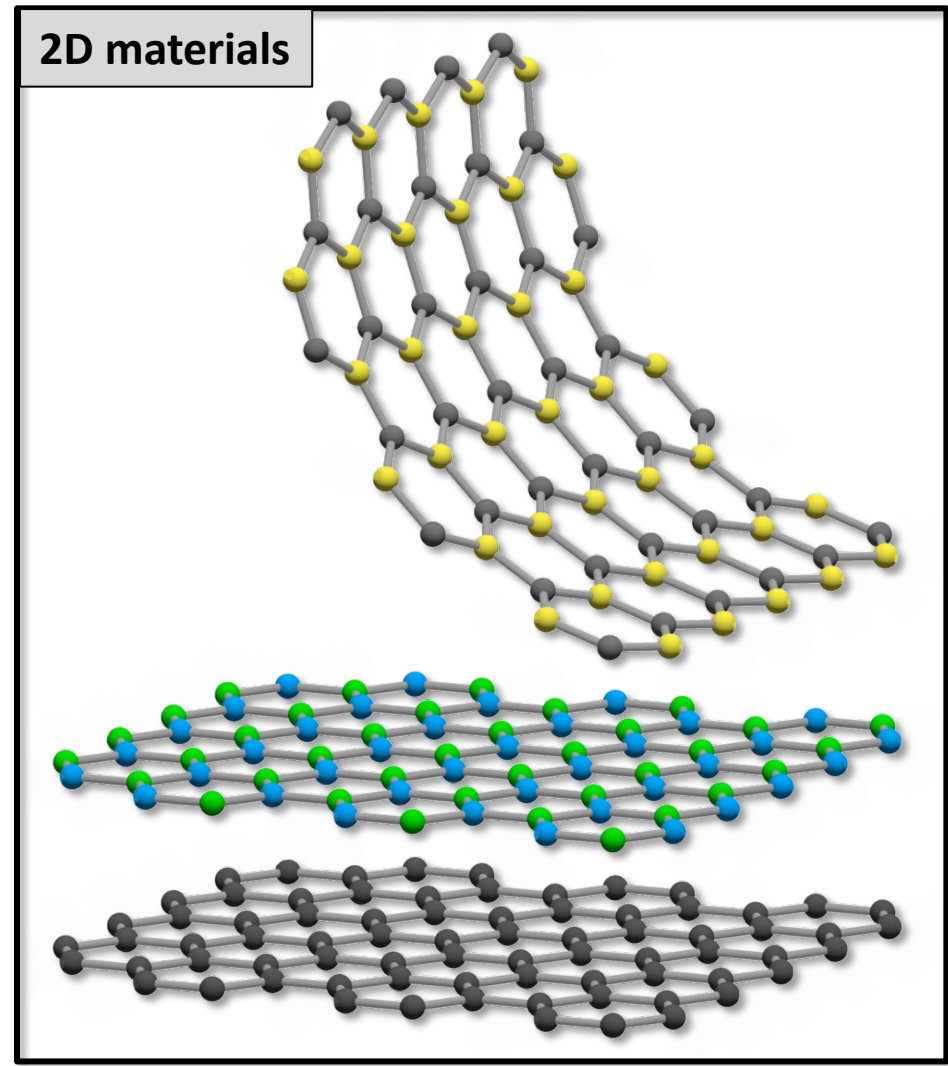
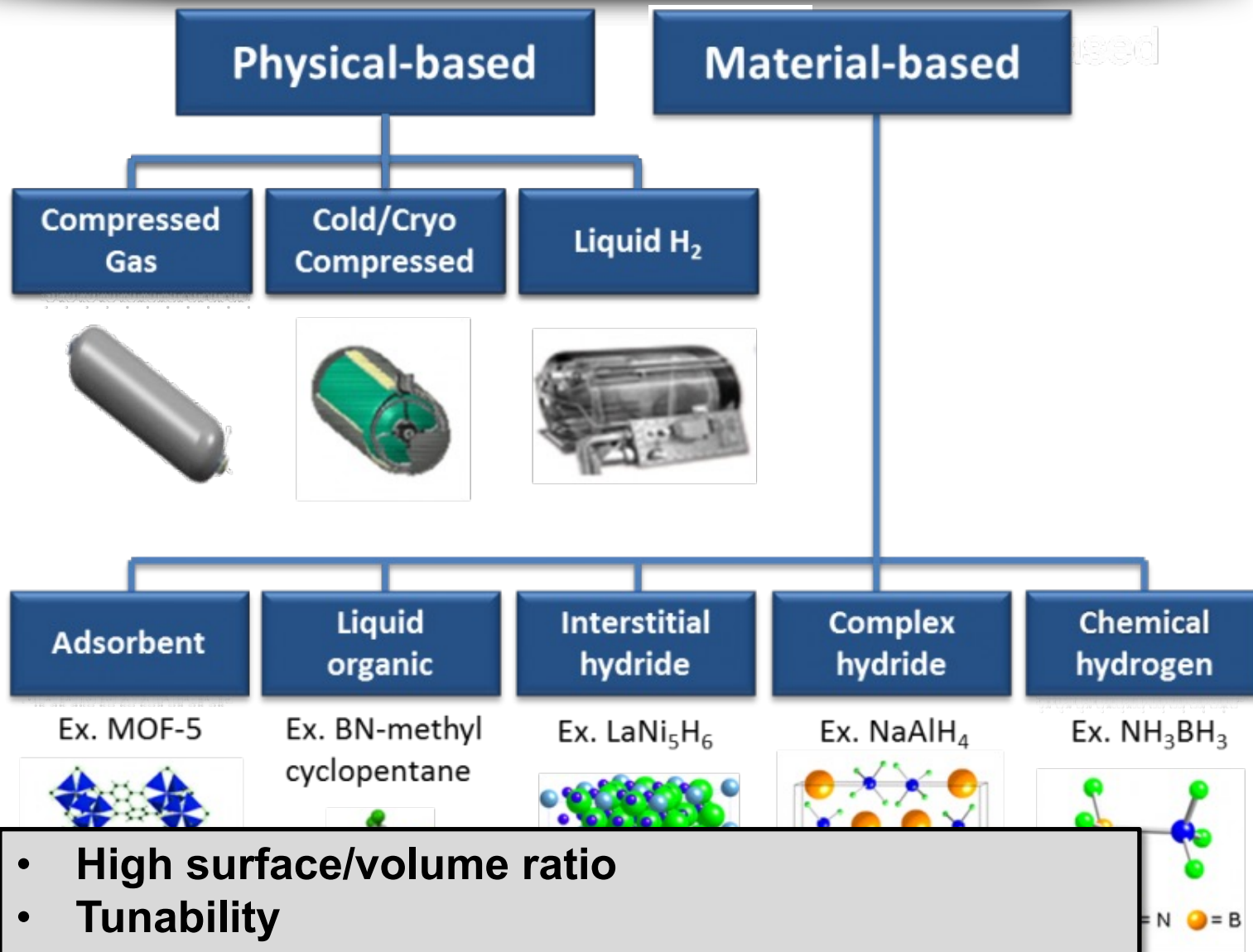


Cryogenic
temperature

H STORAGE



H STORAGE



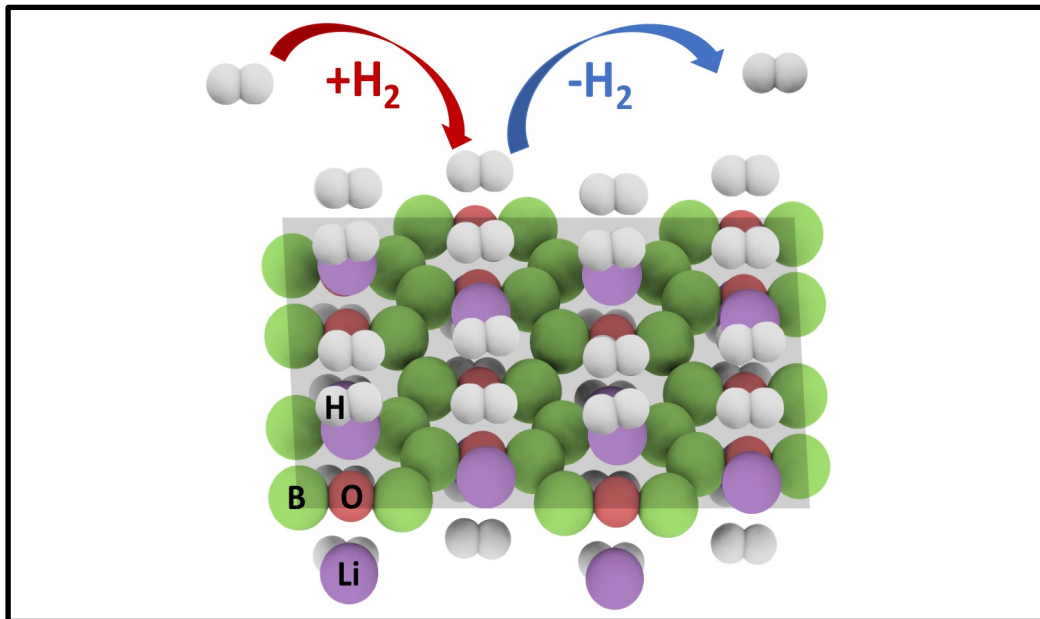
- High surface/volume ratio
- Tunability
- Promising for both chemisorption/physisorption



Mr. Parsa Habibi

BOROPHENE OXIDE WITH LITHIUM

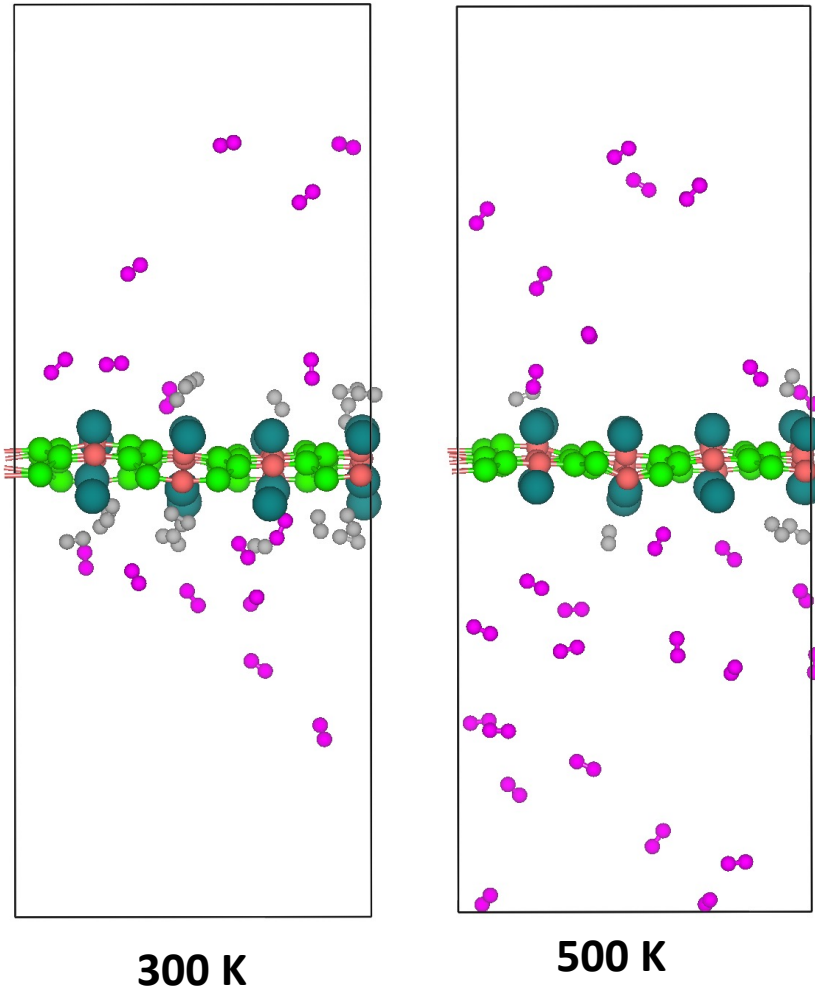
- Each Li binds to two H₂ molecules – average binding energy of -0.24 eV/H₂



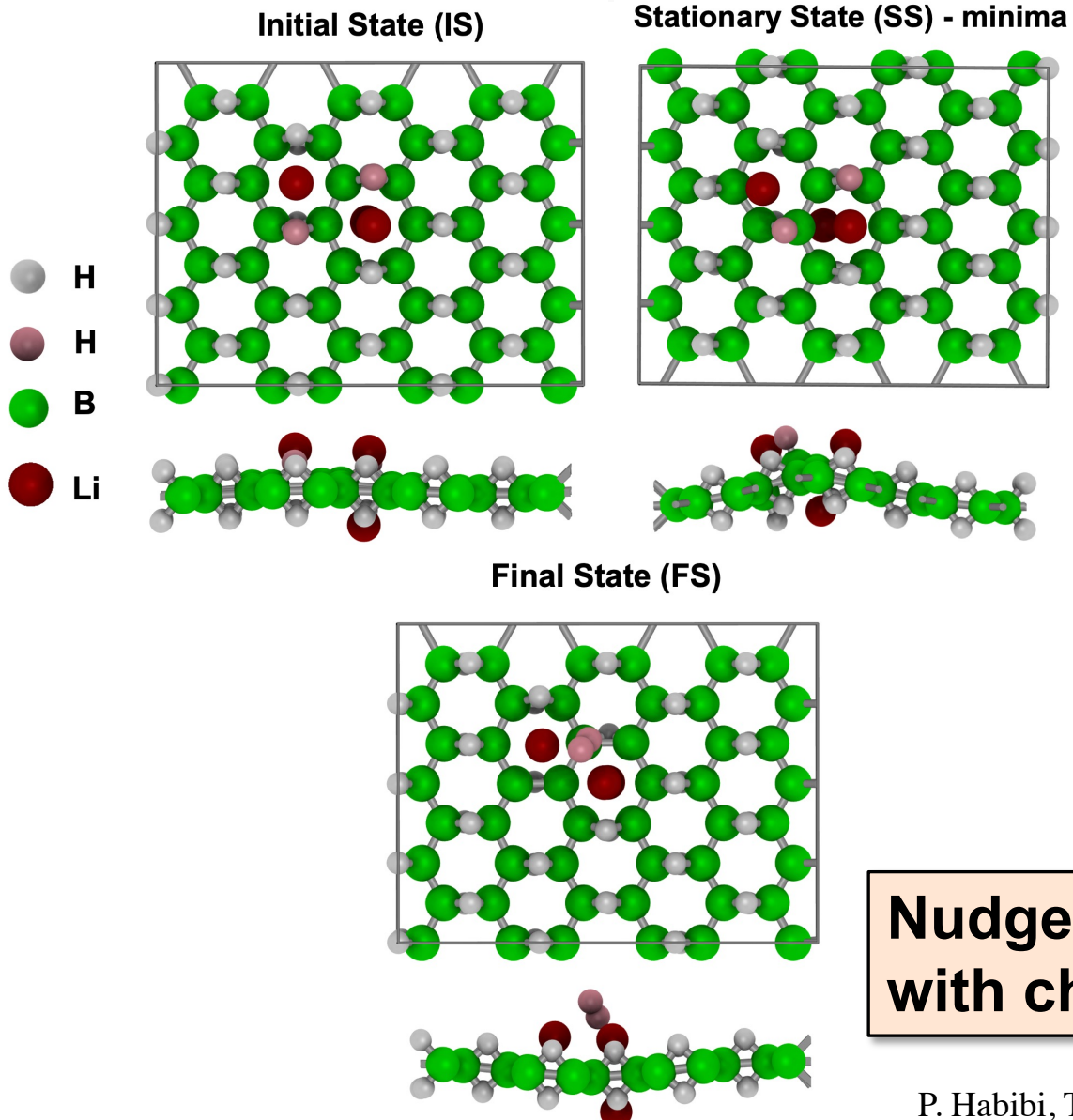
AB-INITIO MD: T DEPENDENT H DESORPTION



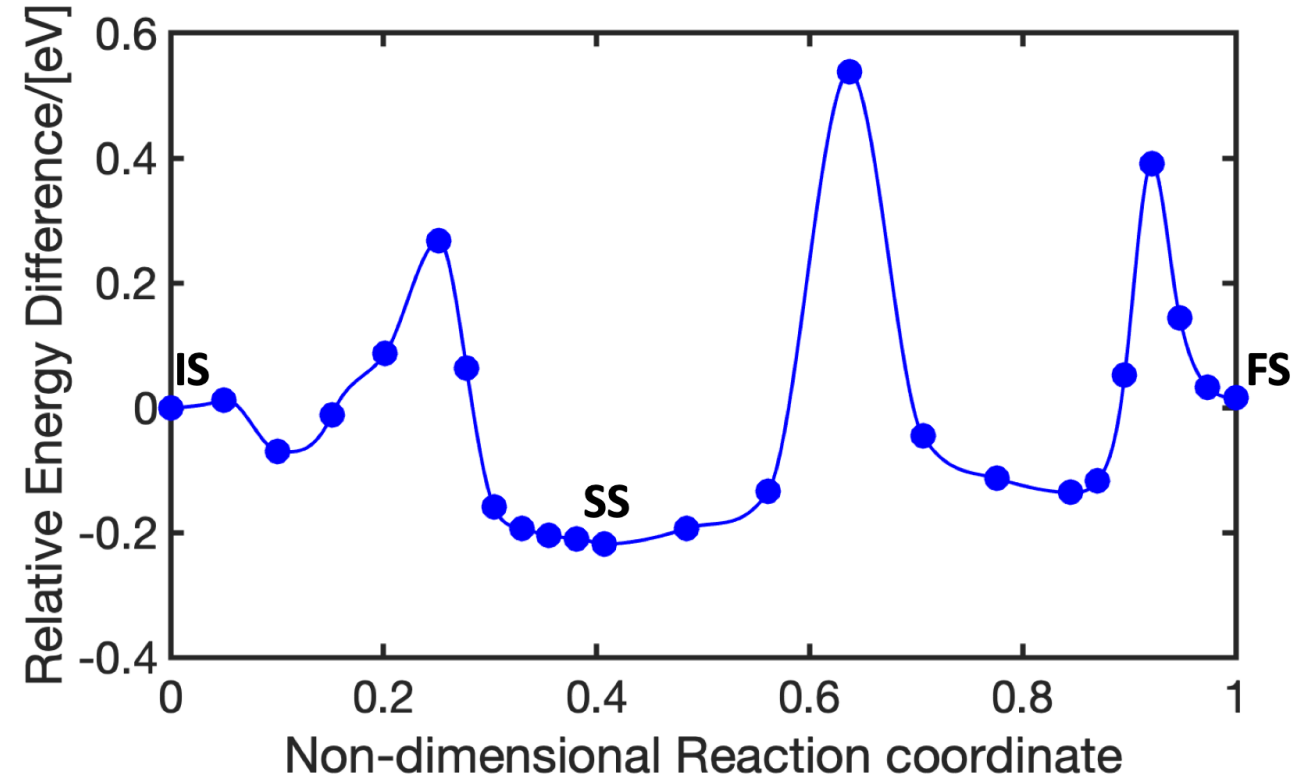
Mr. Parsa Habibi



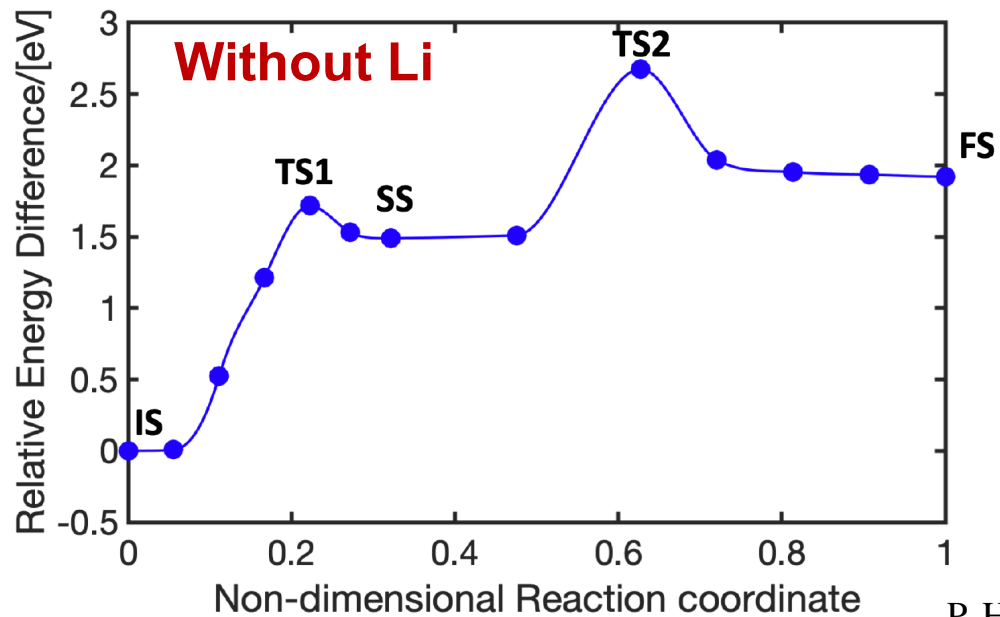
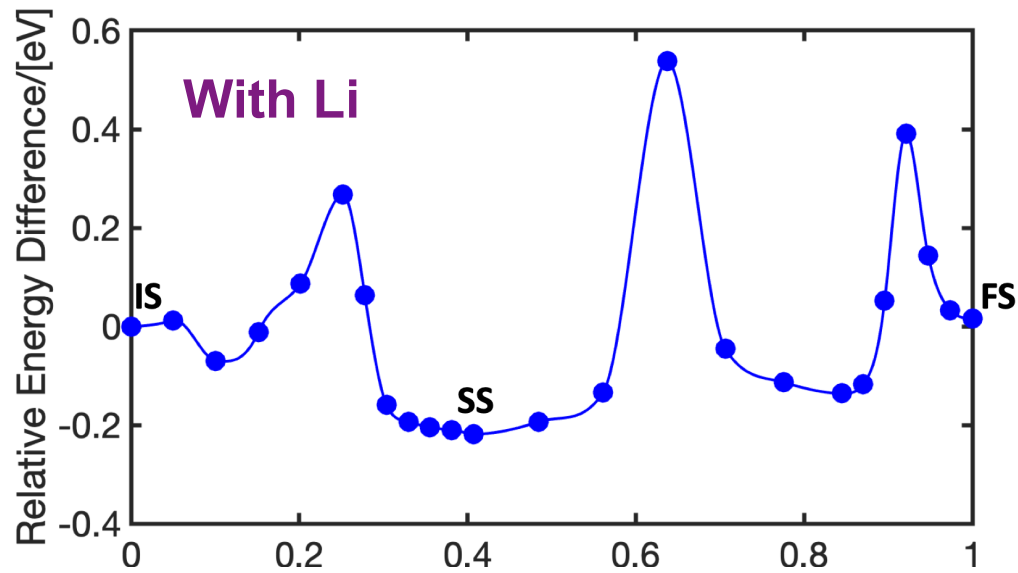
- Each Li binds to two H₂ molecules – average binding energy of -0.24 eV/H₂
- Structural stability tested at temperatures of 200, 300, 400 and 500K
- H₂ bound by van der Waals forces - structure does not undergo irreversible changes
- 53% of H₂ still bound at 300K - 19% bound at 400K



BOROPHENE HYDRIDE WITH LITHIUM



Nudged Elastic Band - Energy barriers associated with chemisorption

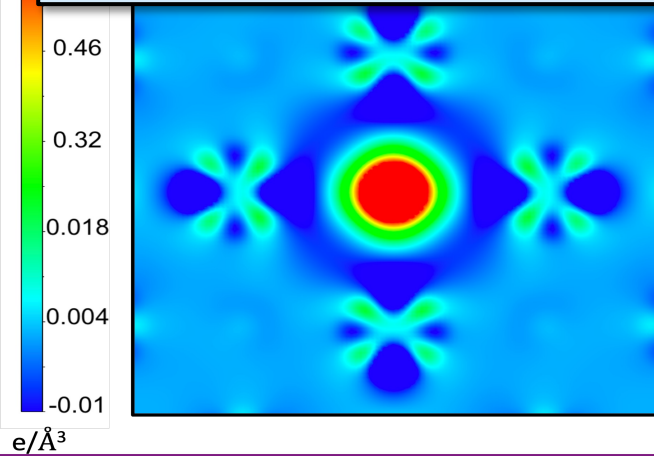


- **Complex potential energy landscape due to the addition of Li**
- **Energy barrier for dehydrogenation reduced significantly in presence of Li**
- **Li weakens the electron deficient 3-center 2 electron bond present in B-H-B**

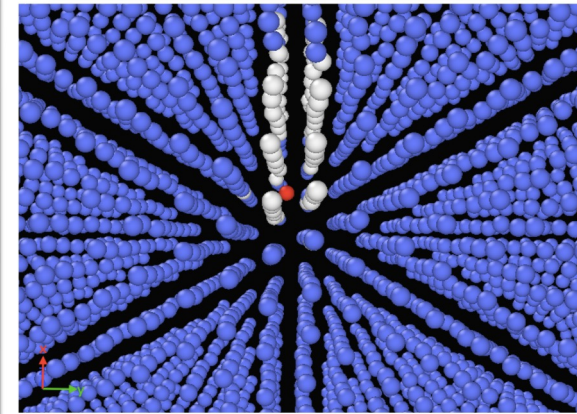
Enhanced adsorption/desorption kinetics by tuning the Li-loading

SUMMARY

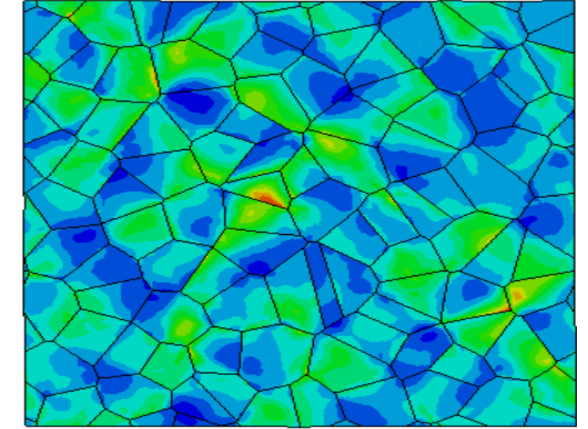
Density Functional Theory



Molecular Dynamics



Crystal Plasticity



- Atomistic insights into H interaction with microstructure to resist HE
- Atomistic insights into surface-H interaction for safe and efficient storage

Multi-scale methodology to understand processes related to energy harvesting

TEAM



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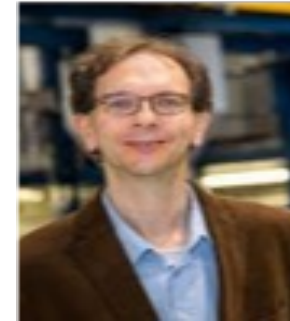
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