Multi-Scale Modelling of the TiFe-H system for Hydrogen Storage

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Summary

Fully understanding the properties of hydrogen-metal systems requires to study them on different length and time scales. Even though there are experimental methods available to perform these studies, corresponding multi-scale modelling can help to disentangle the influence of different effects and predict properties that are difficult to measure. Here, we present our recent work on modelling the TiFe-H system. Starting from the atomic scale, the properties of the relevant bulk phases are determined with Density Functional Theory (DFT). Automated workflows and Ab-initio molecular dynamics (AIMD) allow us to obtain a more realistic picture for models on larger scales. Studying processes at interfaces reveals kinetic barriers and favorable growth directions. Finally, the insights from lower scales are combined in thermodynamic models, which are employed in meso-scale simulations, describing the microstructure evolution during hydrogenation.

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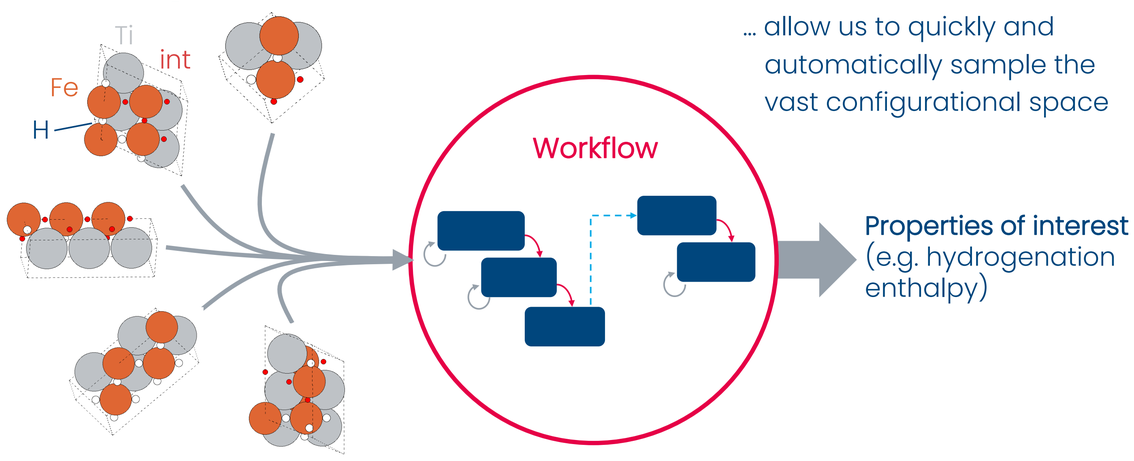
Computational Workflows



… allow us to quickly and automatically sample the vast configurational space

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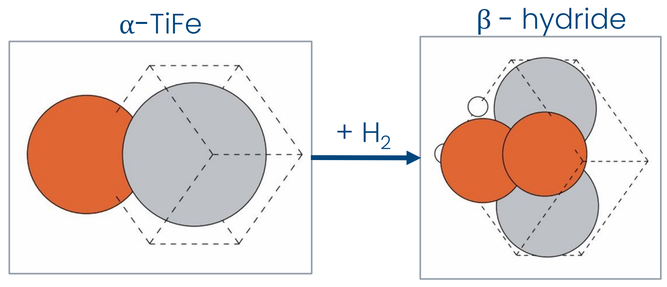
Properties of the Bulk Phases

DFT calculations

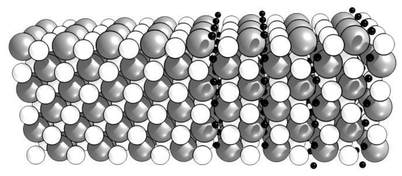
Access to basic properties:
- Hydrogenation enthalpy
- Volume change
- Bulk modulus
- Electronic structure



Modelling of Interfaces

TiFe – hydride interface

- Very coherent interface with the hydride
- Interface energy vs orientation gives preferred growth direction



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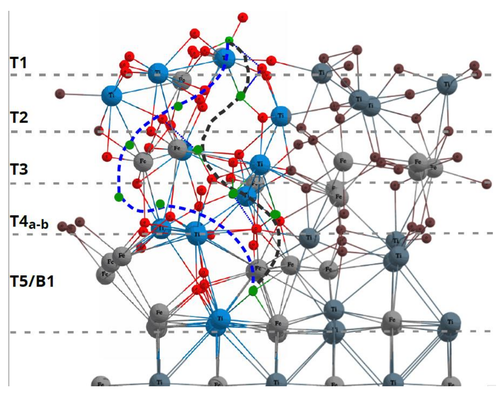
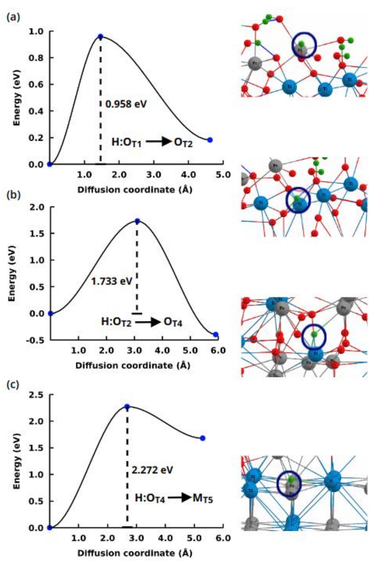
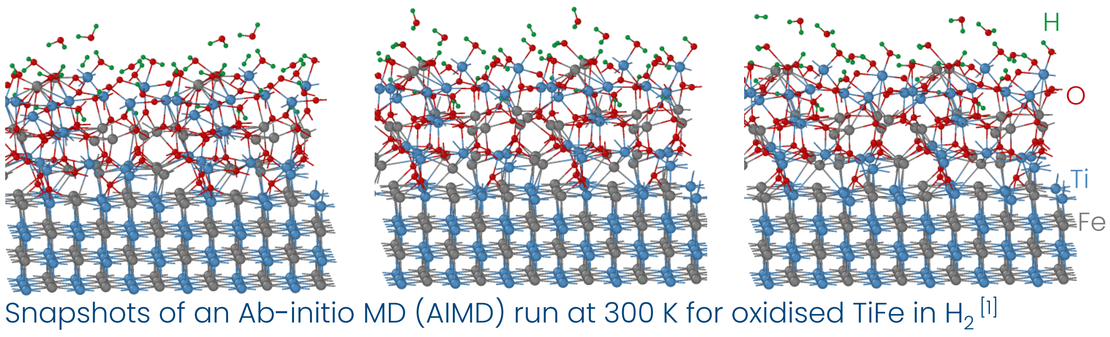
TiFe – oxide interface[1]

- Amorphous oxide layer is formed
- Oxide is large barrier for hydrogen migration
- Layer needs to be cracked, e.g. thermally [2]





Insights from Molecular Dynamics



Snapshots of an Ab-initio MD (AIMD) run at 300 K for oxidised TiFe in H_2 [1]

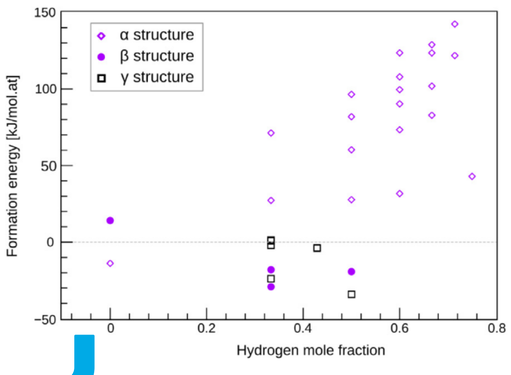
- First oxide layer hydroxylates and impedes further adsorption of hydrogen
- Large migration barriers inhibit movement of hydrogen to subsurface layers

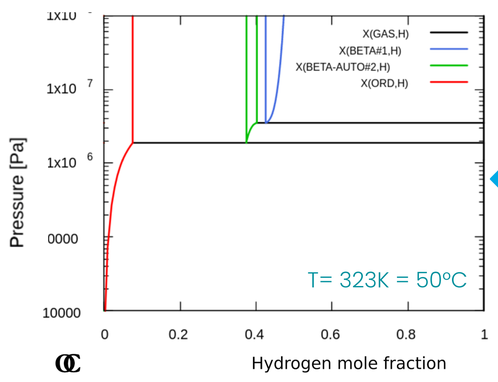
Breaking scale limitations of AIMD with machine learning

see poster by A. Santhosh

Thermodynamic modelling

- DFT gives access to energies of unstable structures
- Possible to disentangle chemical and strain contributions





Combination of DFT and experimental data leads to improved thermodynamic model [3]

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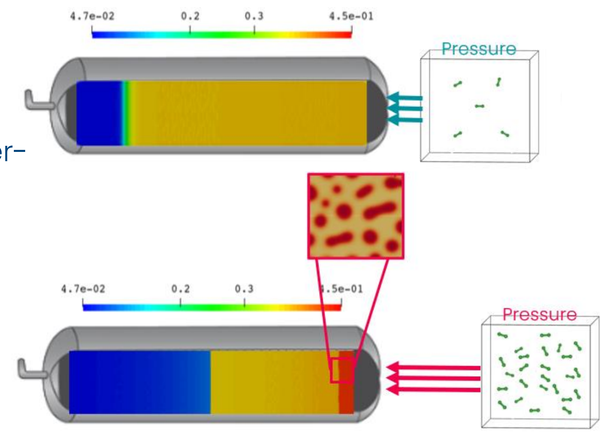
Mesoscale simulations

- Microstructure modelling based on thermodynamic model
- Additional parameters (e.g. inter-face energies, diffusion rates) determined experimentally or computationally
- Large pressure gradients can slow down kinetics due to shielding effect



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[1] A. Santhosh et al., preprint on ChemRxiv (to be published in a journal soon), doi: 10.26434/chemrxiv-2023-7zhj3
[2] D. M. Dreistadt et al., Journal of Alloys and Compounds 919 (2022), 165847, doi: 10.1016/j.jallcom.2022.165847
[3] E. Alvares et al., Calphad 77 (2022), 102426, doi: 10.1016/j.calphad.2022.102426

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