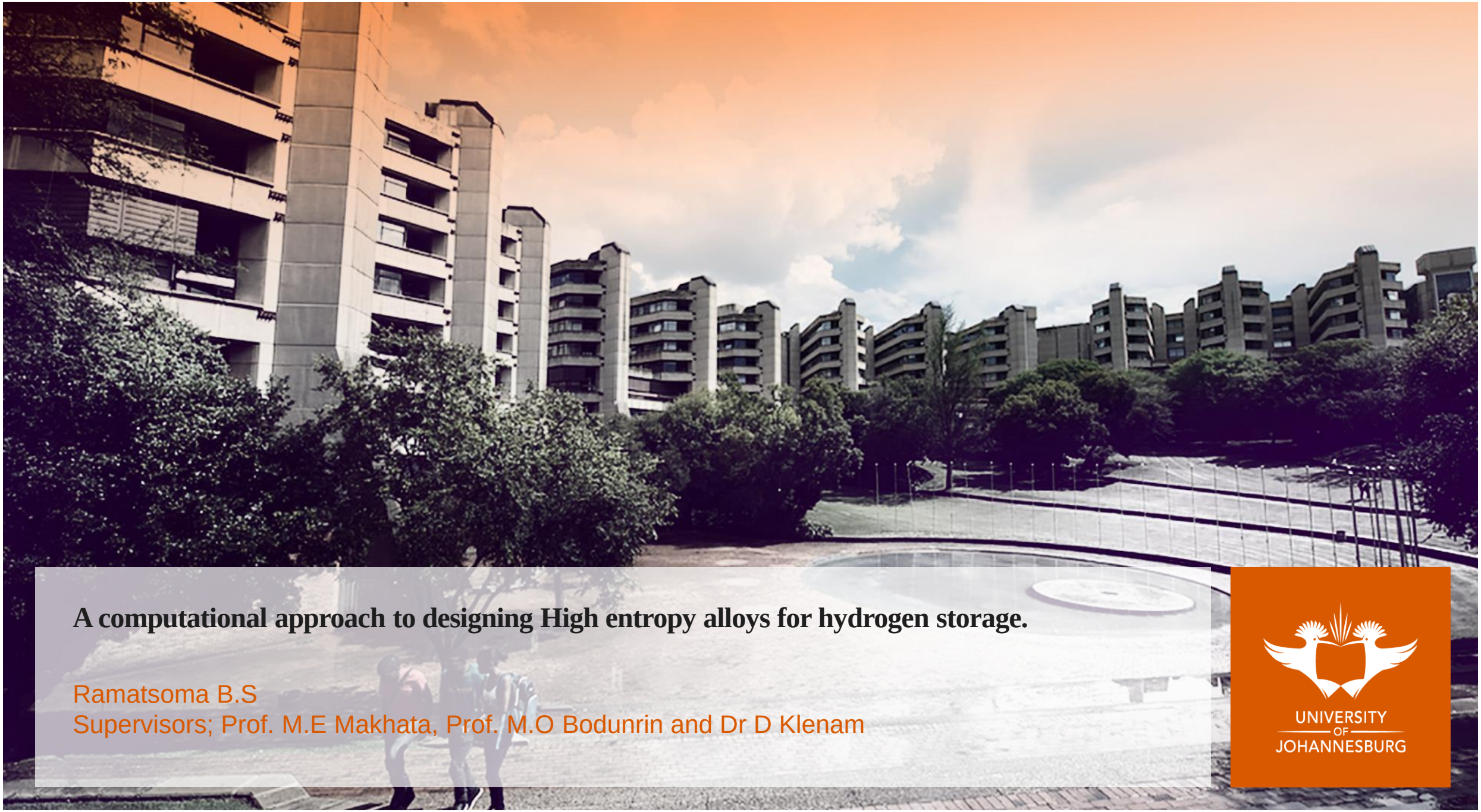

A computational approach to designing High entropy alloys for hydrogen storage.

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UNIVERSITY OF JOHANNESBURG

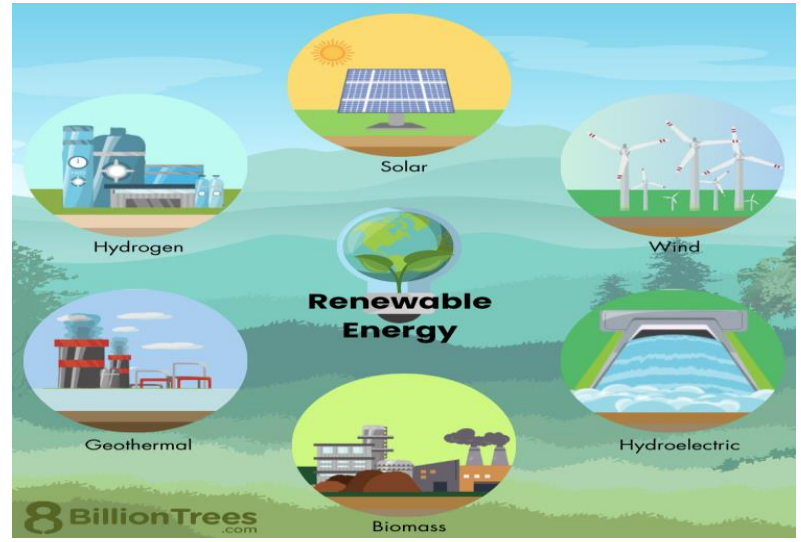
TIME TO GO GREEN

GREENHOUSE GASES

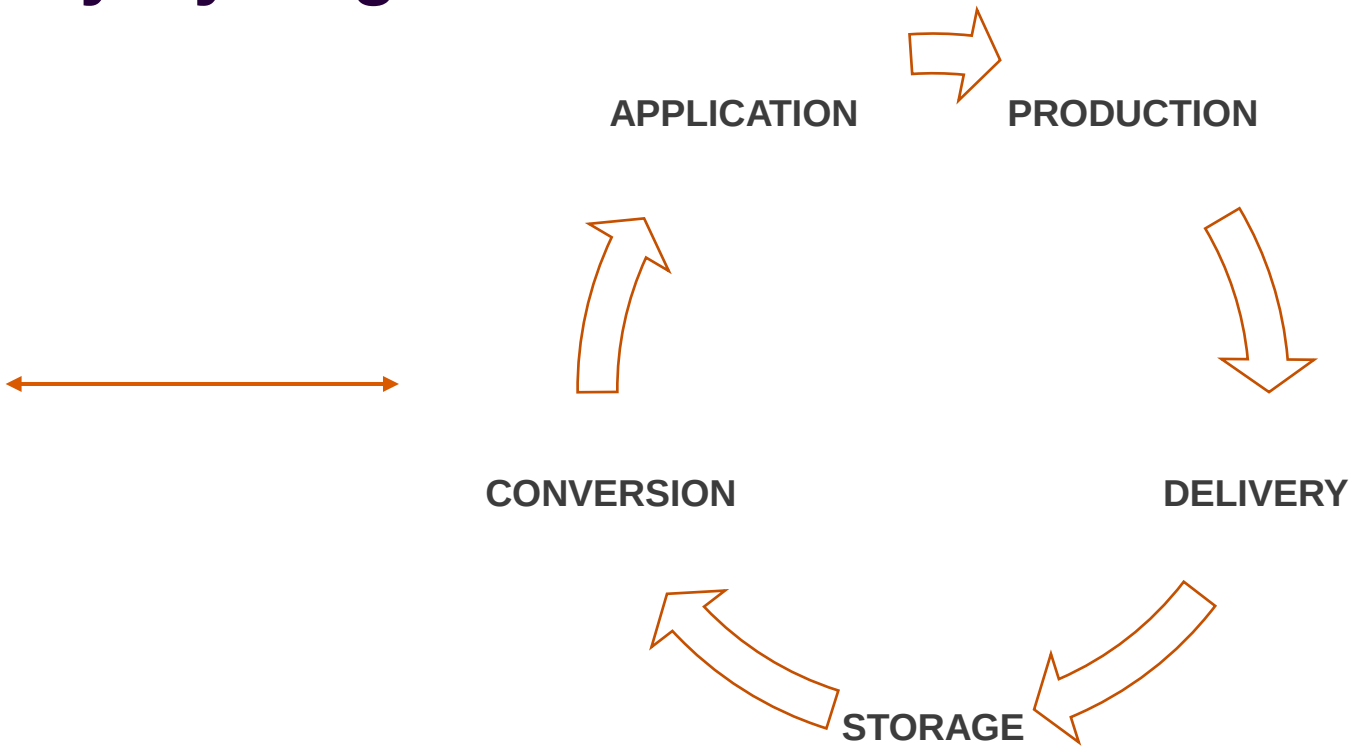
CLIMATE CHANGE

RENEWABLE ENERGY

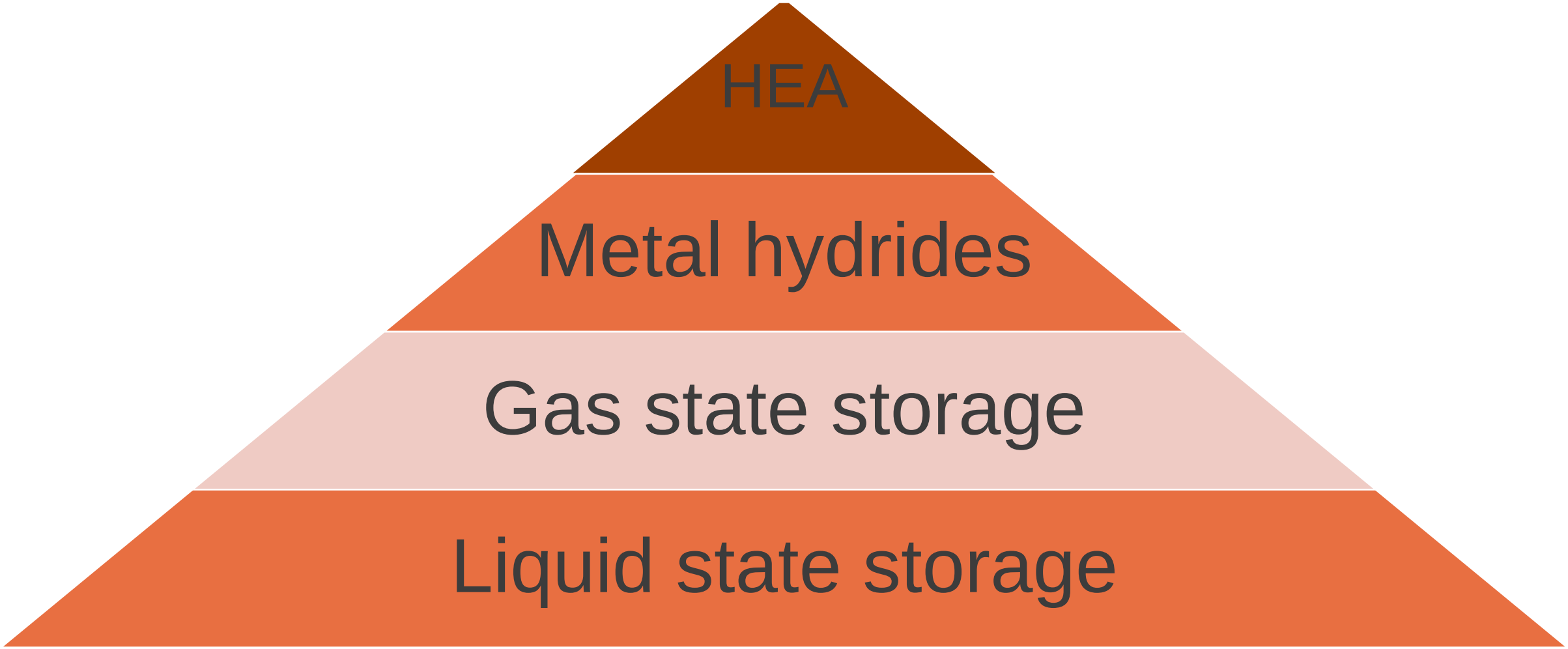
- Fawzy *et al*, 2020



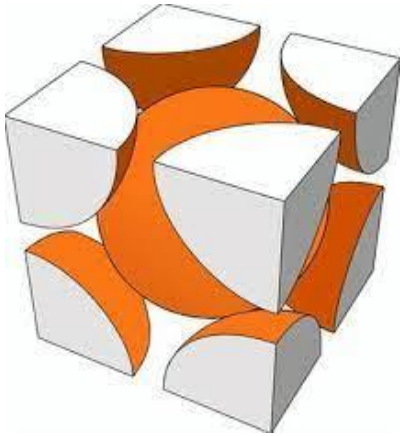
Why Hydrogen?



Why High entropy alloys?

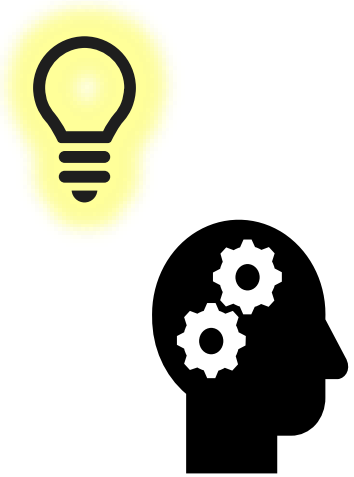


High entropy metal hydrides

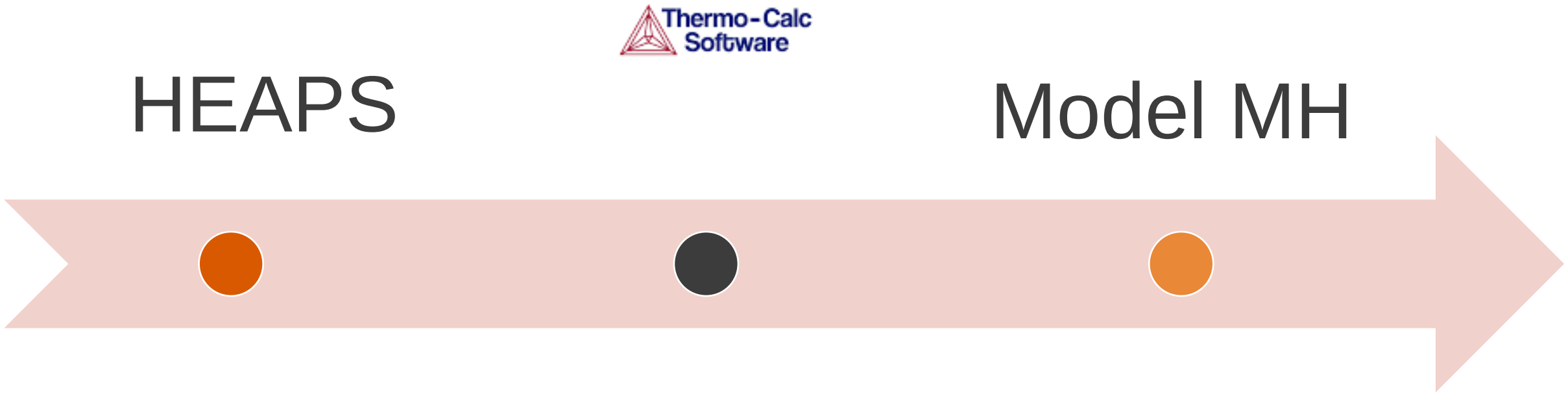


Alloys	wt%	Author
TiZrFeMnCrV	1.80 wt.%	Chen et al., 2022
TiZrNbFeNi & $Ti_{20}Zr_{20}Nb_5Fe_{40}Ni_{15}$	1.64wt% & 1.38wt% respectively	Floriano et al., 2020
$Ti_{27.5}V_{27.5}Nb_{20}Cr_{12.5}Mn_{12.5}$	3.38 wt%	Serrano et al., 2023
$Mg_{0.10}Ti_{0.30}V_{0.25}Zr_{0.10}Nb_{0.25}$	2.7 wt.%	Montero, Sahlberg & Zlotea, 2021
$Ti_{0.30}V_{0.25}Zr_{0.10}Nb_{0.25}Mo_{0.10}$	2.8 wt.%	Bouzidi et al., 2021
$Ti_{0.30}V_{0.25}Cr_{0.10}Zr_{0.10}Nb_{0.25}$	3.0 wt.%	Bouzidi et al., 2022
$Ti_4V_3NbCr_2$	3.7 wt%	Chen et al., 2023

Importance of Computational modelling of metal hydrides



Modelling Tools



Approach

HEAPS

- Calculate thermodynamic properties of HEAs

Thermo-calc

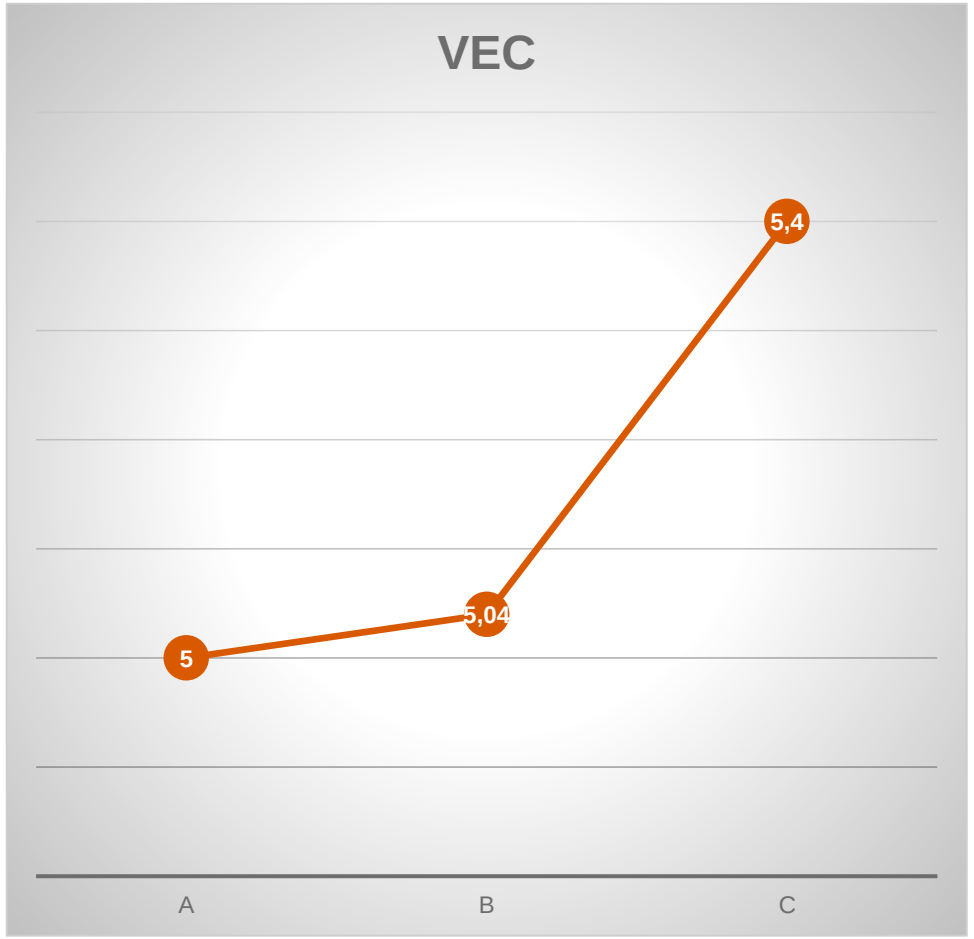
- Calculate Phases of HEAs

Model MH

- Simulate hydrogen storage capacity

Importance of Valence electron concentration in HEA metal hydrides

ALLOY	COMPOSITION
A	$Ti_{25}V_{25}Nb_{25}Cr_{25}$
B	$Ti_{32}V_{26}Nb_{16}Cr_{17}Mn_{9}$
F	$Ti_{20}V_{20}Nb_{20}Cr_{20}Fe_{10}Mn_{10}$



Impact on thermodynamic properties on hydride formation

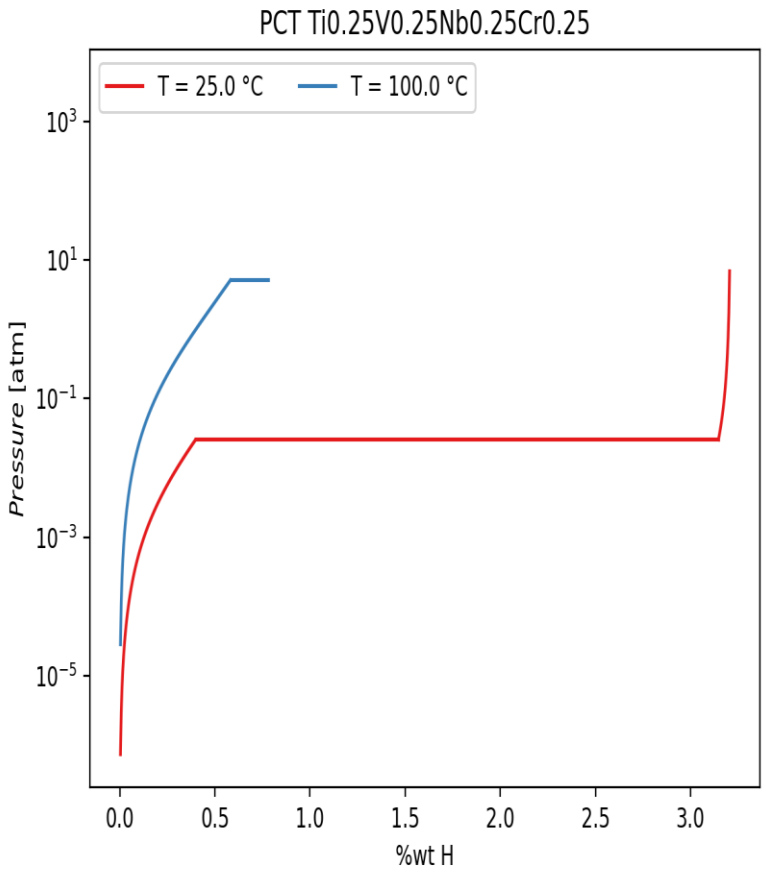
ALLOY	COMPOSITION	VEC	ΔH^{ic} (kJ·mol^{-1})	S^{xs} (bcc) (J·mol^{-1}·K^{-1})
A	$Ti_{25}V_{25}Nb_{25}Cr_{25}$	5	-6.39	-0.85713
B	$Ti_{32}V_{26}Nb_{16}Cr_{17}Mn_{9}$	5.04	-10.6	-0.7545
C	$Ti_{20}V_{20}Nb_{20}Cr_{20}Fe_{10}Mn_{10}$	5.5	-15.78	-0.86654

Phase fraction Of HEA metal hydrides

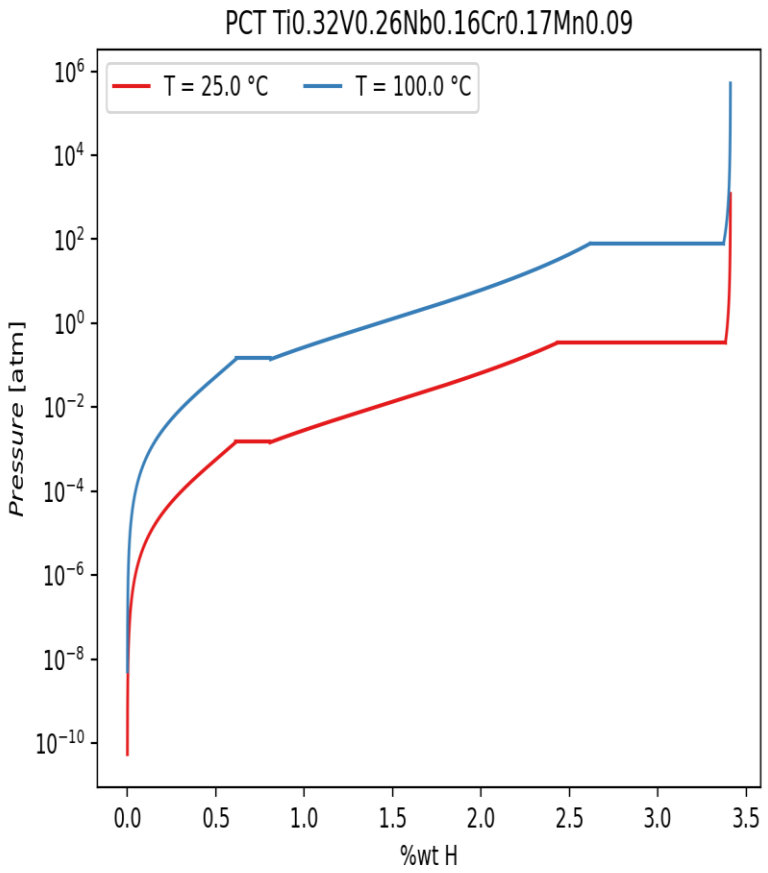
Sample	Temperature (ºC)	BCC (%)	Laves phase (%)	HCP (%)
A	25	54.3	20.7	24.9
	400	68.6	12.5	18.8
B	400	68.5	18.8	12.7
C	25	60.1	30.9	9
	400	68.9	31.1	0

PCT results

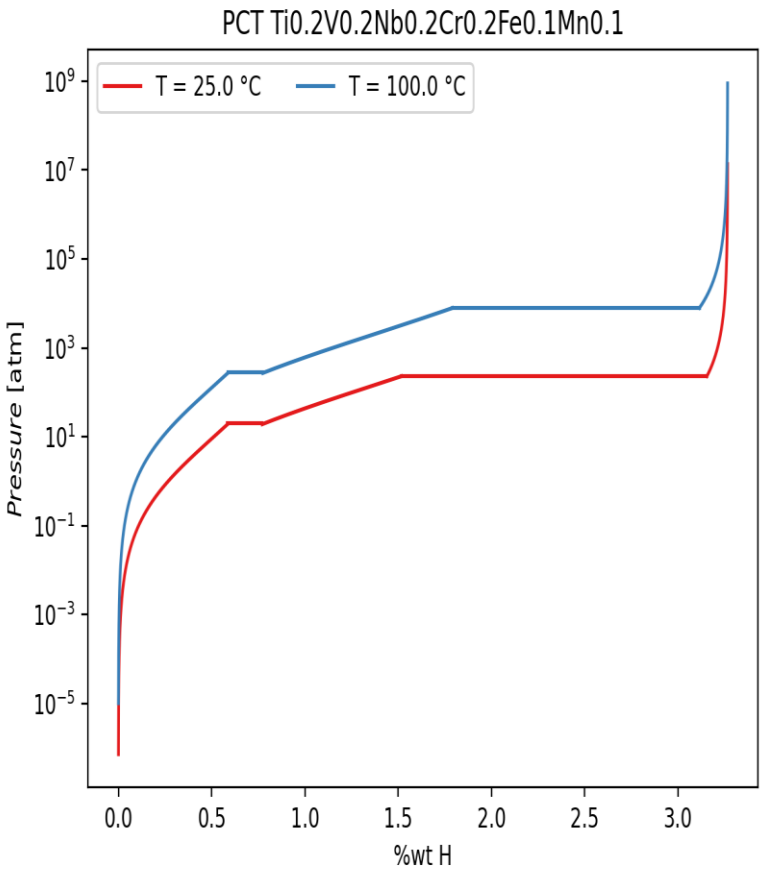
A



B



C



Conclusion

- **Key Findings**:
  - The HEA alloys demonstrated a hydrogen storage capacity exceeding **3 wt%** at room temperature and various pressures while B showed the best storage capacity exceeding **3.5 wt%.**
  - The computational approach significantly reduced reliance on traditional trial-and-error methods, saving time and costs.
- **Advantages of Computational Approach**:
  - Enables prediction and optimisation of hydrogen storage properties before experimental work.
  - Streamlines alloy development and allows targeted exploration of new materials.
  - Simulates and refines hydrogen absorption/desorption behaviours of HEA alloys.
- **Future Applications**:
  - Validate computational data with experimental work.
  - The computational methods can be extended to other HEA metal hydrides.

Acknowledgements

1. Supervisors; Prof. M.E Makhata, Prof. M.O Bodunrin and Dr D Klenam

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Thank you

Any Questions?

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