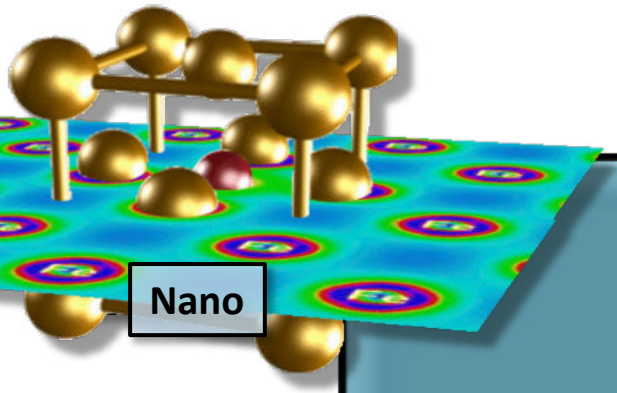
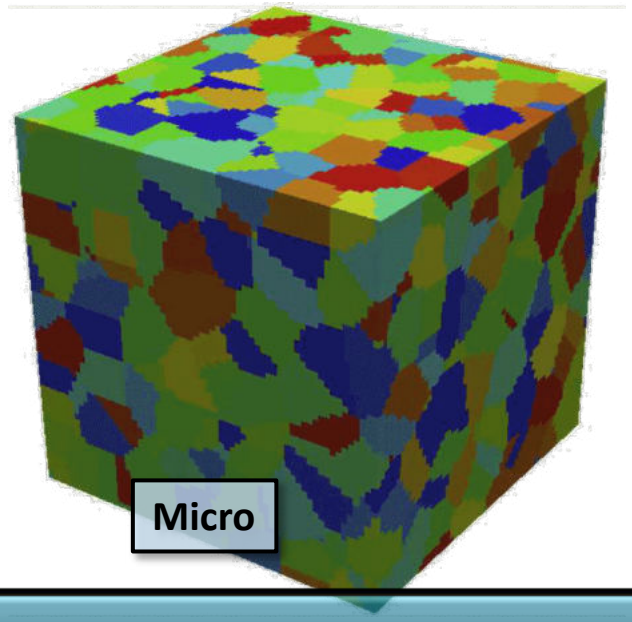
Computation-guided materials designing for sustainable & renewable energy applications



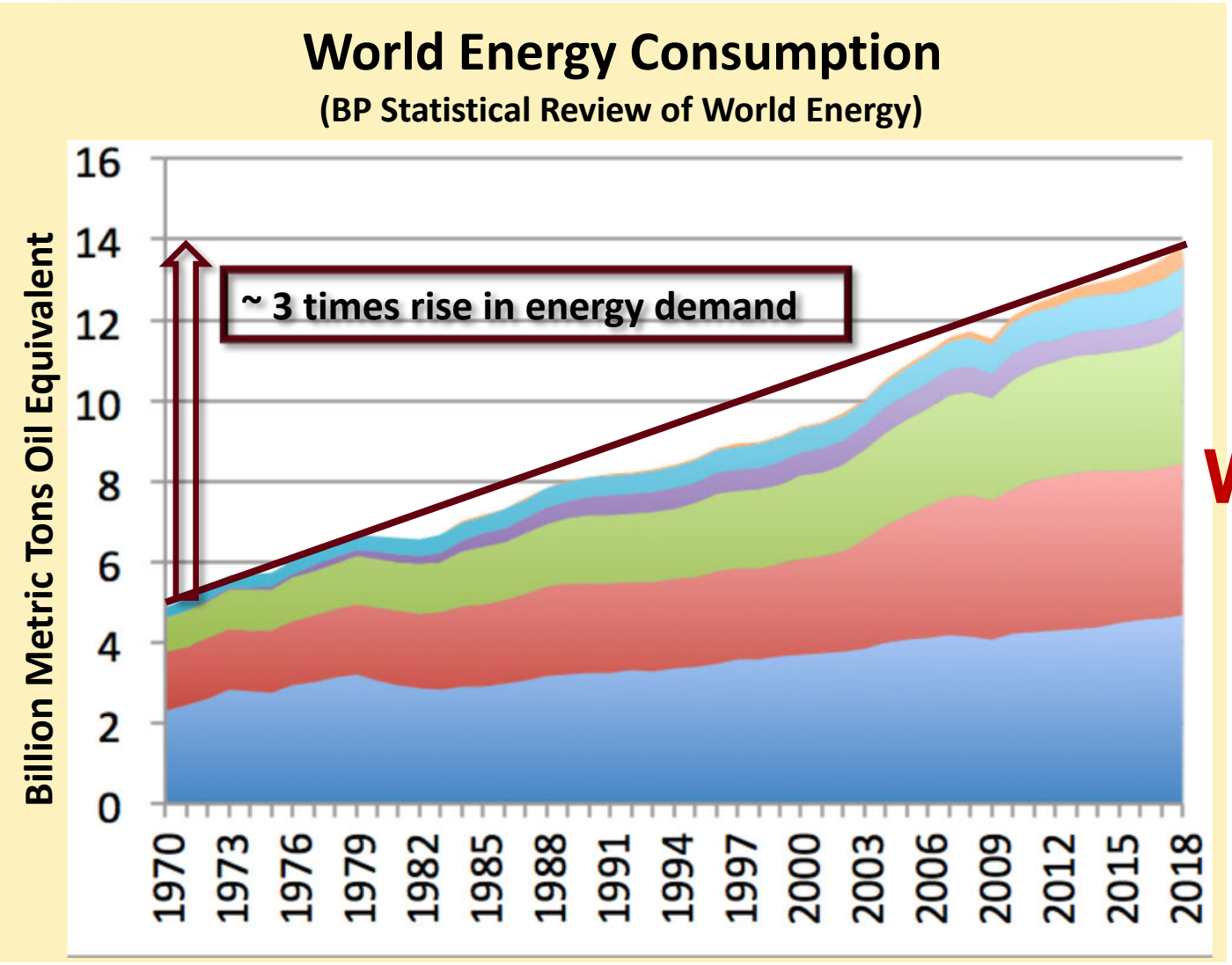


Poulumi Dey

Materials Science and Engineering

TU Delft

Rising Global Energy Demand



What is the need of the hour?

D. Vuuren *et al.*, Nat. Sustain. **2**, 1132 (2019)

SUSTAINABLE SOURCES

TU Delft

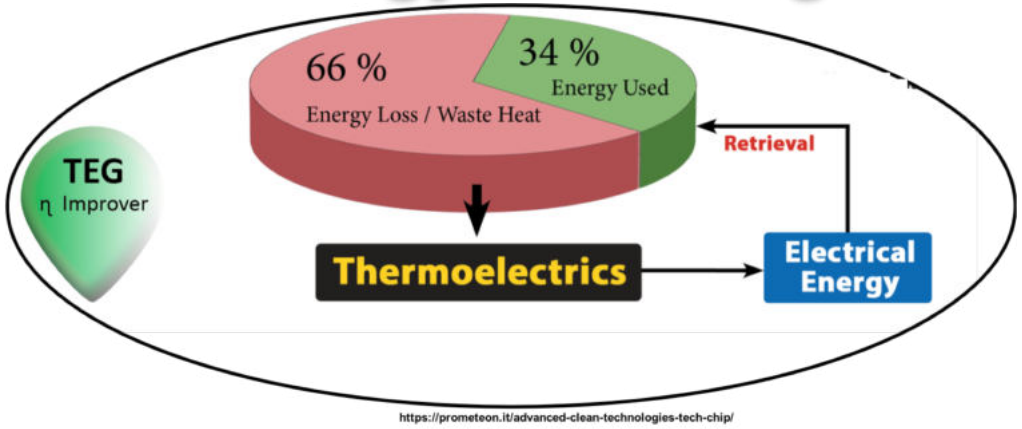
Transition to sustainable sources of energy

Hydrogen Energy

Storage & Transport

Research challenges?

Thermoelectricity – energy & cooling



Heat to energy conversion

HYDROGEN EFFECTS

Hydrogen Embrittlement (HE)….

West Berlin Congress Hall, 1980

Hydrogen intake causing collapse of roof

San Francisco-Oakland Bay Bridge, 2013

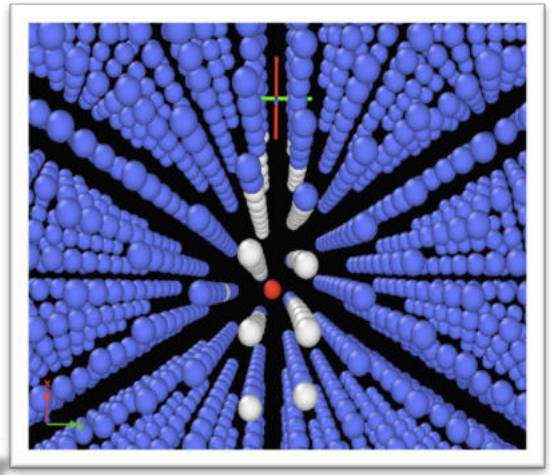
Brittle bolts and cracking due to hydrogen contamination

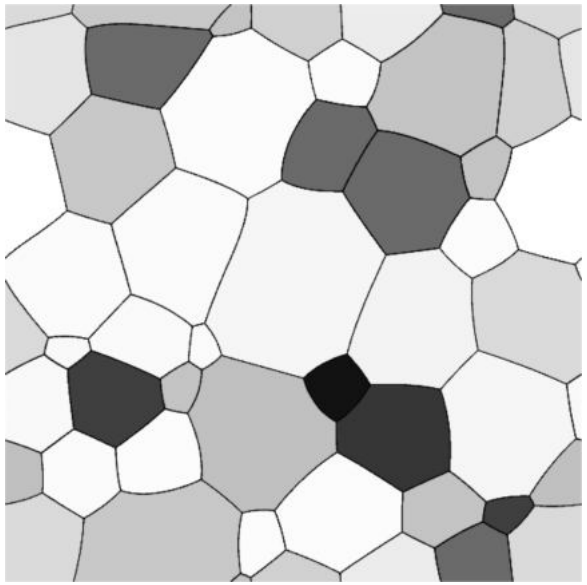
….big threat!

WHAT IS NEEDED?

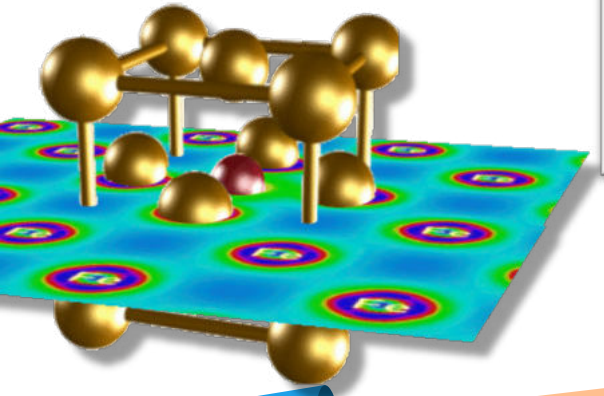
TU Delft

Fundamental atomistic insights beyond experimental resolution





Hydrogen induced degradation

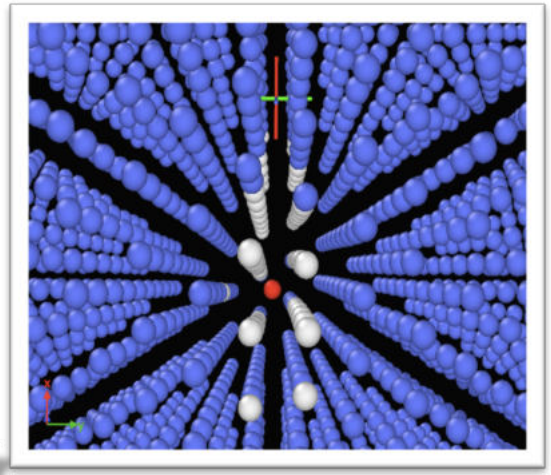


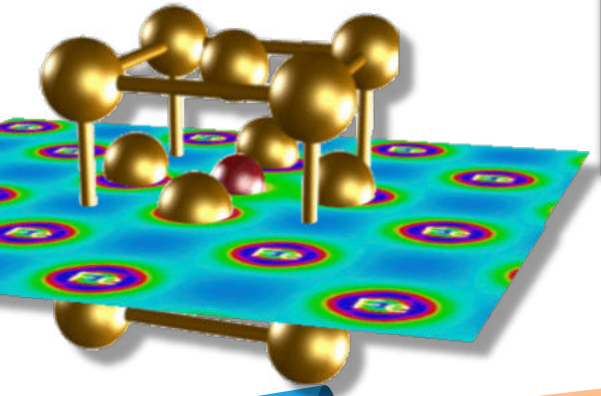
WHAT IS NEEDED?

TU Delft

HYDROGEN FUEL

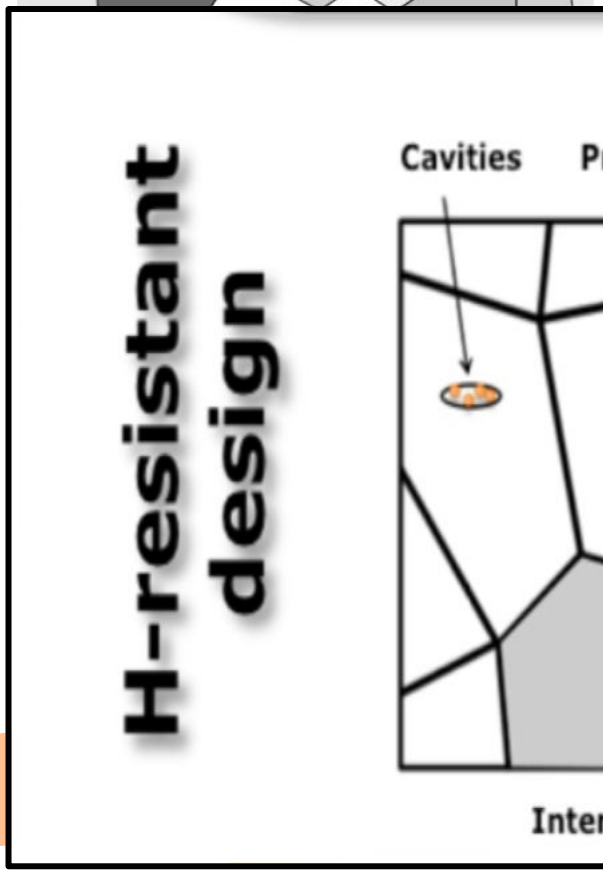
Fundamental atomistic insights beyond experimental resolution





Å

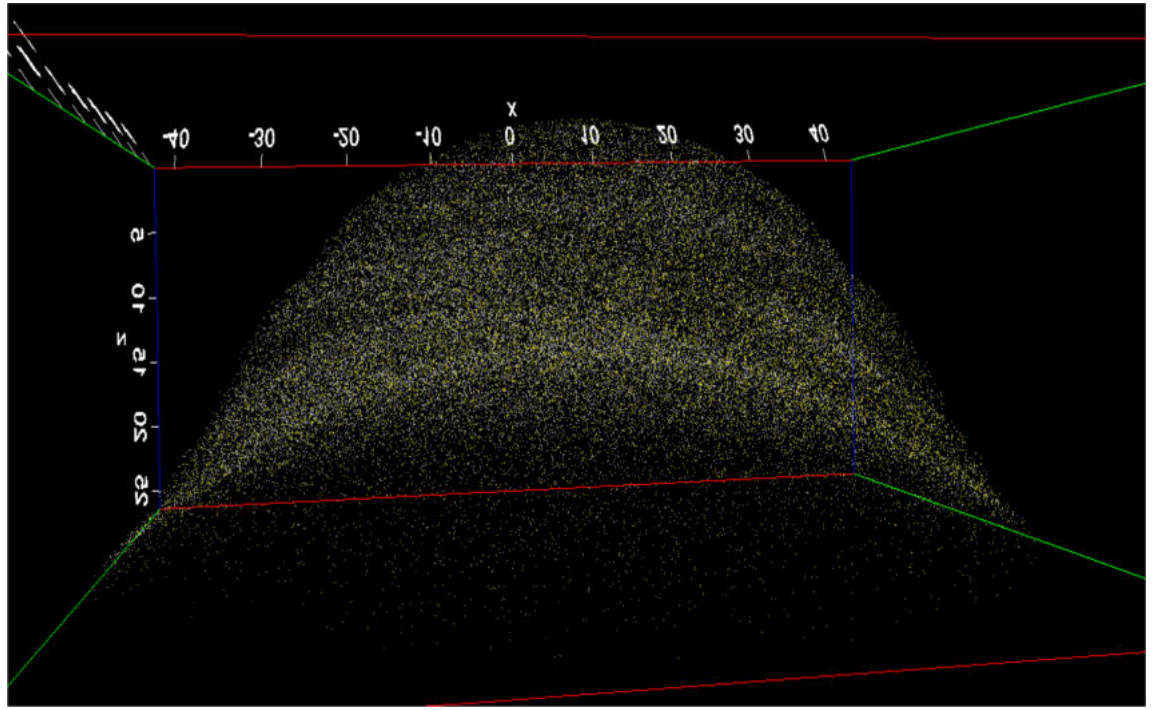
μm



H TRAPPING – APT STUDY

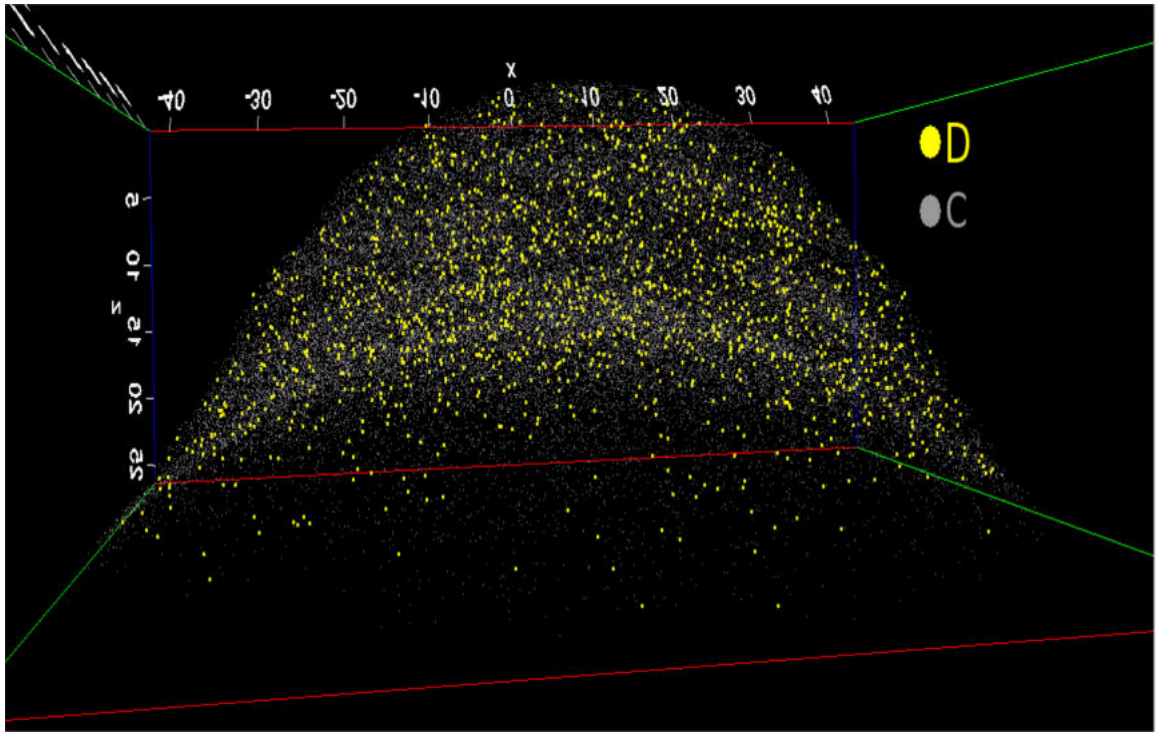
TU Delft

Before D charging (15 hrs aged)



❖ Variation in C concentration – spinodal decomposition

After D charging (15 hrs aged)



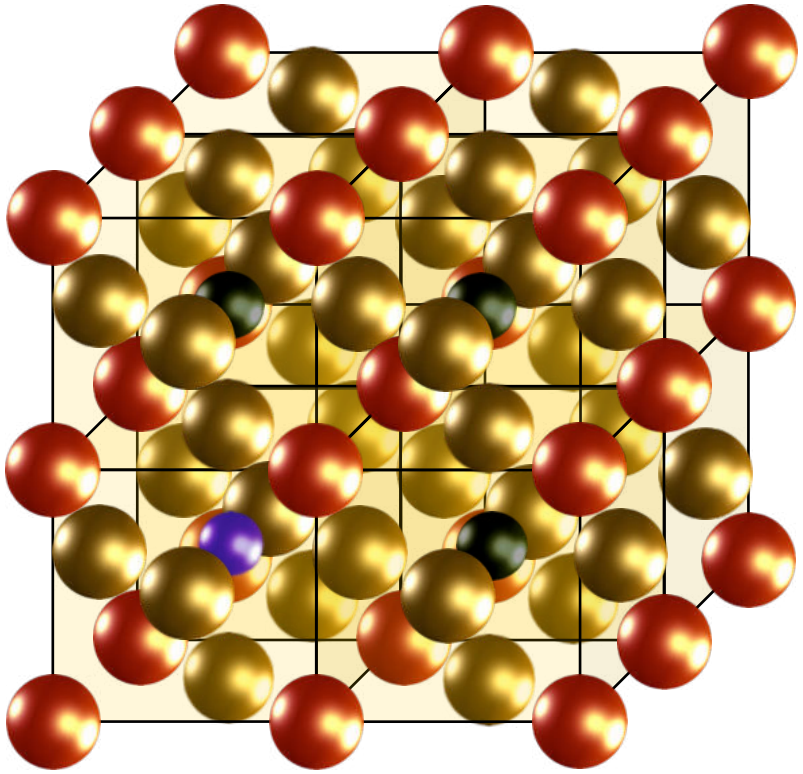
❖ No clear D localization to C-rich region visible

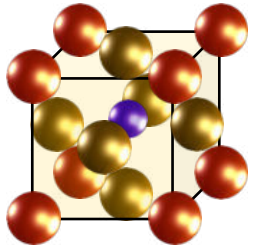
Significant amount of Deuterium in the sample – precipitate increases H solubility!

D. Haley, P. –P. Choi, D. Raabe, MPIE, Düsseldorf

H TRAPPING – DFT STUDY

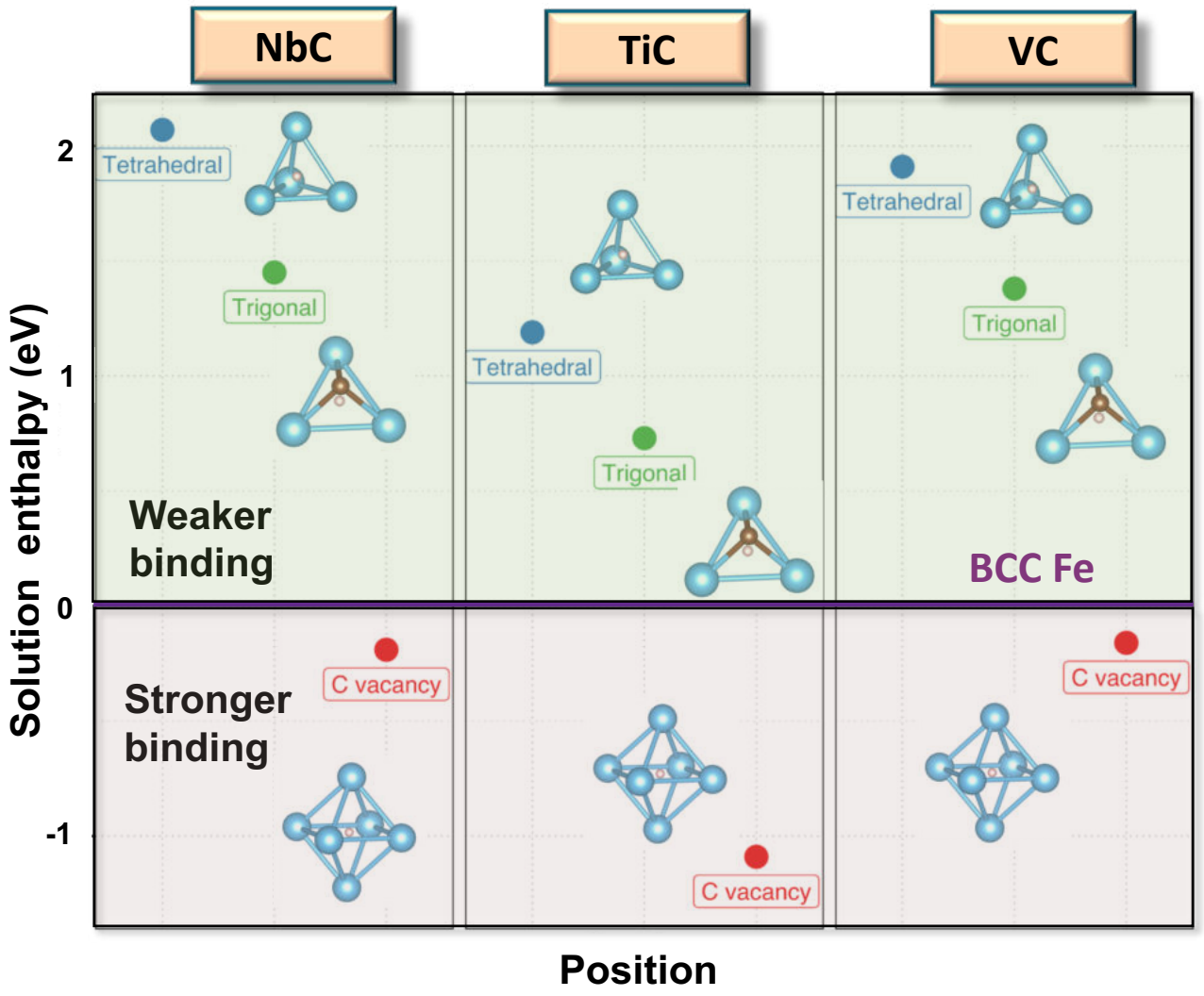
Hydrogen solubility in FeAlC: $\Delta H_H = E$[FeAlCH] – E[FeAlC with one vacancy] - μ_H



H in OS	Solution enthalpy (eV)
	-0.30

C-vacancies in κ carbides trap H!

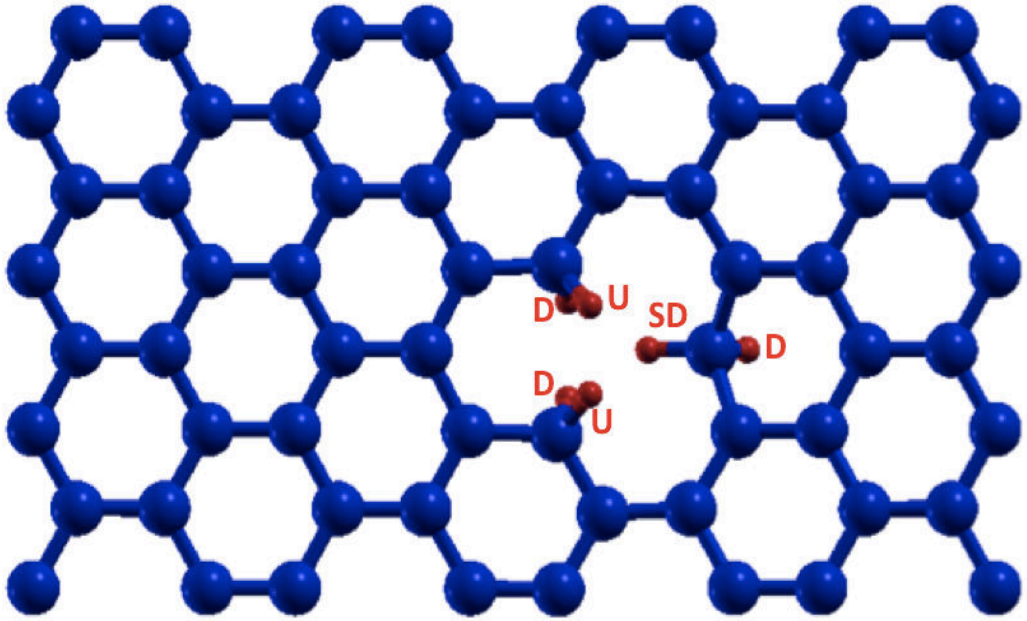
COMPARATIVE DFT STUDY: H TRAPPING

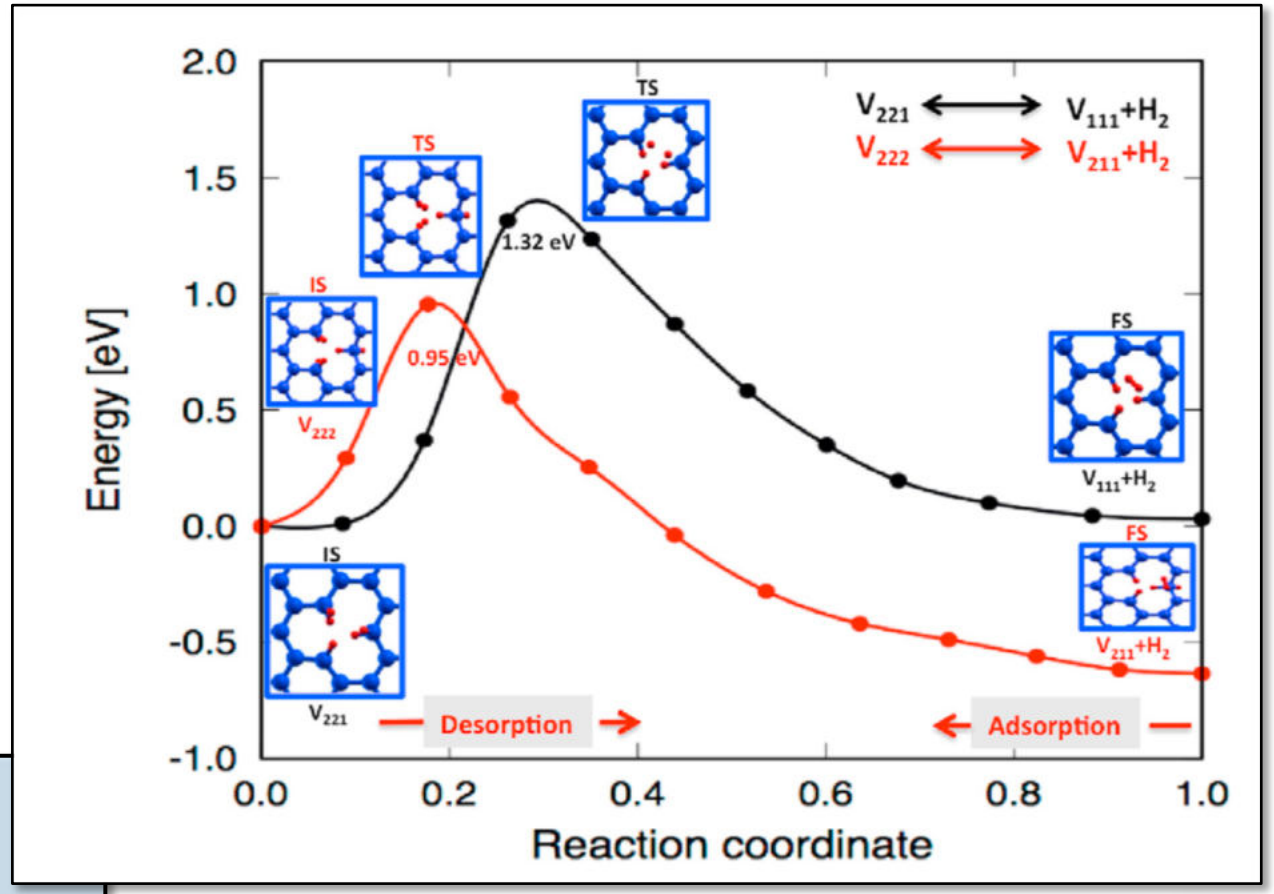


- Negative solution enthalpy means H dissolution from Fe into carbide is exothermic
- Dissolution in interstitial sites endothermic - trigonal site favoured over tetrahedral site
- Strong binding at C vacancy sites - Comparable solution enthalpies for NbC and VC and exceptionally high for TiC

H STORAGE: ADSOPRTION AND DESORPTION

EXAMPLE: GRAPHENE



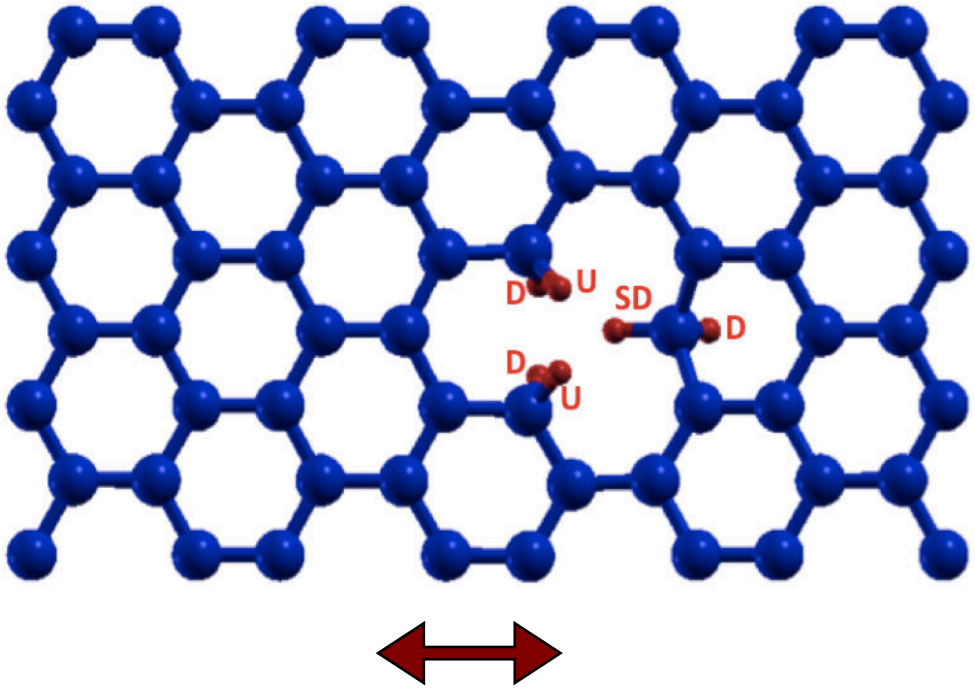


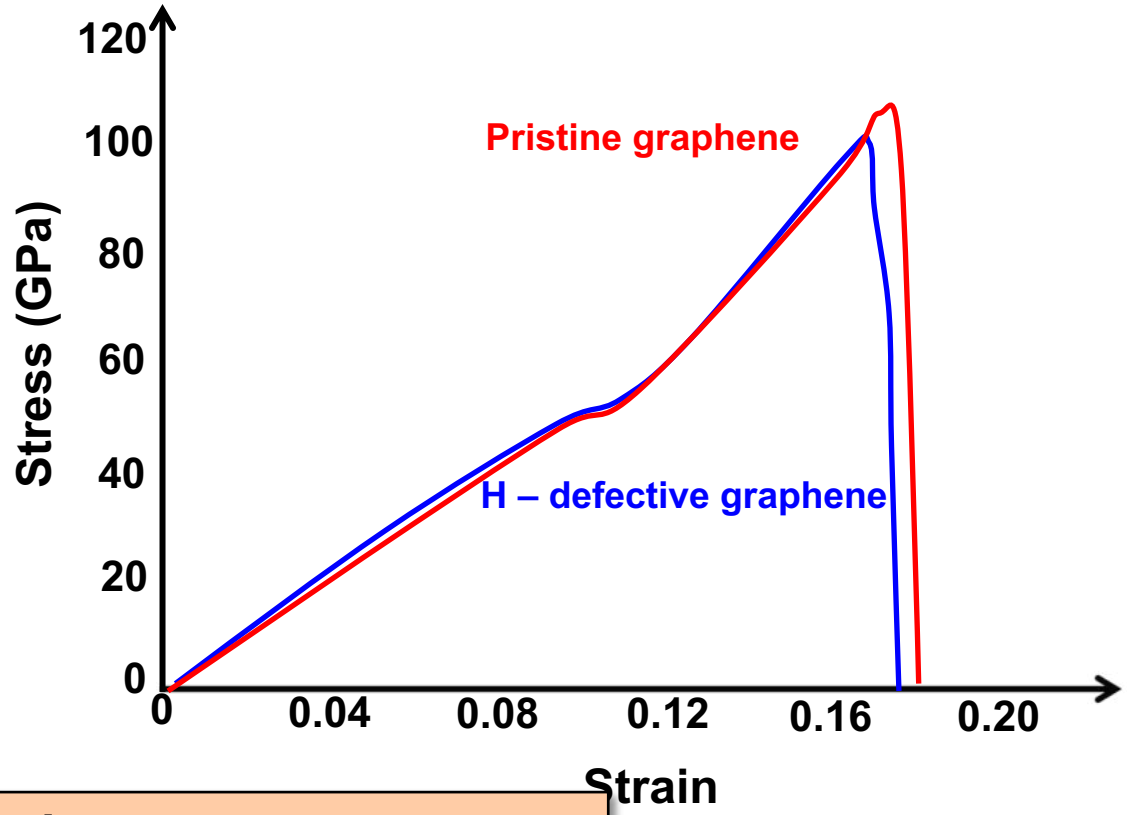
Energy barriers associated with H decorated defective graphene

G. K. Sunnardianto, G. Bokas, A. Hussein, C. Walters, O. A. Moultos, **P. Dey**, International Journal of Hydrogen Energy **46**, 5485 (2021)

H EFFECT ON MECHANICAL PROPERTY

EXAMPLE: GRAPHENE





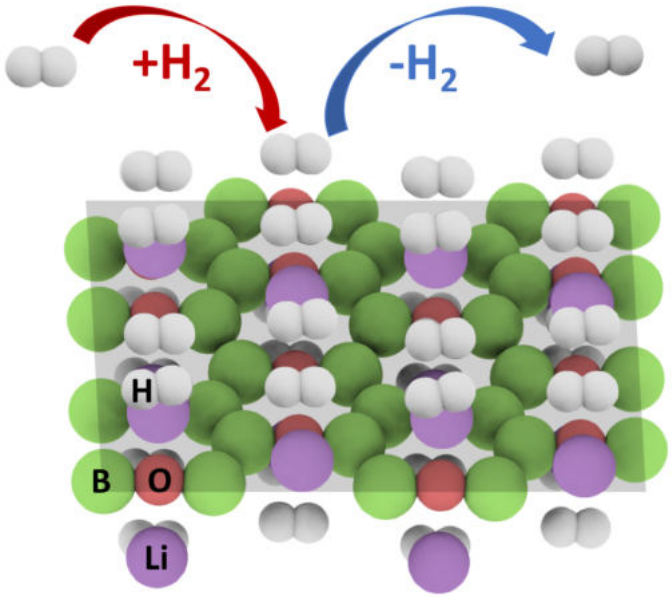
- Not much effect of the presence of H on stress-strain curve
- Slight reduction in the value of the fracture strain and tensile strength

G. K. Sunnardianto, G. Bokas, A. Hussein, C. Walters, O. A. Moultos, **P. Dey**, International Journal of Hydrogen Energy 46, 5485 (2021)

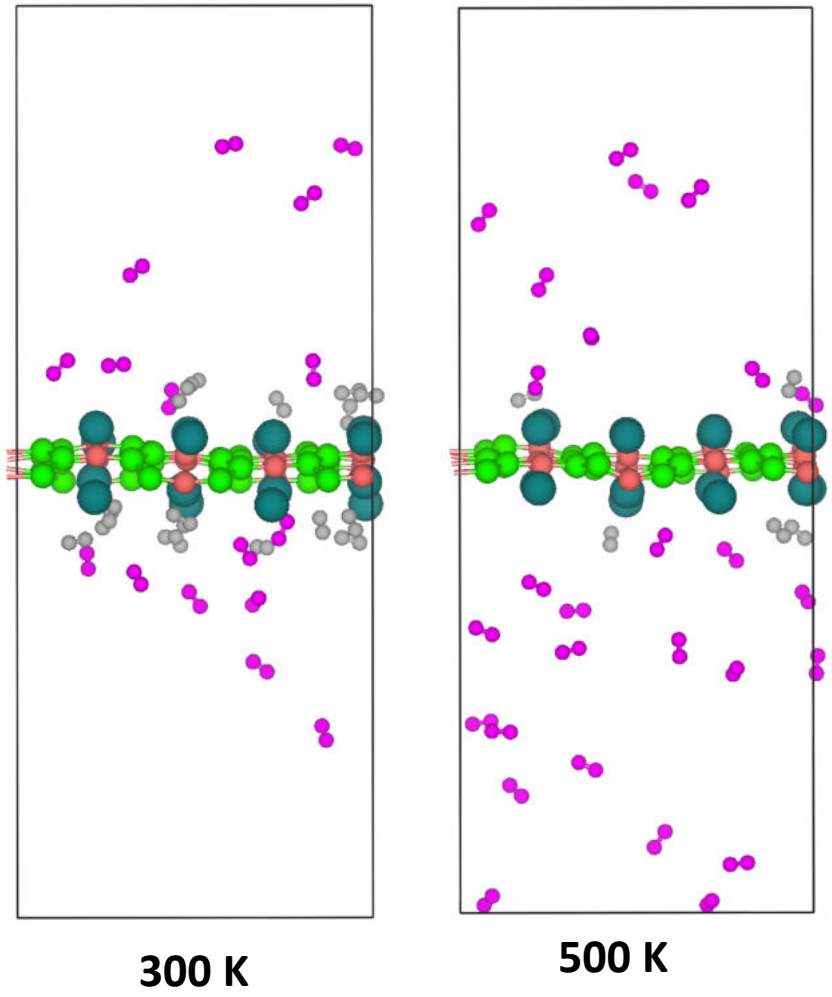
H STORAGE: ADSOPRTION AND DESORPTION

EXAMPLE: BOROPHENE OXIDE WITH LITHIUM

- Li is introduced to enhance interactions with H_2
- Attractive theoretical hydrogen gravimetric density is obtained
- Ab-initio molecular dynamics simulations to test stability and H_2 desorption at finite temperatures



AB-INITIO MD: T DEPENDENT H DESORPTION



EXAMPLE: BOROPHENE OXIDE WITH LITHIUM

- Each Li binds to two H_2 molecules – average binding energy of -0.24 eV/H_2
- Structural stability tested at temperatures of 200, 300, 400 and 500K
- H_2 bound by van der Waals forces - structure does not undergo irreversible changes
- 53% of H_2 still bound at 300K - 19% bound at 400K

P. Habibi, T. J. H. Vlugt, **P. Dey** et al., ACS Appl. Mater. Interfaces **36**, 43233 (2021)

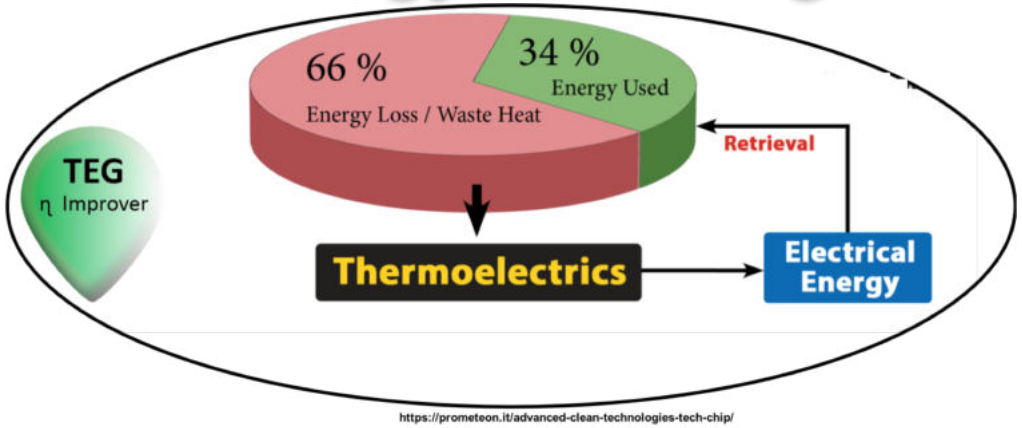
SUSTAINABLE SOURCES

Transition to sustainable sources of energy

Hydrogen Energy

Storage & Transport

Thermoelectricity – energy & cooling



Heat to energy conversion

SUMMARY

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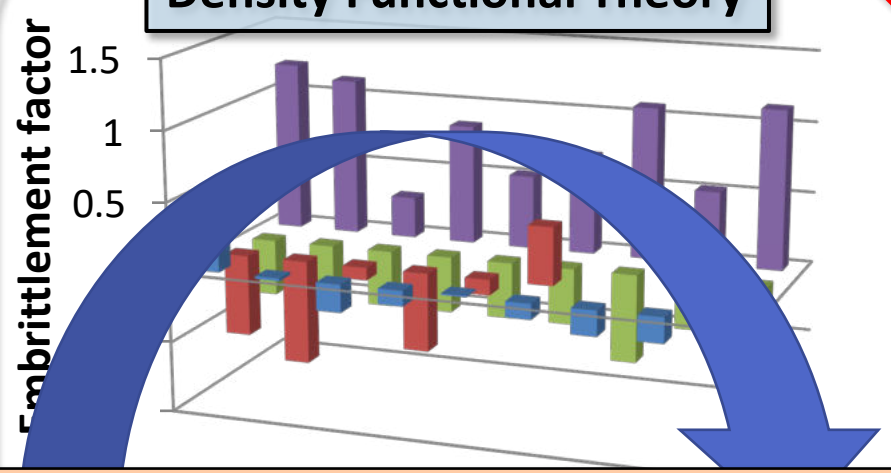
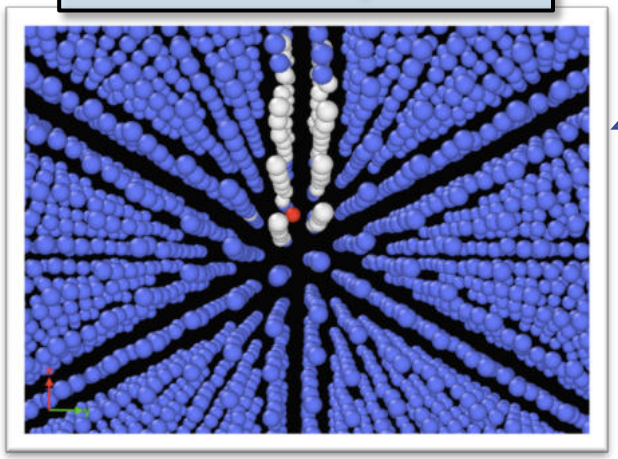
Density Functional Theory

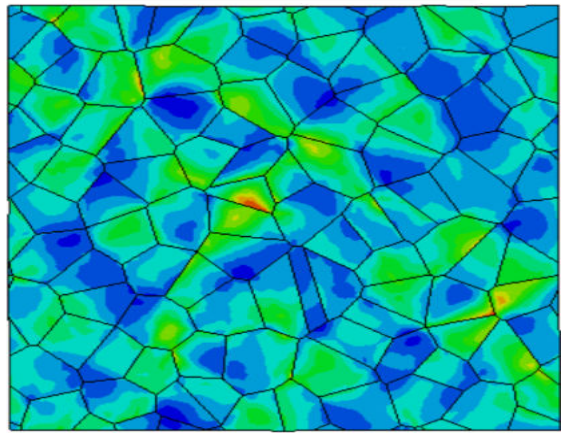


Multi-scale framework to design materials for energy application

Molecular Dynamics



Crystal Plasticity



TEAM

Thank You!

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