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Unlimited Energy? Materials Modeling for Nuclear Fusion

8-10 April 2025

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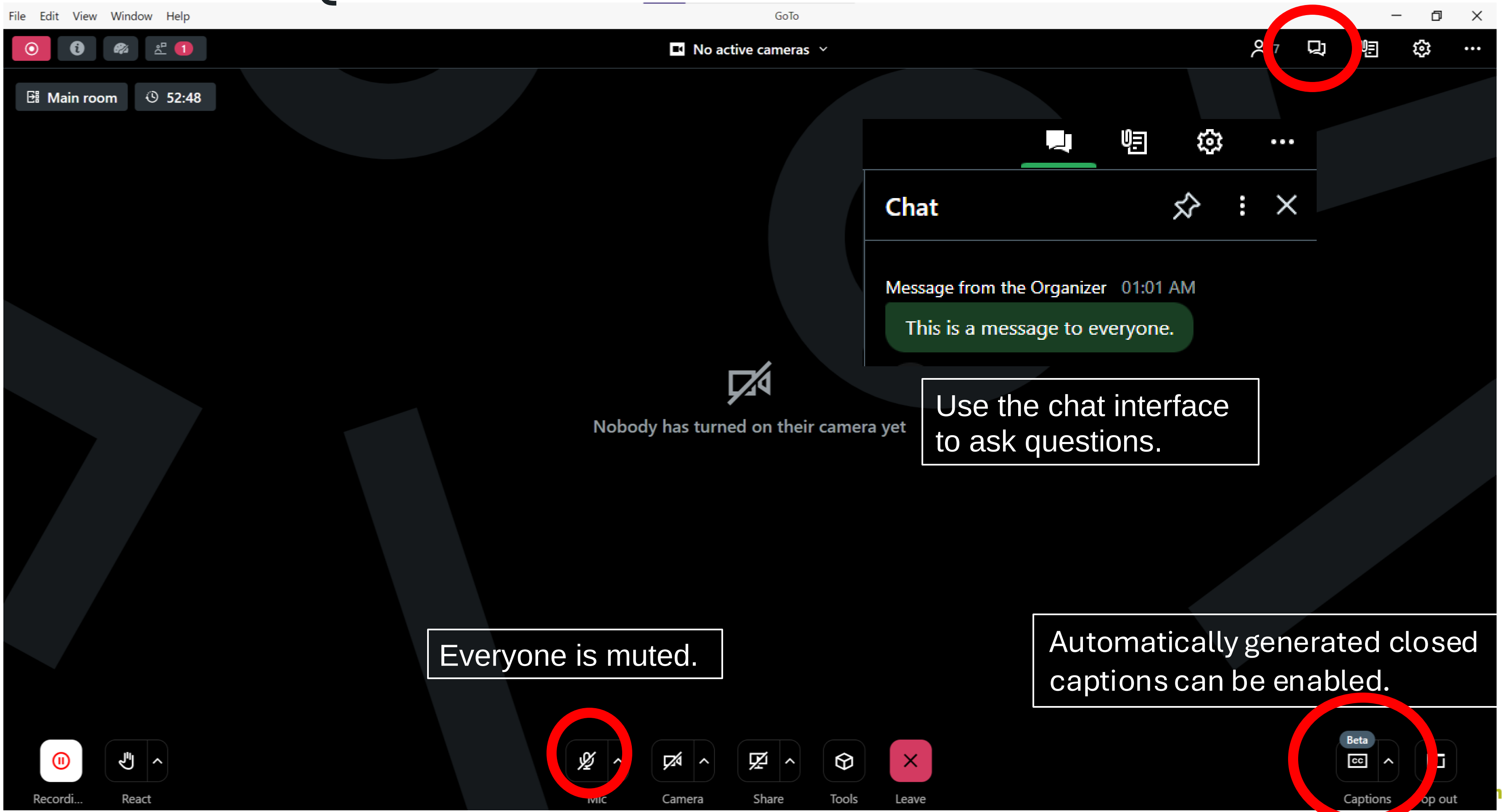

Message from the Organizer 01:01 AM

This is a message to everyone.

Nobody has turned on their camera yet

Use the chat interface to ask questions.

Everyone is muted.

Automatically generated closed captions can be enabled.

Webinar Speakers

Katherine Hollingsworth ***Dr. Erich Wimmer*** ***Dr. Gerhard Engel***

Unlimited Energy?
Materials Modeling for Nuclear Fusion

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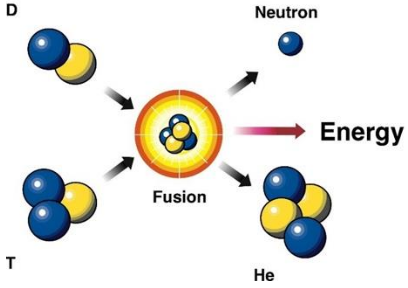
Outline

- Investment in Fusion Energy
- Fusion – Technological Approaches and Challenges
- High-performance Materials Needed in Fusion Reactors
- Computational Materials Engineering: Insight & Predictions
- Materials Design Fusion Alliance
- Q&A

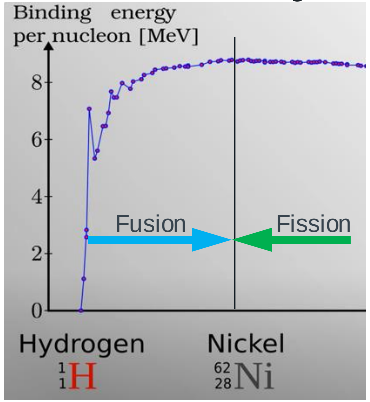
Unlimited Energy? Perhaps, but it's not easy …



https://www.energy.gov/science/doe-explainsfusion-reactions

Combined mass of fusion reaction products is less than the sum of the masses of the reactants, releasing energy:

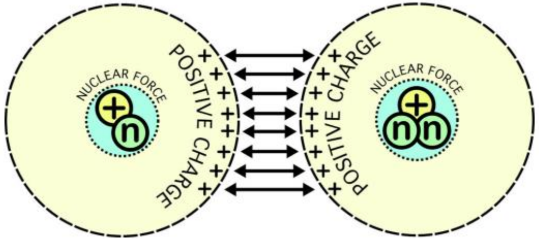
$\Delta E = \Delta m c^2$



The more nucleons bind together, the more energetically favorable the nucleus is – up to Nickel-62.

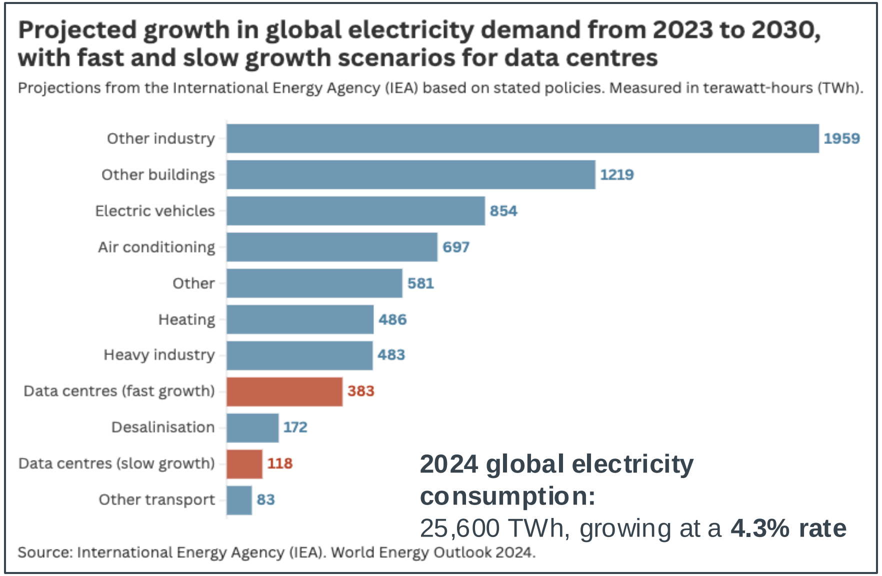
Challenge: Enable atomic nuclei to "quantum tunnel" through the Coulomb barrier and fuse. Requires **High temperature**, **High pressure**, & **Long confinement time**

$$\text{Triple Product} = \underbrace{n}_{\text{Density}} \times \underbrace{T}_{\text{Temperature}} \times \underbrace{\tau}_{\text{Confinement Time}}$$



Investment in Fusion Energy

Increased demand for carbon-free energy outstrips growth of traditional renewables.
This is driving strong public and private sector investment in Nuclear Fusion.



Projected growth in global electricity demand from 2023 to 2030, with fast and slow growth scenarios for data centres

Projections from the International Energy Agency (IEA) based on stated policies. Measured in terawatt-hours (TWh).

2024 global electricity consumption:
25,600 TWh, growing at a **4.3% rate**

Source: International Energy Agency (IEA). World Energy Outlook 2024.

Demand from data centers, while significant, is only a fraction of projected growth globally.

https://www.sustainabilitybynumbers.com/p/ai-energy-demand

Advantages of Fusion Energy

- No greenhouse gas emissions
- 24/7 Availability
- Unlimited fuel supply
- High energy density
- Inherently safe
- Minimal long-lived radioactive waste
- No risk of nuclear proliferation
- Potentially compact and scalable

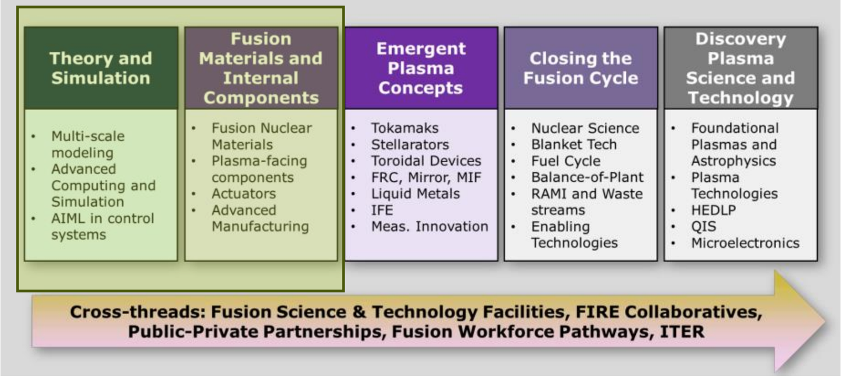
Challenges

- Technical Complexity
- Requires large upfront investments
- Tritium Supply issues
- Neutron damage & materials
- Energy Conversion Bottlenecks
- Cost

Public investment in Fusion:

- **ITER**: > $20B since 2006 (US, China, EU, India, Japan, Korea, Russia)
- **UK** Atomic Energy Authority (UKAEA) 2025 budget > £410M
  - STEP (Spherical Tokamak), LIBRTI (Lithium Breeding), …
- **Europe**: EUROfusion - consortium of national fusion research institutes
- **Japan**’s Moonshot Program, FAST Fusion Project, JT-60SA Tokamak, …
- **South Korea** – e.g., KSTAR, funding > $800M
- **China:** Test Reactor (CFETR), Tokamak (EAST), NIF, …
- **US**: 2024 US DOE for Fusion Energy Sciences budget > $700M
  - DIII-D, ITER, Public-Private partnerships, …

ITER, Southern France



Theory and Simulation	Fusion Materials and Internal Components	Emergent Plasma Concepts	Closing the Fusion Cycle	Discovery Plasma Science and Technology
• Multi-scale modeling • Advanced Computing and Simulation • AIML in control systems	• Fusion Nuclear Materials • Plasma-facing components • Actuators • Advanced Manufacturing	• Tokamaks • Stellarators • Toroidal Devices • FRC, Mirror, MIF • Liquid Metals • IFE • Meas. Innovation	• Nuclear Science • Blanket Tech • Fuel Cycle • Balance-of-Plant • RAMI and Waste streams • Enabling Technologies	• Foundational Plasmas and Astrophysics • Plasma Technologies • HEDLP • QIS • Microelectronics

Cross-threads: Fusion Science & Technology Facilities, FIRE Collaboratives, Public-Private Partnerships, Fusion Workforce Pathways, ITER

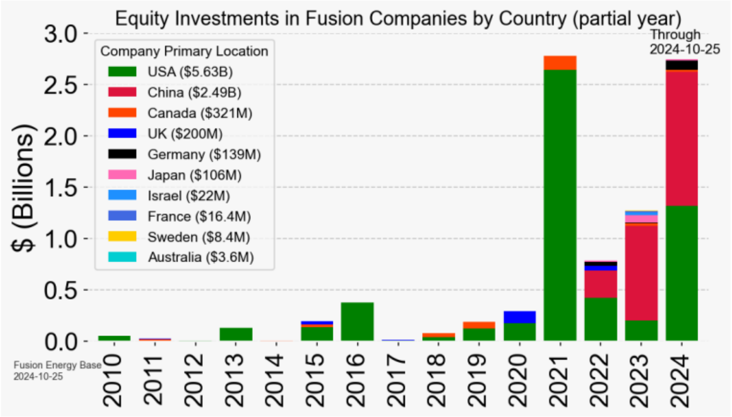
Source: https://www.energy.gov/science/articles/building-bridges-vision-office-fusion-energy-sciences

Private Investment in Fusion:

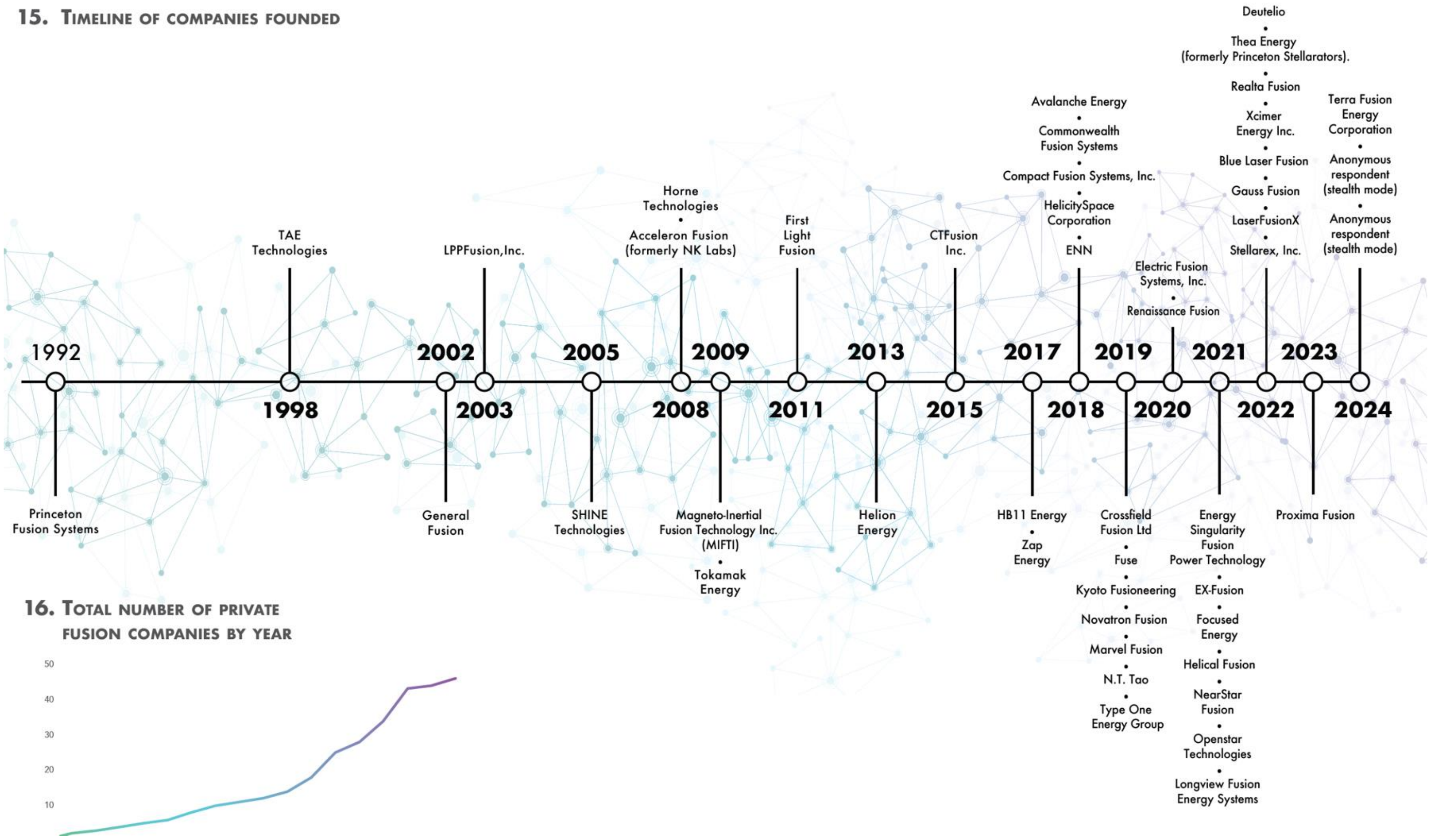
- There are now more than 50 private fusion machine companies globally, plus many more technology developers and suppliers.
- More than 100 research organizations actively contribute to the field
- Total private investment as of 2024: > $7B, >$1B annually (FIA members only)

Source: https://www.fusionenergybase.com/

Source: https://www.fusionindustryassociation.org/



Source: https://www.fusionenergybase.com/



15. Timeline of companies founded

16. Total number of private fusion companies by year

Source: https://www.fusionindustryassociation.org/

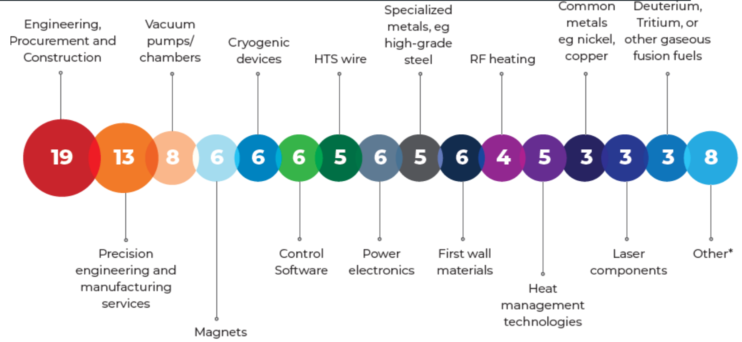
Fusion Companies*:

Acceleron Fusion
Avalanche Energy
Blue Laser Fusion
Commonwealth Fusion Systems (CFS)
Crossfield Fusion
Deutelio
Electric Fusion Systems
Energy Matter Conversion Corporation
Energy Singularity Fusion Power Technology
ENN Energy Research Institute
Ex-Fusion
First Light Fusion
Focused Energy
Fuse Energy Technologies
Gauss Fusion
General Atomics
General Fusion
HB11 Energy
Helical Fusion
Helicity Space
Helion Energy
HHMAX-Energy
Horne Technologies
Innoven Energy
Jupiter Volta
LaserFusionX
LINEA Innovations
Longview Fusion Energy Systems
LPP Fusion
Magneto-Inertial Fusion Technologies
Marvel Fusion
NearStar Fusion
Neo Fusion
Novatron Fusion Group
NT-Tao
OpenStar Technologies
Pacific Fusion
Princeton Fusion Systems
Proxima Fusion
Pulsar Fusion
Realta Fusion
Renaissance Fusion
SHINE Technologies
Startorus Fusion
Stellarex
TAE Technologies
Terra Fusion
Thea Energy
Tokamak Energy
Type One Energy
UK Industrial Fusion Solutions
Xcimer Energy
Xtus Energy
Zap Energy

*As of 2024, partial list

Fusion Suppliers*:

Aerospace Corporation
ALSYMEX
Ampegon Power Electronics AG
Arnold Magnetic Technologies
ASG Superconductors spa
Bechtel Power Company
Bilfinger Nuclear & Energy Transition GmbH
Bruker EST
BUTTING
CleanTech Alliance
Cosylab
Curtiss-Wright
digiLab
Diversified Technologies, Inc.
Eni SpA
ExoFusion
Faraday Factory Japan
Fujikura Ltd.
Fusion Energy Insights
Helixos
High Temperature Superconductors Inc. (HSTI)
IDOM
Interlock Energy LLC
Jacobs
Keller Technology Corporation
Kinectrics
Leonardo Electronics US Inc.
Materials Design
MetOx International
Next Step Fusion
OCEM Power Electronics
Omniseal Solutions
Oxford Sigma
Peak Nano
Pfeiffer Vacuum GmbH
Pillsbury Winthrop Shaw Pittman LLP
RadiaSoft LLC
RI Research Instruments GmbH
Rolf Kind GmbH
SCHOTT
SIGMAPHI
SIMIC SpA
Teledyne Brown Engineering
Triangle Design Group LLC
Westinghouse Electric Company LLC
Absolut System
Air Liquide
Ampleon
Canyon Magnet Energy Inc.
ENERCON
Equinor ASA
Frazer Nash Consultancy Ltd (a KBR Company)
Sapientai LLC
Sumitomo Corporation of Americas
Tecnatom
Thales
TRUMPF Laser



Fusion fuels: Commercially relevant nuclear fusion reactions

Standard fusion – most energy released through neutrons

DT: $\boxed{\mathrm{D} + \mathrm{T} \rightarrow {}^{4}_{2}\mathrm{He}\ (3.52\ \mathrm{MeV}) + n^{0}\ (14.06\ \mathrm{MeV})}$

DD: $\boxed{\mathrm{D} + \mathrm{D} \begin{array}{l} \nearrow {}^{3}_{2}\mathrm{He}\ (0.82\ \mathrm{MeV}) + n^{0}\ (2.45\ \mathrm{MeV}) \\ \searrow \mathrm{T}\ (1.01\ \mathrm{MeV}) + p^{+}\ (3.02\ \mathrm{MeV}) \end{array}}$

Aneutronic fusion – energy released by alpha particles:

p-B11: $\boxed{p^{+} + {}^{11}_{5}\mathrm{B} \longrightarrow 3\ {}^{4}_{2}\mathrm{He}\ (8.7\ \mathrm{MeV})}$

D-He3: $\boxed{\mathrm{D} + {}^{3}_{2}\mathrm{He} \longrightarrow {}^{4}_{2}\mathrm{He}\ (3.6\ \mathrm{MeV}) + p^{+}\ (14.7\ \mathrm{MeV})}$

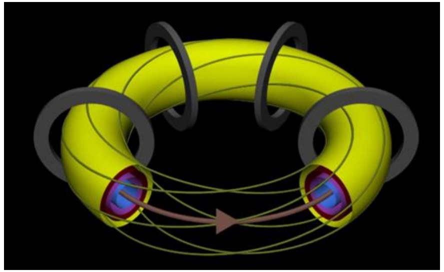
https://en.wikipedia.org/wiki/Nuclear_fusion

⊕	⊖
Highest reactivity Lowest temperature	Neutron damage
Less neutron damage Avoids Tritium fuel	Much less reactive -> higher temperatures and densities needed

⊕	⊖
Direct energy conversion & Little neutron damage and radiation	Much higher temperatures and confinement needed. “Bremsstrahlung”

Fusion Technologies

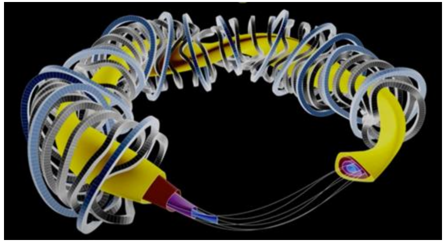
Magnetic Confinement



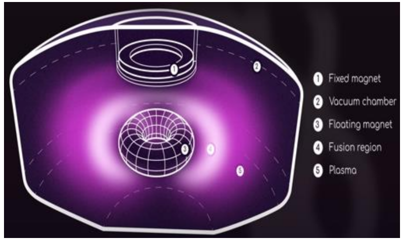
Challenges:
- Plasma instabilities
- Tritium breeding & handling
- Plasma facing materials
- Neutron damage
- Magnets
- Waste handling
- …

Tokamak

Coils + Electric current → *Twisted magnetic field*



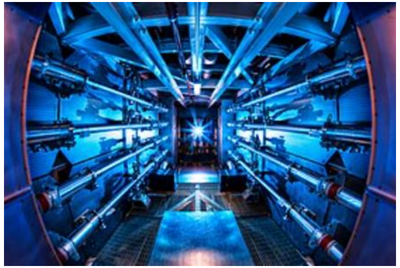
Stellerator



Levitating Dipole (OpenStar)

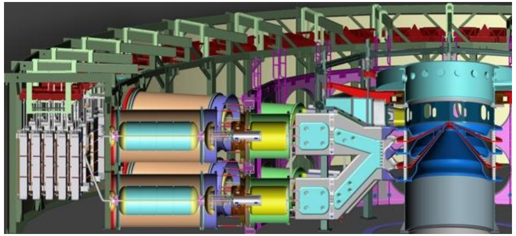
Twisted Coils → *Twisted magnetic field*

Inertial Confinement



Challenges:
- Implosion symmetry
- hydrodynamic stability
- Pellet/target design
- Materials challenges
- Waste handling
- …

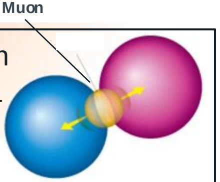
Laser-Driven (National Ignition Facility)



Z-machine (Sandia) – pulsed power

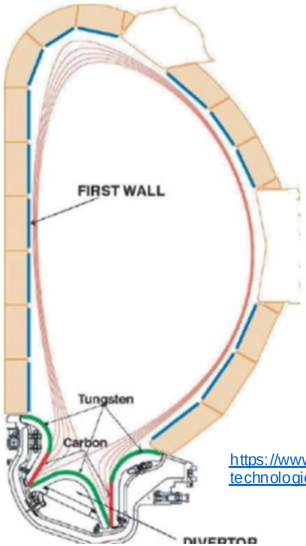
Muon catalyzed fusion

Replace electron in H_2 or DT with a muon. Brings nuclei closer by a factor 200.



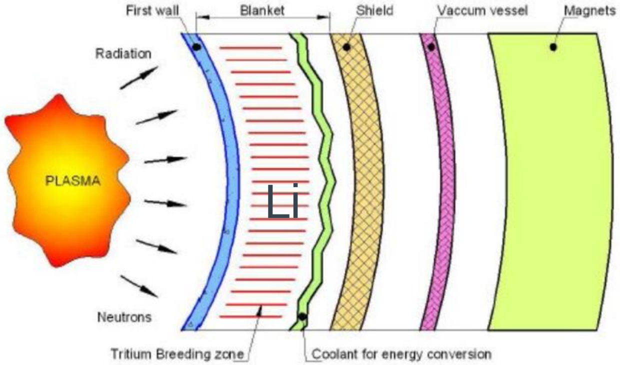
Materials Challenges in Tokamaks

Neutron radiation	Divertor, First wall, Blanket
Temperature & Heat Flux	Divertor, First wall
Magnetic stresses (coils)	Most components
Corrosion	Blanket
Mechanical load	All components
Helium Generation	Divertor, First wall
Cooling fluid pressure	First wall substrate
Plasma erosion	First wall, Divertor
Tritium Absorption	Divertor, First wall, Blanket



Divertor

https://www.climate-and-hope.net/electricity-technologies/divertor-and-limiter



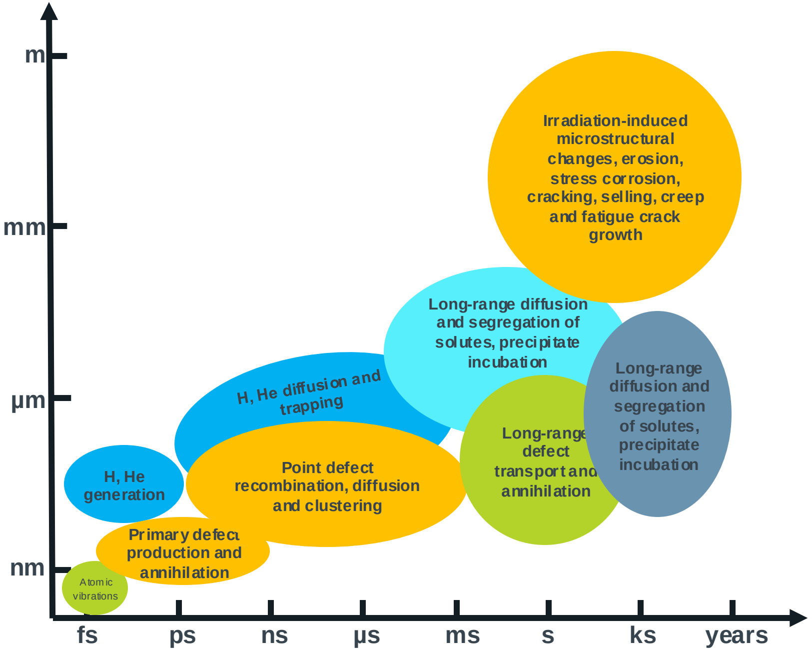
https://www.researchgate.net/publication/231004407_Materials_issues_in_fusion_reactors/figures?lo=1

Neutron damage

- Displacement damage
- Accumulation of hydrogen and helium
- Transmutations

With the present status of materials available for fusion reactors it will be necessary to replace certain components on a regular basis. Estimates:

- Limiters, once per year
- Divertor, once every two years
- Breeder Blankets, once every four years
- Vacuum Vessel, unknown



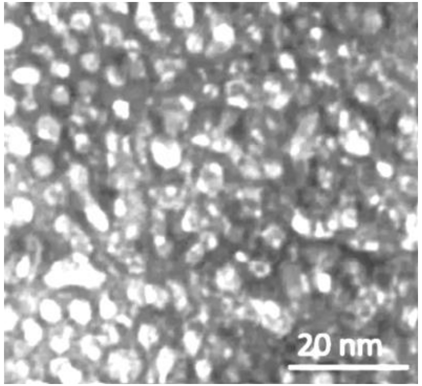
https://www.climate-and-hope.net/electricity-technologies/materials-and-radiation-damage?c=nuclear-fusion

Materials used in Fusion Reactors

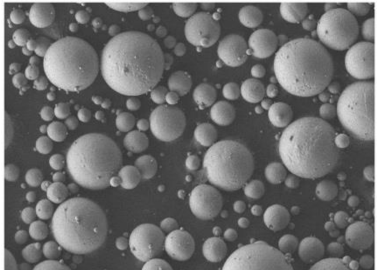
Materials for Extreme Environments

- **Metals & Alloys (Structural/Divertor/First Wall)**
  - W, Be, Ti, Zr, V, Cr alloys
  - High entropy (HEA), Multi Component (MCA), Compositionally Complex (CCA)
  - Powder metallurgy variants (e.g., Oxide Dispersion Strengthened, ODS)
  - Steels (boron-strengthened, RAFM, …)
  - …
- **Ceramics & Coatings (Blanket walls, circuit coatings, flow separators)**
  - SiC, TiC, ZrC, HfC, WC, ….
  - Coatings: AlO_x, Er_2O_3, CrN, BN (corrosion resistance)
- **Ceramics (Breeders and Amplifiers)**
  - Li Orthosilicate, …
- **Magnets and Insulators**
  - Superconducting magnetic materials
  - Resistive magnetic materials
  - Insulators/Shielding
- **Lasers**

Source: UK_Fusion_Materials_Roadmap_Interactive.pdf



Helium bubbles in tungsten



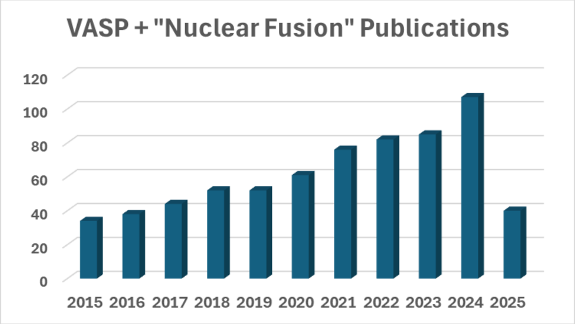
High entropy alloy powder

Materials Design Software in Nuclear Fusion Publications

More than 800 publications VASP + “Nuclear fusion”

Examples:

- **A quinary WTaCrVHf nanocrystalline refractory high-entropy alloy withholding extreme irradiation environments.**
  Atwani et el, Nature Communications **14**, Article 2516 (2023)
  Combines experiment and modeling (VASP and a cluster expansion) to design a new nanocrystalline refractory high-entropy alloy (RHEA).
- **Multi-Resolution Characterization of the Coupling Effects of Molten Salts, High Temperature and Irradiation on Intergranular Fracture**
  Dingreville et al, SANDIA REPORT SAND2021-11224
  Use of VASP and Ab initio Molecular Dynamics in combination with experiment
- **Ab initio study of tungsten-based alloys under fusion power-plant conditions**
  Qian et al, J. Nuclear Physics **581,** 154422 (2023)
  Use of atomistic modeling (VASP) to characterize effect of transmutations on the properties of plasma-facing tungsten alloys during the operational life.



Google Scholar Results

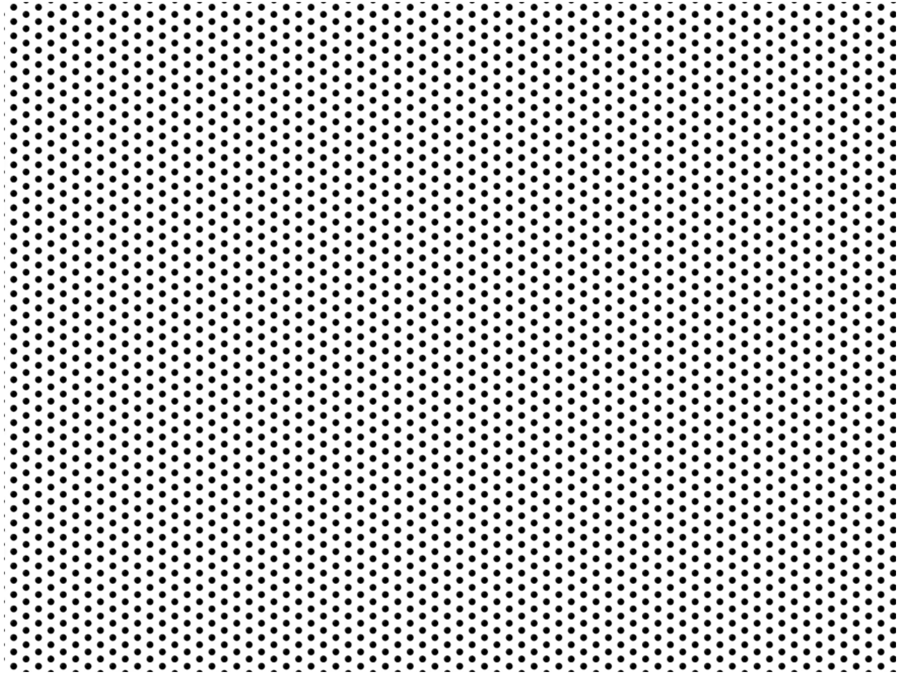
Topic	**VASP Pubs**
Alloy	55,600
Tungsten	16,100
Composite	42,900
Ceramics	18,800
HEA	18,300
ODS	3,060
Superconductor	18,200
Coating	35,400
Calphad	5,590
Inertial Confinement	471

Computational Materials Engineering: Insight & Predictions

Illustrative examples:

- Effect of irradiation on materials properties
- Dynamics of H(D,T): diffusion, release, and trapping
- Effect of transmutations
- Phase transformations
- Microstructure evolution

Impact of High-Energy Neutrons on Tungsten



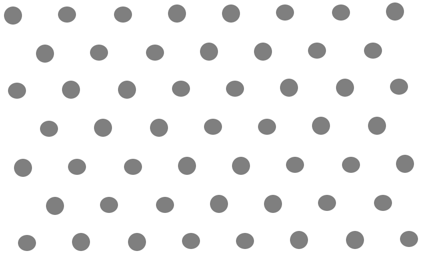
Simulation of collision cascade in tungsten

- Formation of crowdions after healing of initial damage
- Initiation by high momentum of knock-on atom
- Molecular dynamics with adaptive time steps
- Interatomic potential by Mason et al. (2023)
- *LAMMPS* in *MedeA* environment

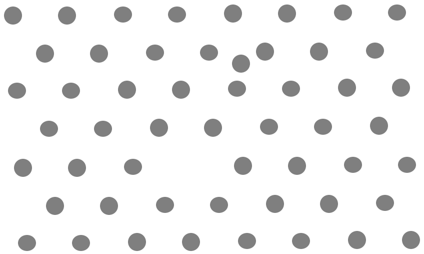
Structure of Defects in W

Computational protocol:

- Take a W supercell
- Introduce Frenkel pairs
- Relax structure
- Compute properties

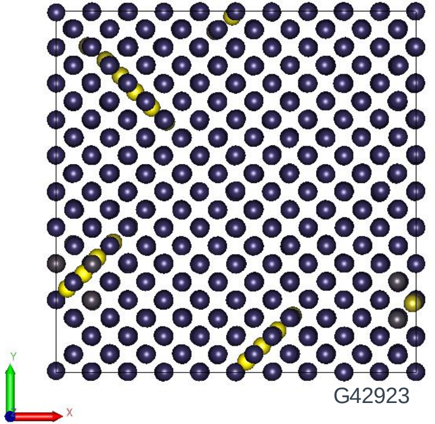


Perfect crystal



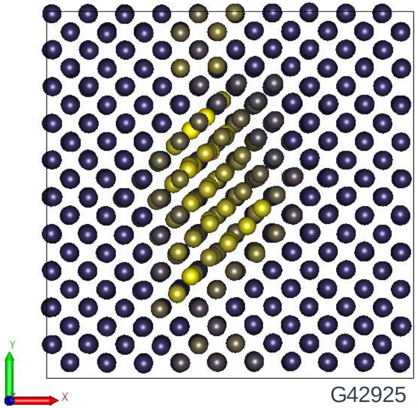
Crystal with Frenkel pair
(vacancy + interstitial)

Fraction of Frenkel pairs: 0.0025

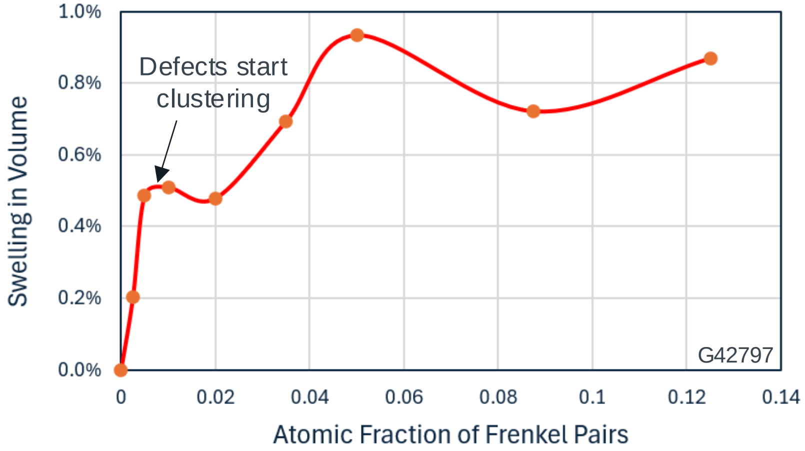


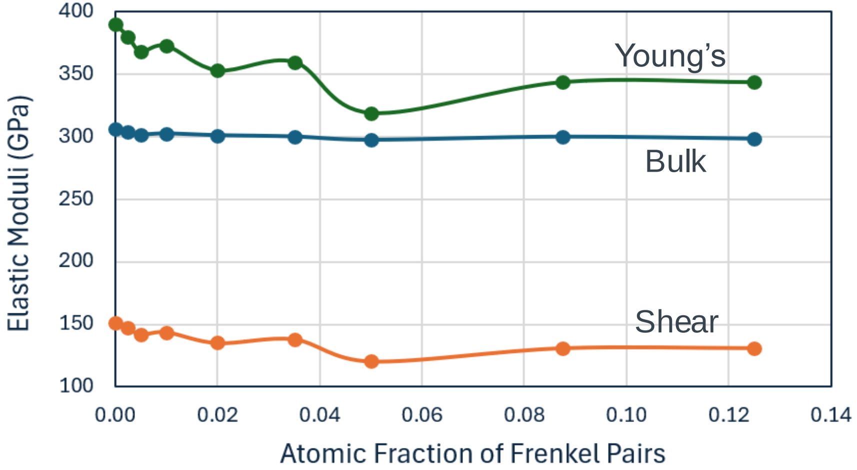
Fraction of Frenkel pairs: 0.02

Fraction of Frenkel pairs: 0.0875



Defect-Induced Property Changes





Under the specific conditions of this simulation, the swelling and changes in elastic coefficients as a function of defect concentrations is linear at very low concentrations but reaches a plateau at higher concentrations due to clustering of defects.

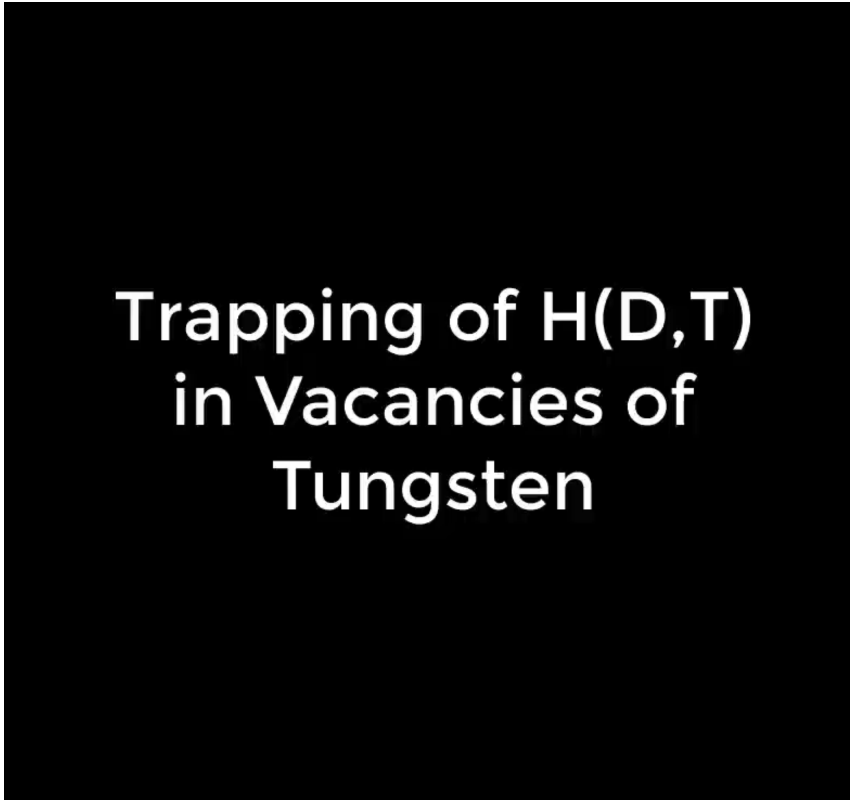
Computations:
DFT-PBE trained machine-learned potential (M. Christensen, unpublished)
Initial random generation of Frenkel pairs
Relaxation with NPT ensemble at 300 K in molecular dynamics simulations of 100 ps
Elastic coefficients computed for minimized ground state structures
Software: LAMMPS within *MedeA* materials modeling environment

Dynamics of H(D,T) in W

Heating of
Tungsten
Crack with H

- H(D,T) tend to migrate to W surfaces
- At high-temperatures and low partial pressure of H in the gas phase, H tends to escape first in the form of atoms which later recombine forming molecules

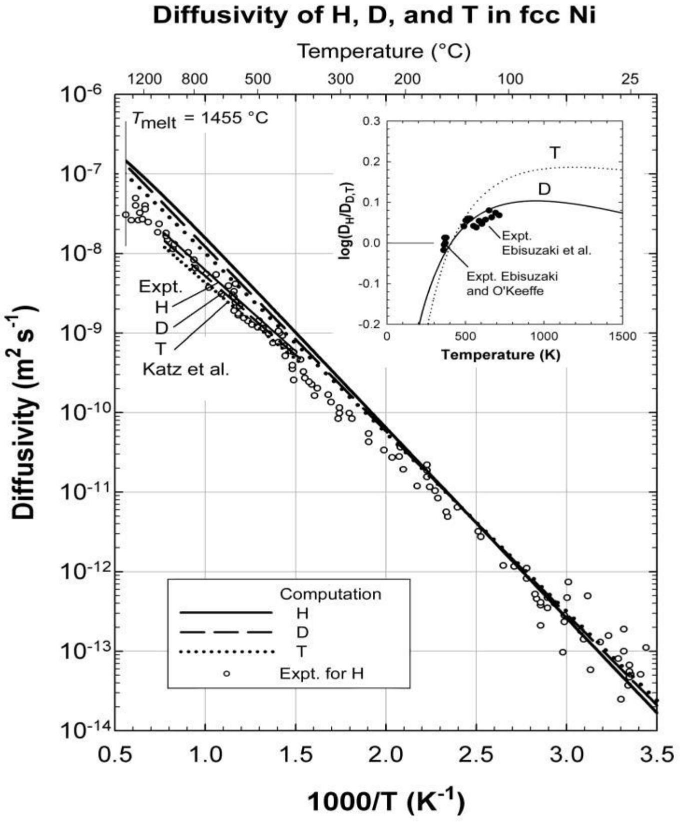
Trapping of H(D,T) in Vacancies of W



Trapping of H(D,T) in Vacancies of Tungsten

- Diffusing interstitial H(D,T) atoms in W are trapped in vacancies.
- A single vacancy in a bcc-W lattice can trap up to six H(D,T) atoms

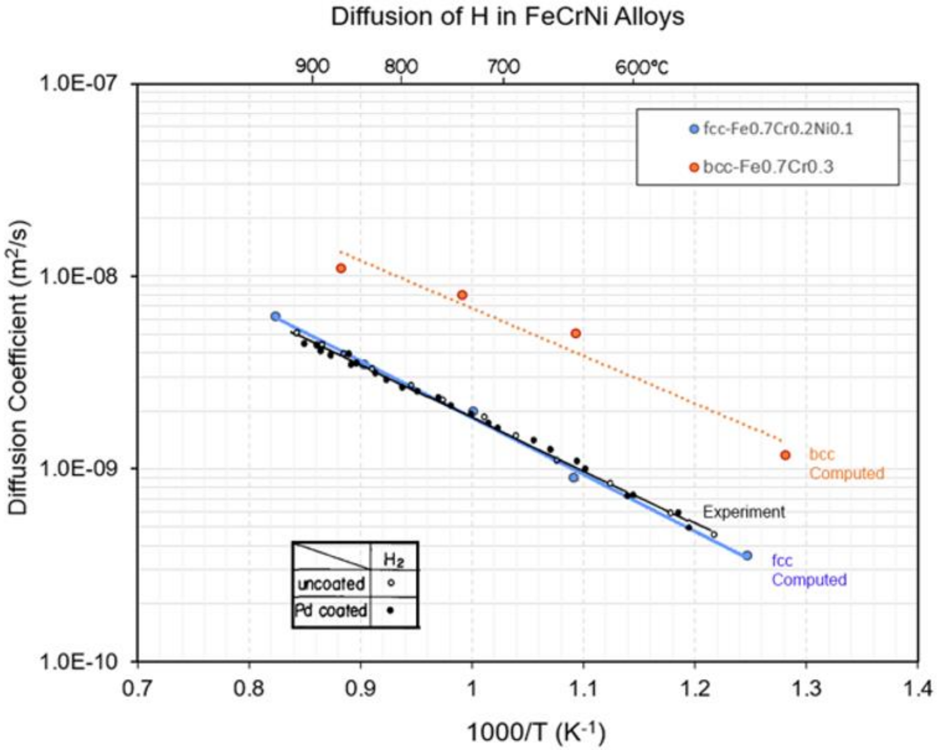
Diffusion: Isotope Effects



- The diffusion coefficient of H in Ni computed from first-principles has similar accuracy as experimental data at ambient and medium temperatures.
- Present computational method capture subtle isotope effects.

E. Wimmer, W. Wolf, J. Sticht, P. Saxe, C. B. Geller, R. Najafabadi, and G. A. Young, “Temperaturedependent diffusion coefficients from *ab initio* computations: Hydrogen, deuterium, and tritium in nickel”, Phys. Rev. B **77**, 134305 (2008)

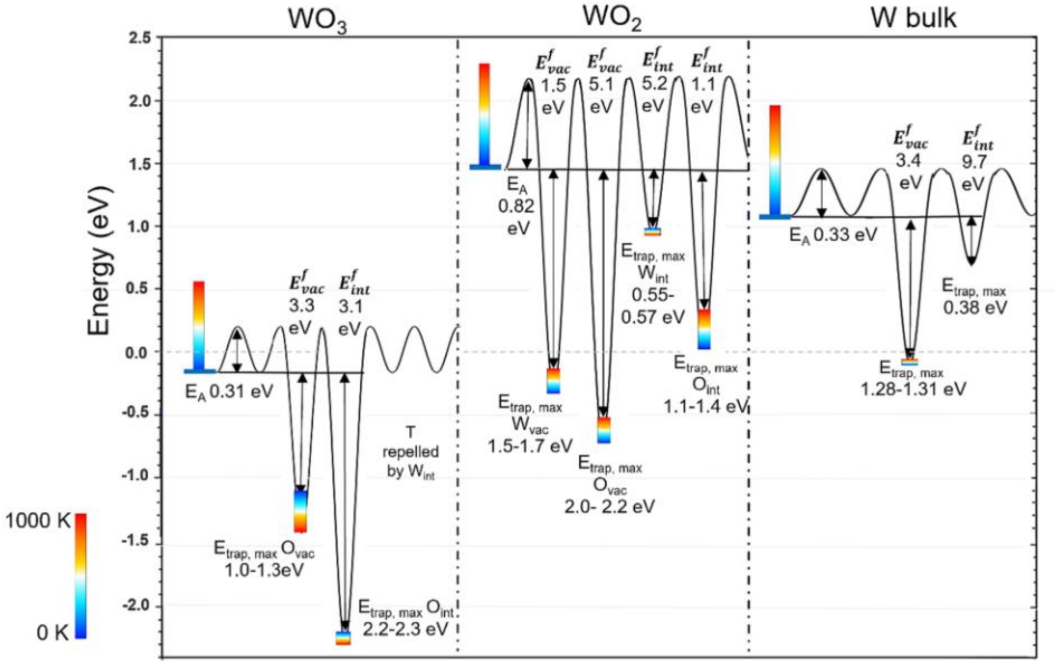
Diffusion of H in Steel



- The computation of diffusion coefficients is well established
- In the present case, computed results are within the experimental uncertainty
- High-quality interatomic potentials are essential.
- *MedeA* offers the tool to create and optimize such potentials

M. Christensen (unpublished)

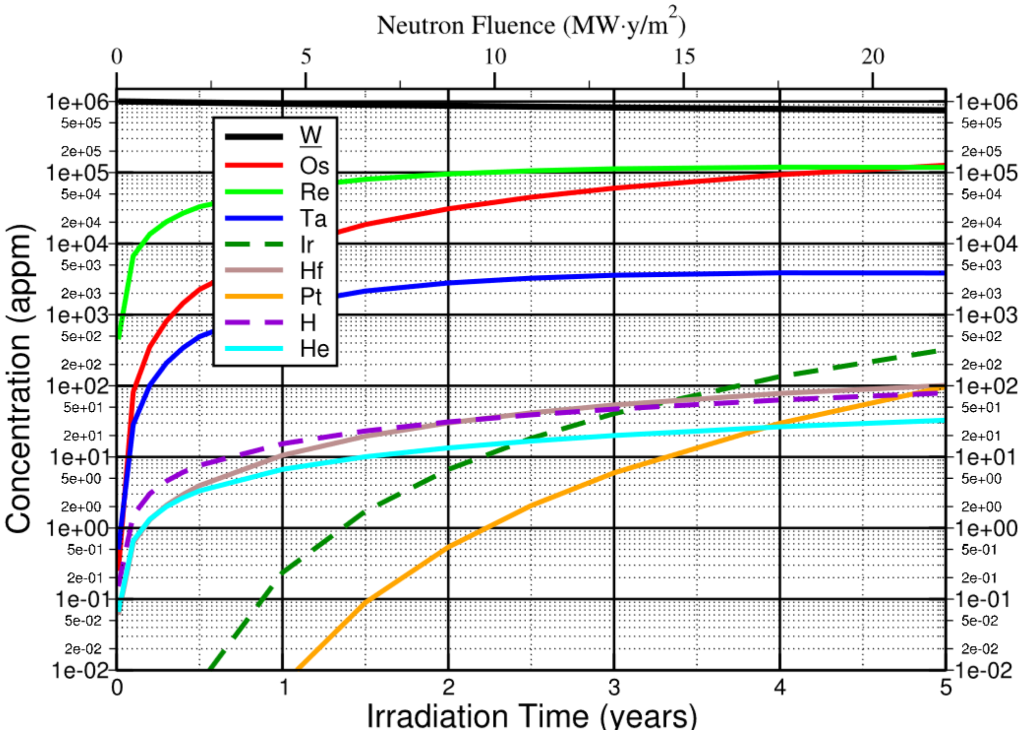
Tritium in W and W-Oxides



M. Christensen, E. Wimmer, M. R. Gilbert, C. Geller, B. Dron, and D. Nguyen-Manh, Atomistic modelling of tritium thermodynamics and kinetics in tungsten and its oxides, Nuclear Materials and Energy **38**, 101611 (2024)

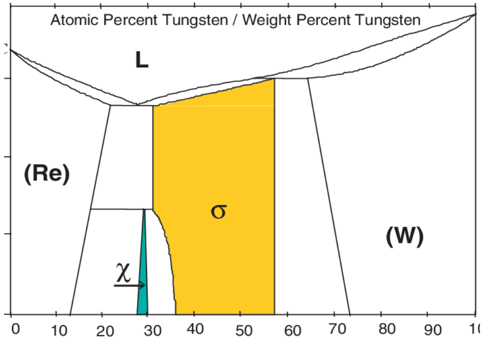
- Detailed DFT computations of hydrogen in W and its oxides reveal WO_2 as a barrier for H(D,T) to escape from bulk W while WO_3 is a “window”.
- Diffusion barriers for H in WO_2 are large compared with those in bulk W and WO_3.
- Oxygen vacancies in WO_2 and WO_3 are deep traps for H(D,T).

Transmutations

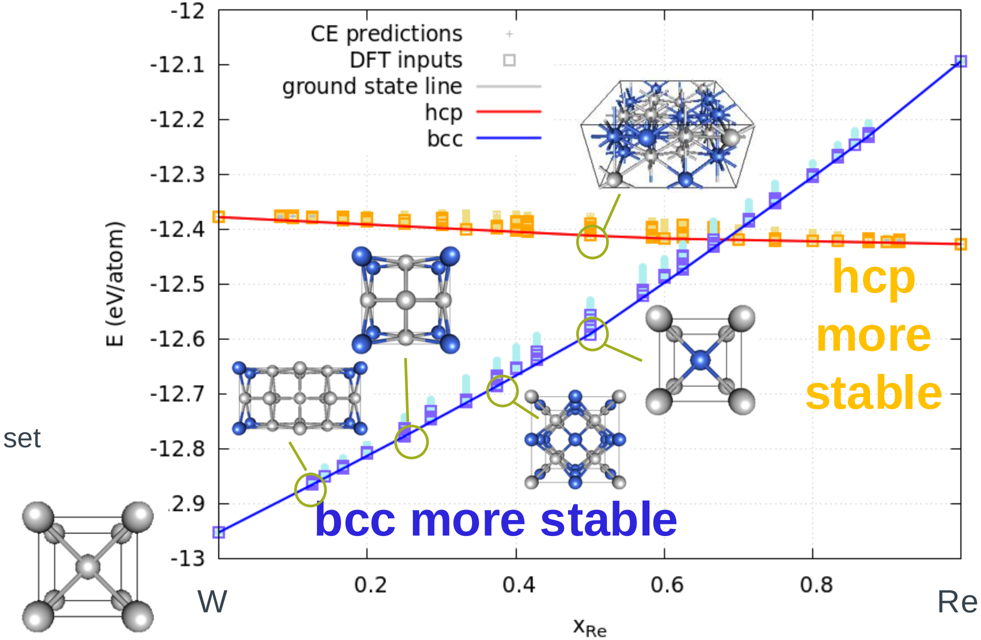


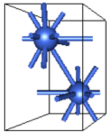
M. R. Gilbert, Culham Centre for Fusion Energy, CCFE-R(10)01 (2011)

W-Re Cluster Expansion



Berne et al., J. Phys.: Condens. Matter 13 (2001) 9433–9443



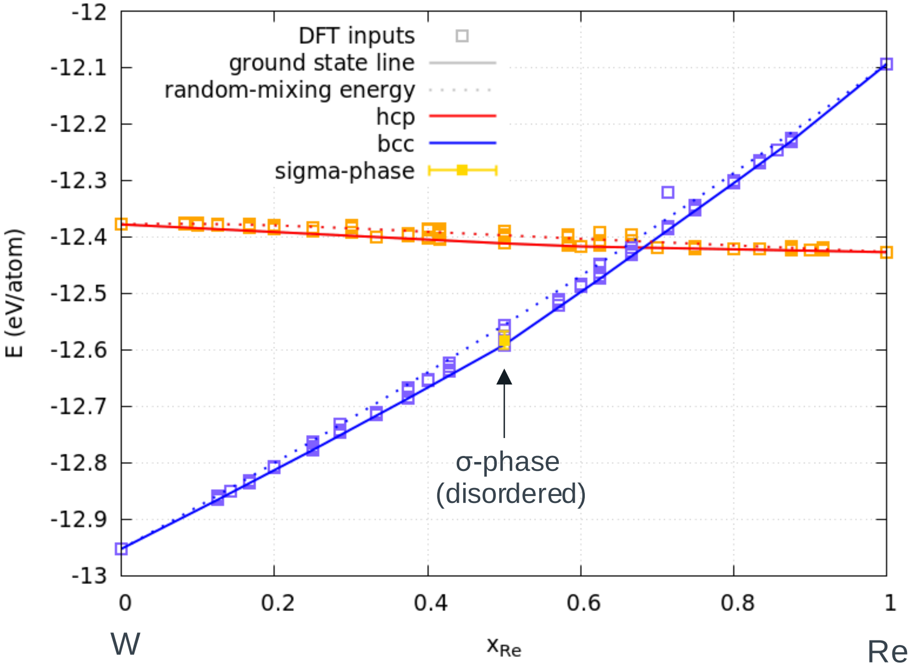


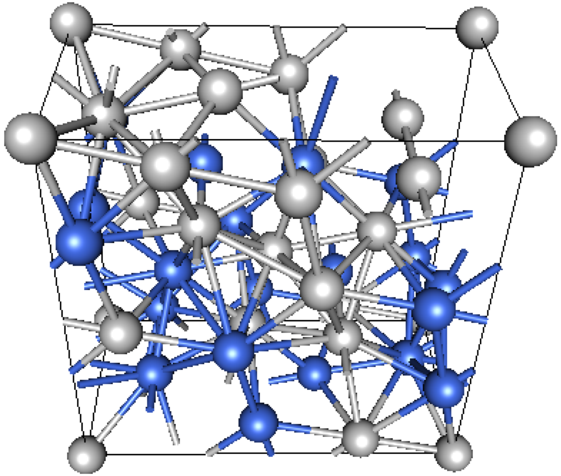
bcc cluster expansion:
isotropic relaxation
87 structures in the training set
631 predicted structures

hcp cluster expansion:
isotropic relaxation
80 structures in the training set
5777 predicted structures

- Cluster expansion on bcc and hcp lattice without prior knowledge on stable W-Re phases
- Wide solubility range for both pure phases

W-Re Cluster Expansion: Random-Mixing Energy





Disorder stabilizes σ-phase vs. random bcc phase

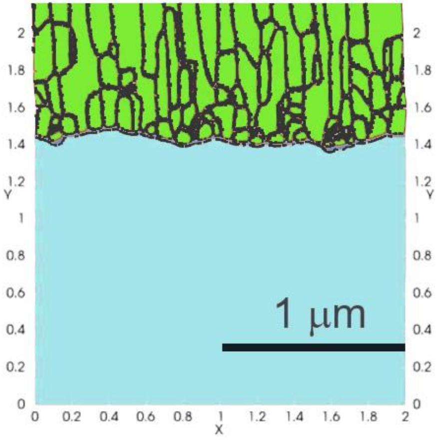
Phase Transition

Heating of m-ZrO_2

Stoichiometric and with 5% O-Vacancies

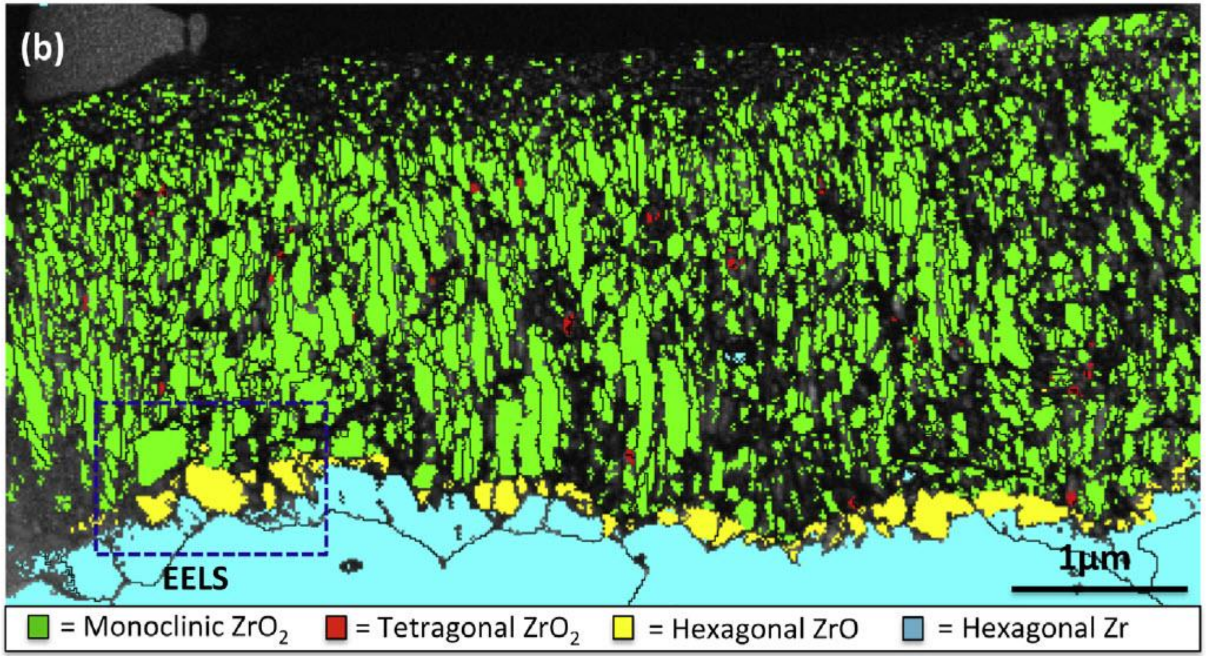
Reproducing the Microstructure of ZrO_2 Corrosion Film

Simulation with *MedeA PhaseField* using ab initio-based computed materials properties



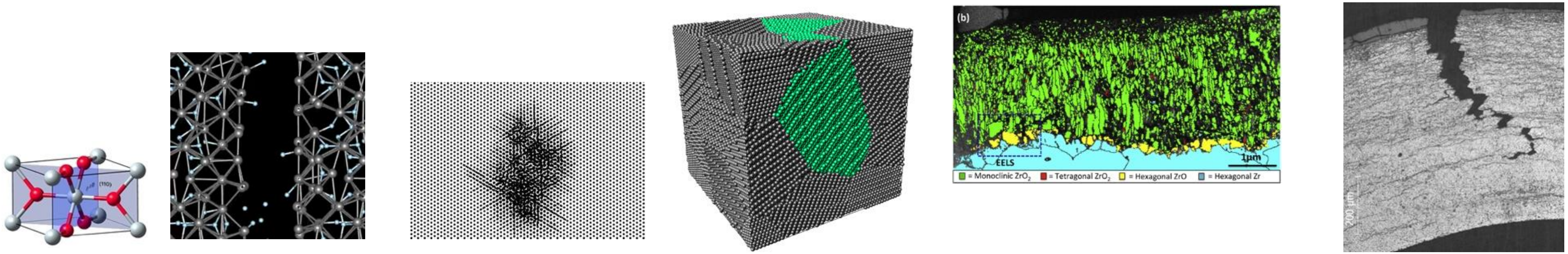
40 days

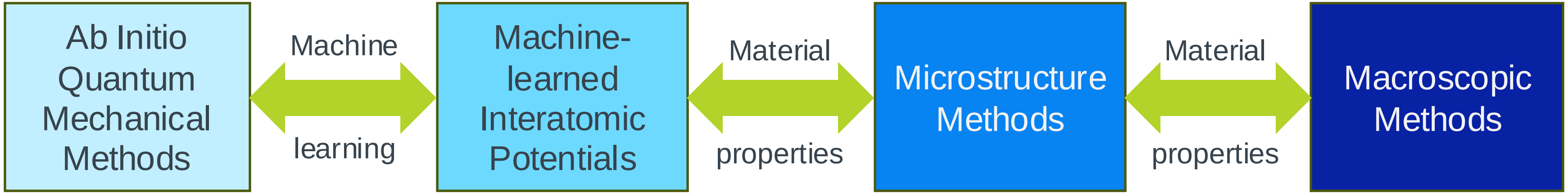
Experiment



360 days

Multiscale Materials Modeling





Ab Initio Quantum Mechanical Methods

Machine learning

Machine-learned Interatomic Potentials

Material properties

Microstructure Methods

Material properties

Macroscopic Methods

MedeA

Databases

Direct access to more than 1,1 million experimental and calculated structure entries

Builders

Rich set of builders for crystalline/amorphous/ordered systems, molecules, interfaces, nanoparticles, polymers, fluids, solids, hybrid materials, composites…

Compute Engines

DFT, classical MD and MC, semiempirical: VASP, GAUSSIAN, MOPAC, LAMMPS, GIBBS, PhaseField

Forcefields + Forcefield Optimizer + MLPG

Access to state-of-the-art Forcefields (non-reactive & reactive); open access to all FF parameters; addition of user-defined FFs; FF optimization, Machine Learning Potential Generator

Workflow Editor and Property Modules

Graphical workflows & pre-configured computational protocols, to facilitate modeling, analysis, and property prediction

High Throughput

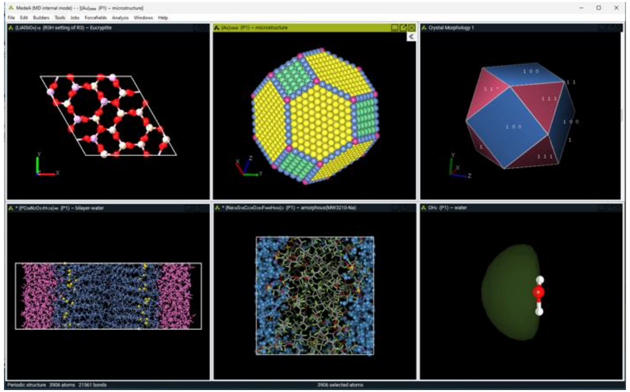
Generation of large and consistent sets of computed data & descriptors

Analysis Tools

On-the-fly analysis, post-processing for system characterization and visualization, QSAR/QSPR

JobServer & TaskServer

Automated processing of compute protocols & workflows; Reliable long-term archiving & accounting of computed data



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Materials Design Fusion Alliance

- Immediate access to state-of-the-art multiscale materials modeling software, tuned to the needs of the fusion community
- Knowledge transfer from a team of materials modelers with many years of experience
- Professional, long-term technical and scientific software support
- Ability to direct development in areas of critical need
- Access to a pre-competitive forum for the exchange of know-how in the modeling of fusion-related materials
- Option to use the software on premise or in the cloud
- Preferred access to contract research services provided by Materials Design

Acknowledgements

All customers of Materials Design

All science and technology partners, especially

- Prof. Georg Kresse (Univ. Vienna) and the entire VASP team
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- Prof. Gus Hart (Brigham-Young Univ.)
- Prof. K. Parlinski (Univ. Cracow)

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- René Windiks
- Shubham Pandey
- Volker Eyert
- Walter Wolf
- Xavier Rozanska

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Unlimited Energy? Materials Modeling for Nuclear Fusion

8-10 April 2025

Related *MedeA* Webinars

From the Femtoscale to the Mesoscale and Back: An Integrated Multiscale Approach

https://www.materialsdesign.com/webinars/recorded/from-the-femtoscale-to-the-mesoscale-and-back-an-integrated-multiscale-approach

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On-the-fly Machine Learning Forcefields with MedeA VASP

https://www.materialsdesign.com/webinars/recorded/medea-training-on-the-fly-machine-learning-forcefields-with-medea-vasp

Highlighted *MedeA* Modules

***MedeA Environment*:** The *MedeA*] software package is the leading environment for the atomistic simulation of materials. *MedeA* enables professional, day-to-day deployment of atomic-scale and nano-scale computations for materials engineering, materials optimization and materials discovery. In *MedeA*, world-class simulation engines are integrated with elaborate property prediction modules, experimental databases, structure builders and analysis tools, all in one user-friendly environment.

***MedeA VASP*:** Comprehensive access to the VASP Code via a graphical user interface (GUI) to set up, run and analyze multi-step VASP calculations

***MedeA LAMMPS*:** Full access to the LAMMPS Code via a graphical user interface based on flowcharts to perform forcefield calculations using MLPs generated by *MedeA* MLPG

***MedeA UNCLE*:** expands access to materials and properties at the meso and micro scales. Maintaining the predictive power and accuracy of abinitio Density Functional methods, *MedeA UNCLE* lets you determine stable multi-component crystal structures and rank metastable structures by enthalpy of formation.

***MedeA Phonon*:** allows you to explore the temperature dependence of free energies and heat capacities, the vibrational motions that lead to reactions and phase transitions, as well as Infrared and Raman spectra of structural models with ease and computational efficiency. The module can operate with VASP, LAMMPS or MOPAC as a computational engine.

***MedeA Microstructure Builder*:** creates microstructure models for atomistic simulations using a *Seed & Growth* algorithm with starting points either placed randomly or at user-specified coordinates within a supercell. Each such point is used as an origin to grow a crystalline grain by adding atoms from that seed point outwards, until a grain boundary is encountered.

***MedeA MLPG*:** Fully integrated workflow from training-set generation (using *MedeA* HT) and MLP generation to MLP application using *MedeA* LAMMPS

***MedeA High Throughput*:** Generation of large and consistent sets of computed data for input to machine learning procedures

***MedeA PhaseField*:** MedeA PhaseField models material microstructures over larger length and time scales than atomistic simulations. It combines MedeA's advanced tools to solve phase field, mass transport, and elasticity equations, predicting grain growth, phase separation, diffusion, and stress changes. It’s used to predict the properties of alloys, ceramics, and organic materials at engineering scales and timescales.

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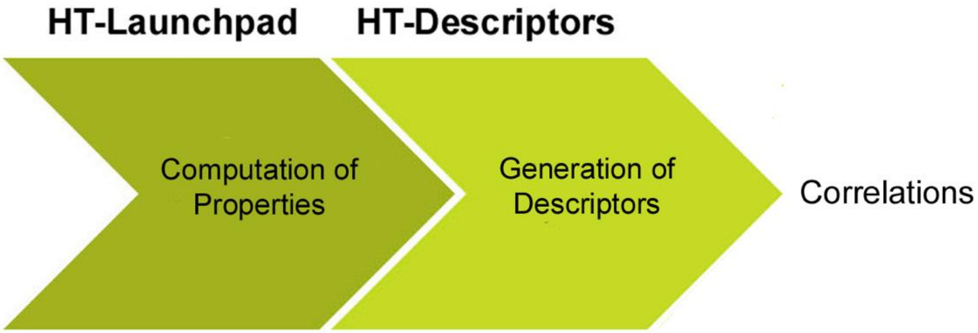
HT Training

April 29, 2025

8 am -12 pm Pacific

Registrations opening soon

https://www.materialsdesign.com/webinars



VIENNA

The Materials Design annual user event will be in Vienna for 2025

October 6-8, 2025

Registrations open soon

Question and Answer Session

Erich Wimmer

Materials Design

Gerhard Engel

Materials Design

Questions about Materials Design Webinars

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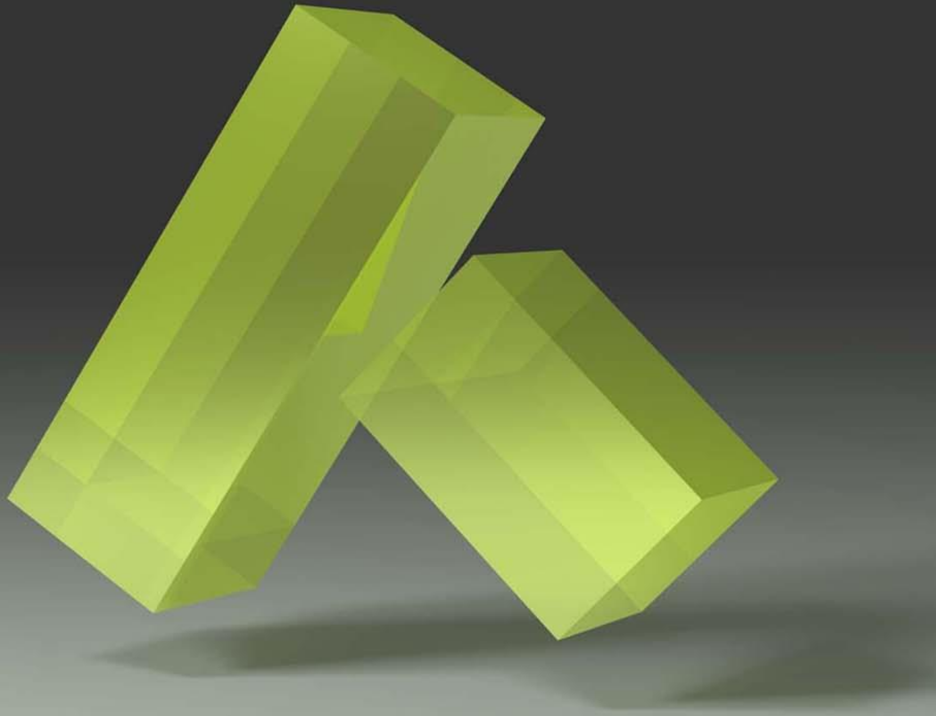

MedeA

Innovation by Simulation