Training: Advanced Atomic Model Building Based on Comprehensive Databases

René Windiks
Materials Design

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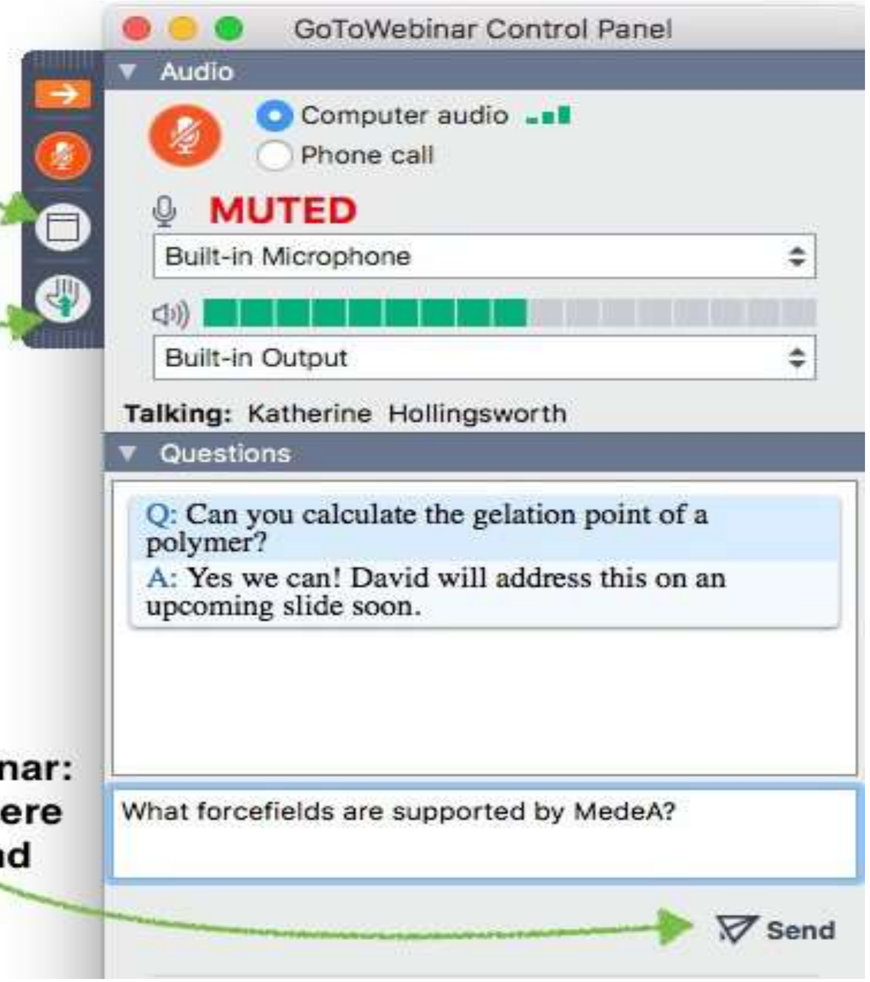

Speakers

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Training: Advanced Atomic Model Building Based on Comprehensive Databases

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Outline

- Explore MSI Phase Diagrams and extract essential structural data with *MedeA InfoMaticA*
- Convert and transform less practical structures with various *MedeA Builders*
- Visualize facets of macroscopic crystals with *MedeA Morphology*
- *MedeA Surface Builder*: Create realistic surface models for complex structures
- *MedeA Interface Builder*: Construct models with minimal strain & lattice mismatch
- *MedeA Nanobuilder*: Build particles, tubes, pipes, and rods
- *MedeA Docking*: Deposit molecules on surfaces or in nanopores

MedeA Software Environment: Overview

Engines

VASP, GIBBS, LAMMPS, GAUSSIAN, MOPAC

Databases

ICSD, Pearson's, NIST, COD, InfoMaticA Query Engine

Binary & ternary phase diagrams

Builders

Crystals, nanoparticles, amorphous materials, interfaces, molecules, polymers, conformers, thermosets, docking

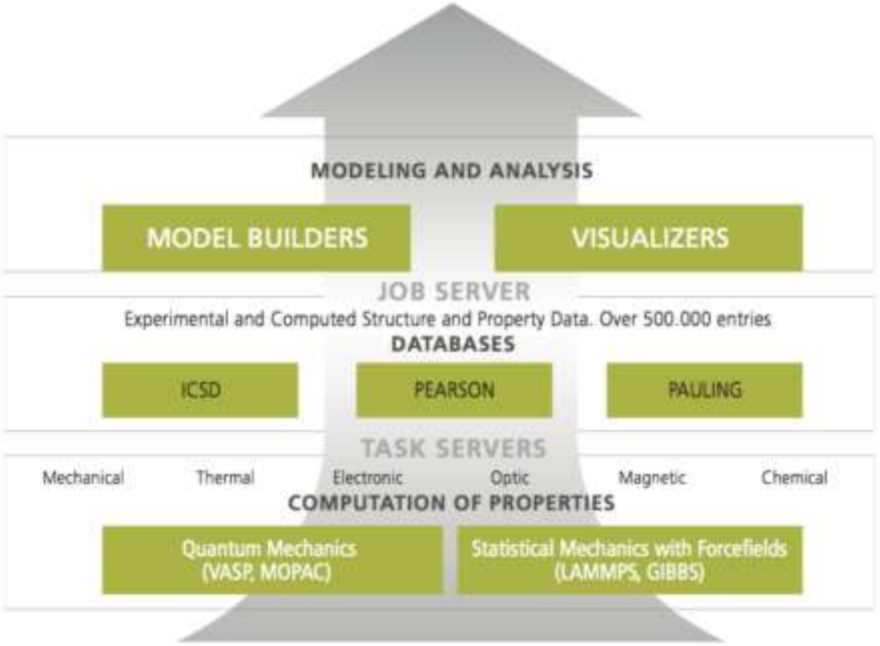
Forcefields

Forcefields bundle, Forcefields Optimizer

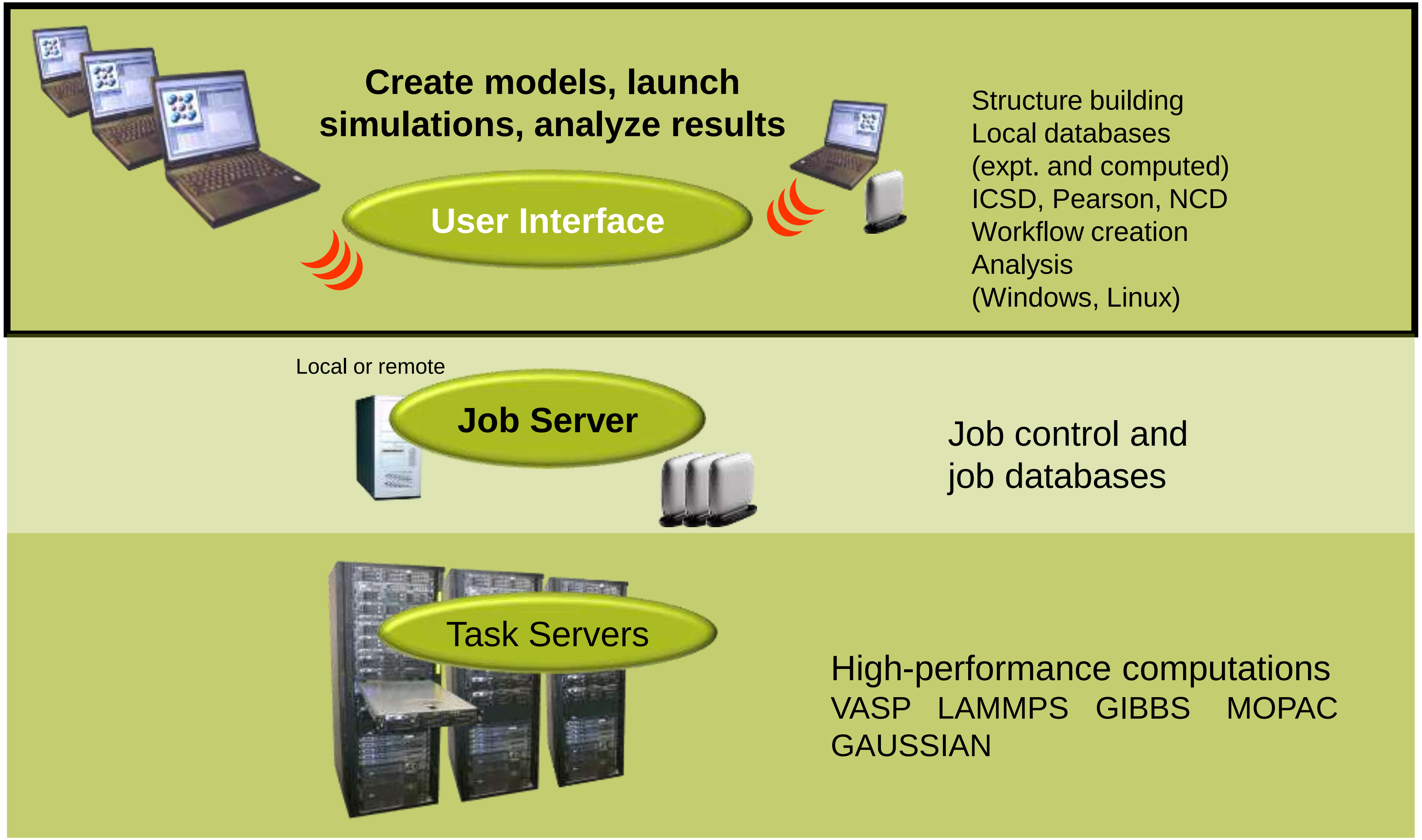
Property Modules

MT, TSS, Phonon, Electronics, UNCLE, LAMMPS (Diffusion, Thermal Conductivity, Viscosity, Cohesive Energy Density, Surface Tension, Deposition, Deformation), QT, P3C, QSPR

- High Throughput
  - HT-Launchpad, HT-Descriptors, HT-Correlation
- Analysis
  - Broad range of analysis tools
- JobServer & TaskServer



MedeA 3-Tier Architecture



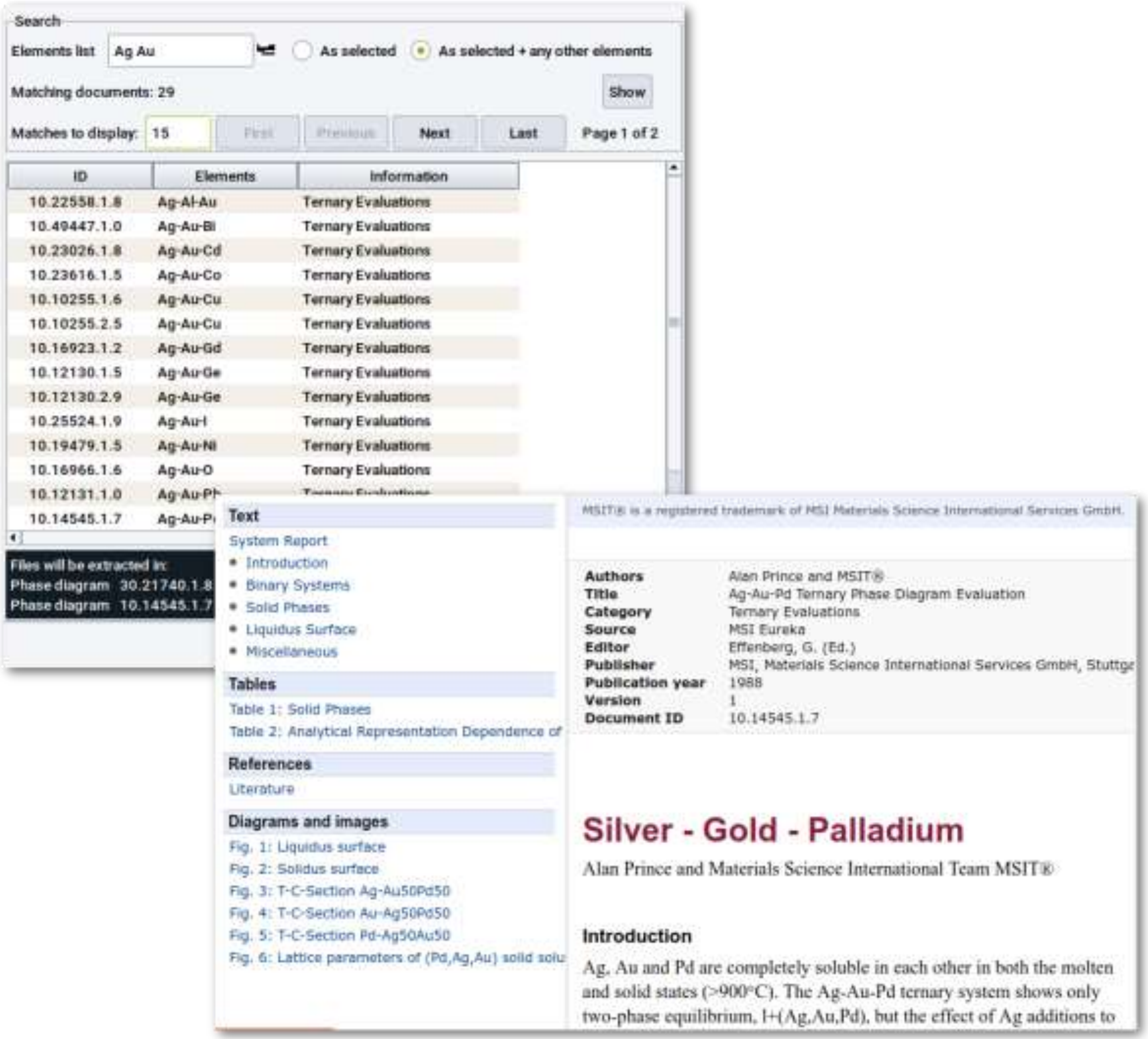
Explore MSI Phase Diagrams and Extract Essential Structural Data With *MedeA InfoMaticA*

Comprehensive Materials World Literature Search in *MedeA*

- MSI Phase Diagrams greatly enhances *MedeA*'s modeling capabilities for your materials discovery, design, and optimization projects

- Key benefits
  - Build your modeling strategy on expertly validated thermodynamic data
  - Swift access to factsheets and critical evaluation reports
  - Seamless integration with *MedeA*

- Key features
  - Full integration with *MedeA* provides on-disk, database search
  - Quick, efficient factsheet retrieval using an intuitive, menu-based query language
  - Complements *MedeA* builders, compute engines, and analysis tools



Convert and Transform Less Practical Structures With Various *MedeA Builders*

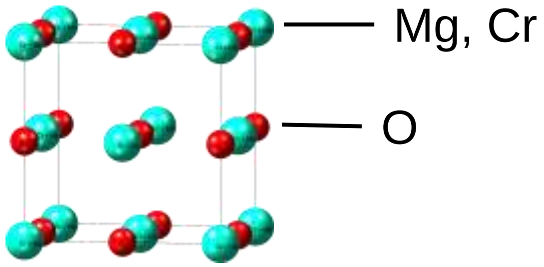
Crystal Structures With Partial Site Occupancies

- Issue: crystal structures of $Mg_{0.25}Cr_{0.5}O$ have partial occupancies for Mg and Cr, e.g. Pearson.551644

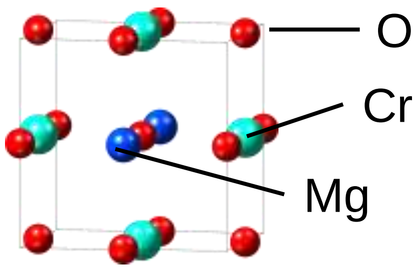
Site	Wyckoff Position	Element	X	Y	Z	Occupancy
O1	4b	O	0.50000	0.50000	0.50000	1.0
M	4a	Cr	0.00000	0.00000	0.00000	0.5025
M	4a	Mg	0.00000	0.00000	0.00000	0.2475

- Requirement: Compute engines such as VASP, LAMMPS, and GIBBS require that lattice sites are occupied or empty
- Solution: Convert crystal structures with *MedeA* features
  - Substututional Search
  - Supercell Builder
  - Random Substitution

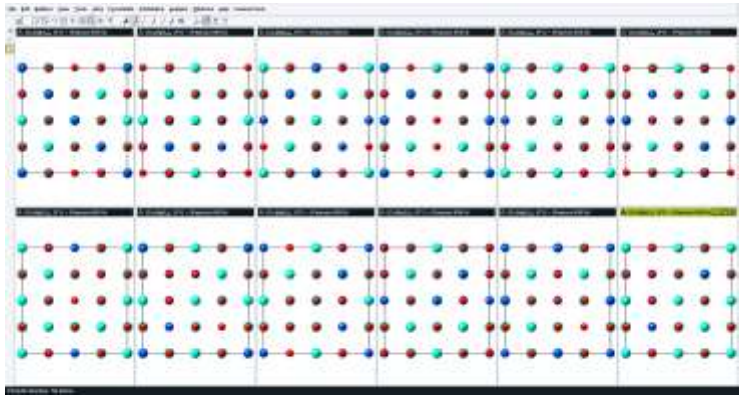
- (Mg,Cr)O, s.g. Fm-3m



- $Mg_{0.25}Cr_{0.5}O$, i.e. $MgCr_2O_4$, s.g. P4/mmm

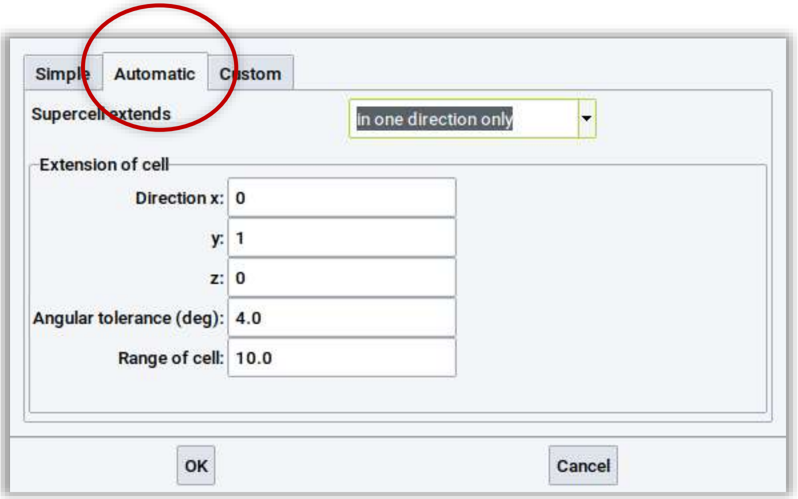


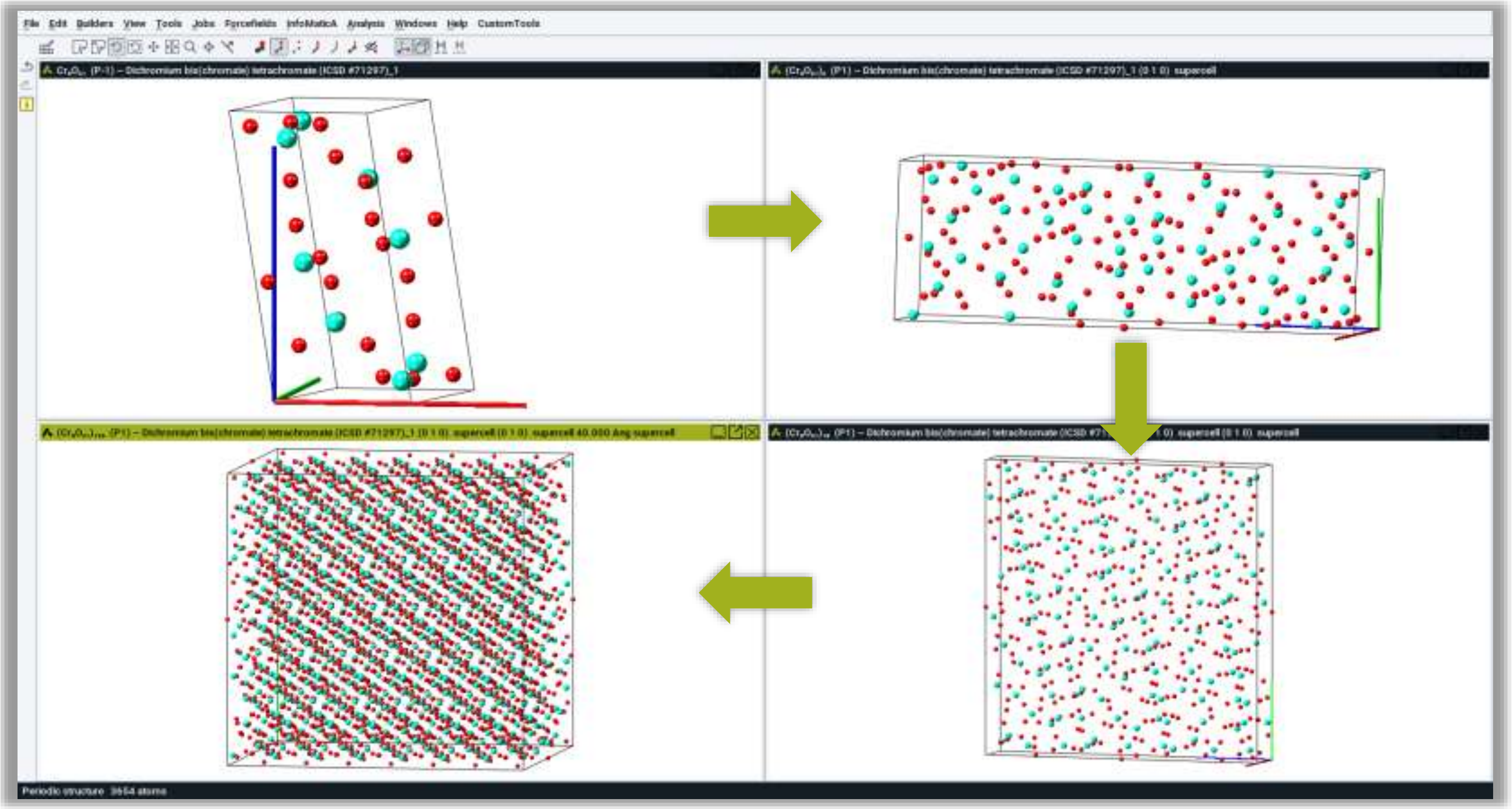
- $(MgCr_2O_4)_8$ with various symmetries



Convert Crystal Structures With Oblique Angles

- Issue: relevant crystal structure is non-orthorhombic
- Advantage: LAMMPS and GIBBS, work best with orthorhombic simulation cells
- Solution: Convert crystal structures with *MedeA* Supercell Builder





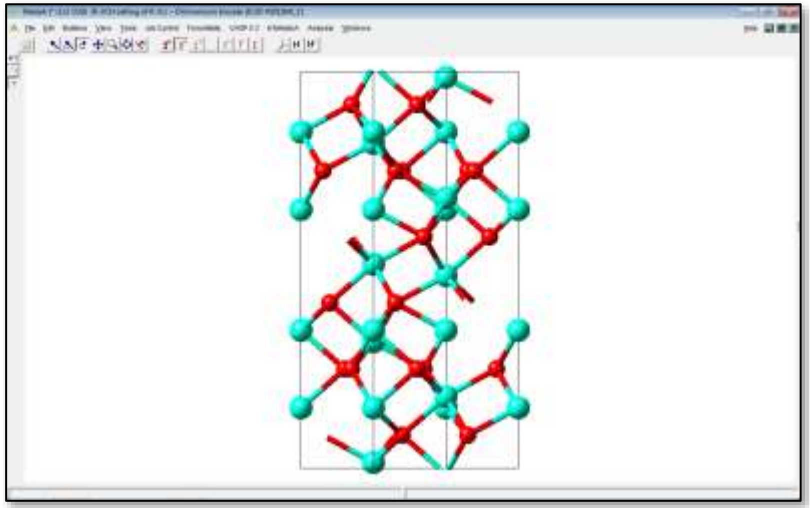
Visualize Facets of Macroscopic Crystals With *MedeA Morphology*

Morphology Simulation: Cr_2O_3

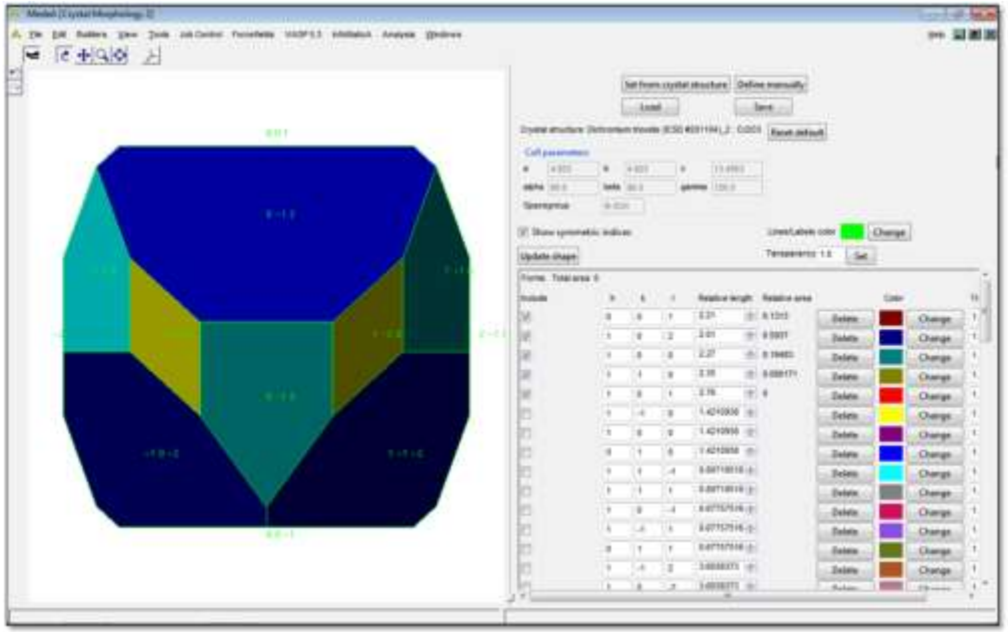
- Surface energies*)

Surface	Energy (J/m^2)
0001	2.21
1012	2.01
1010	2.27
1120	2.35
1011	2.76

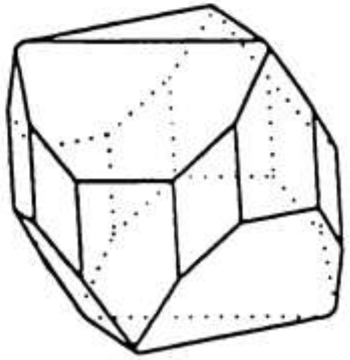
- Crystal structure



- *MedeA Morphology*



- Morphology of Davies et al.*)



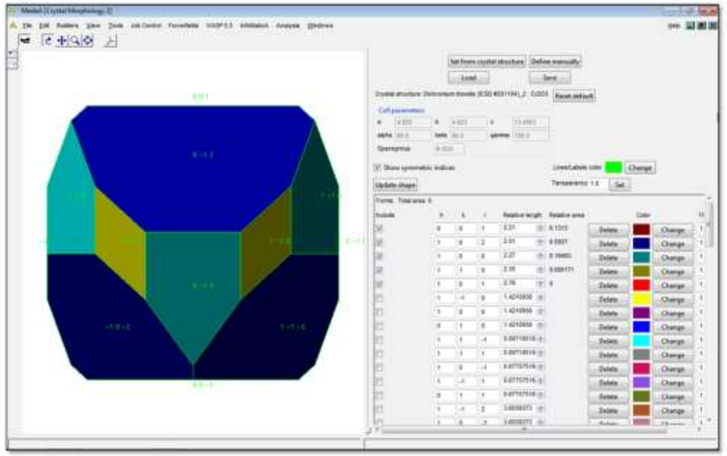
(b)

*)Davies et al. J. Chem. Soc., Faraday Trans. 2: Mol. Chem. Phys., **85**(5), 555-563 (1989).

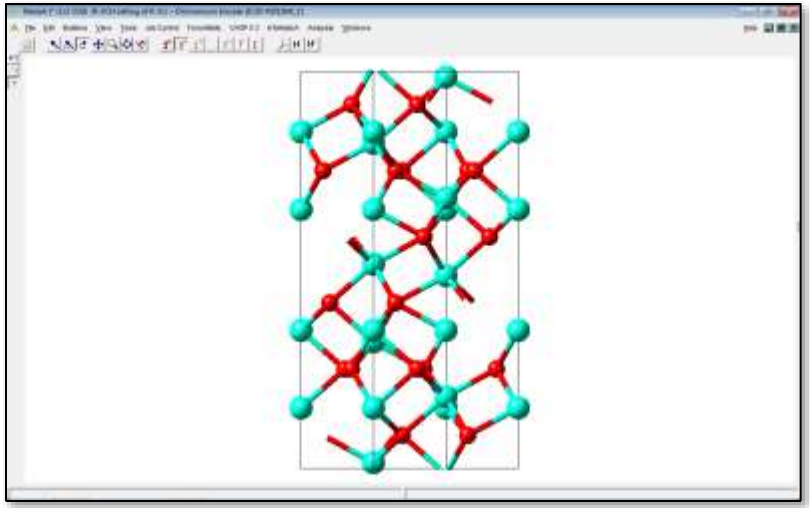
MedeA Surface Builder: Create Realistic Surface Models for Complex Structures

Model for (102) Surface of Cr_2O_3

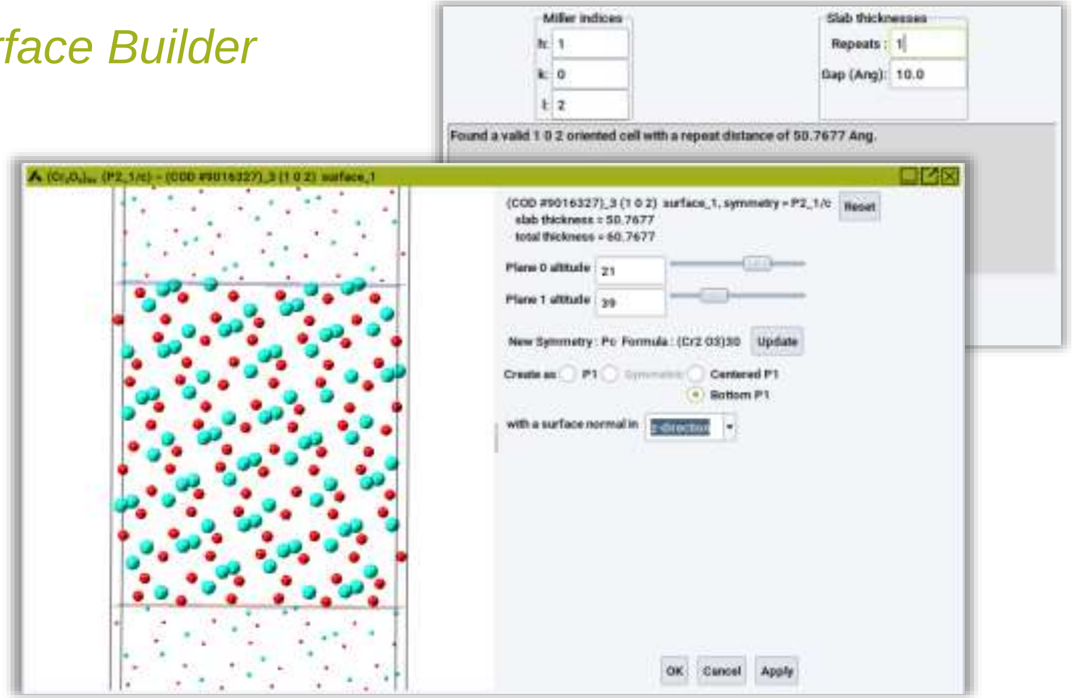
- *MedeA Morphology*



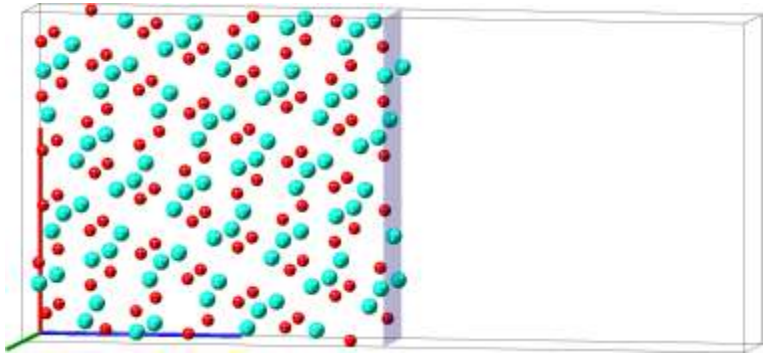
- Crystal structure



- *MedeA Surface Builder*



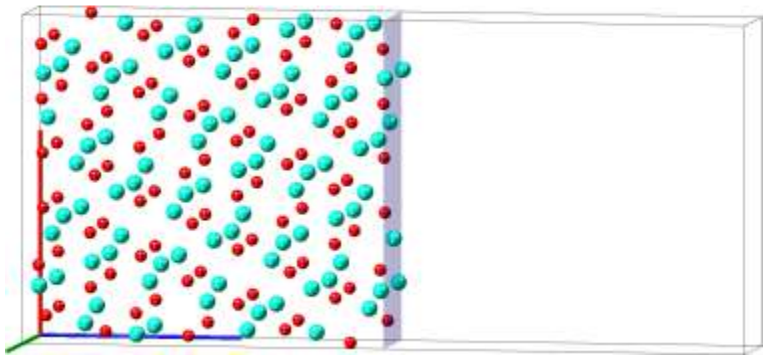
- (102) Surface model



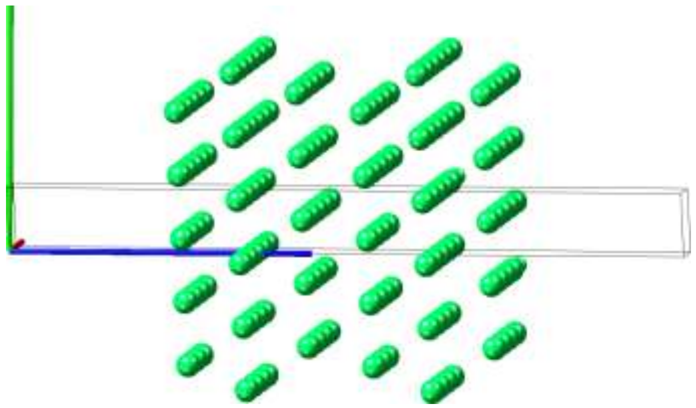
MedeA Interface Builder: Construct Models With Minimal Strain & Lattice Mismatch

Model Cr_2O_3 (102) / Fe(111) Interface

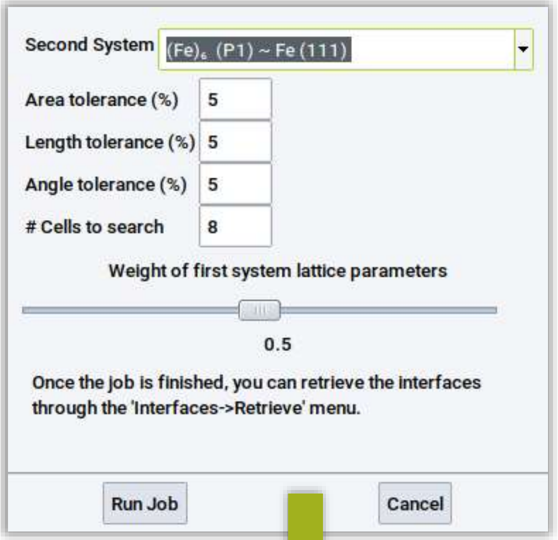
- Cr_2O_3 (102) Surface model



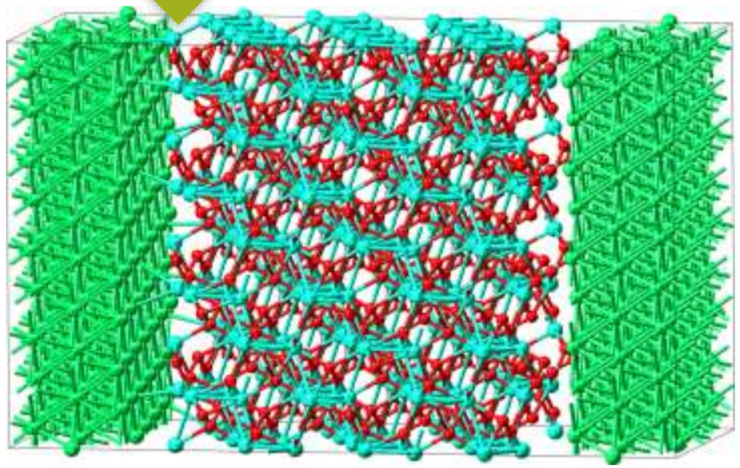
- Fe (111) surface model



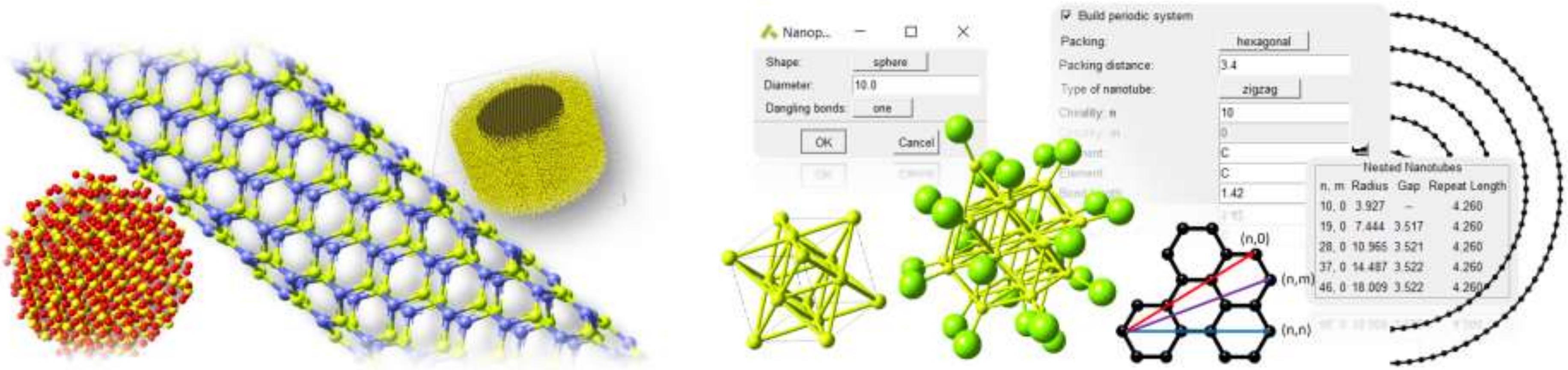
- *MedeA Interface Builder*



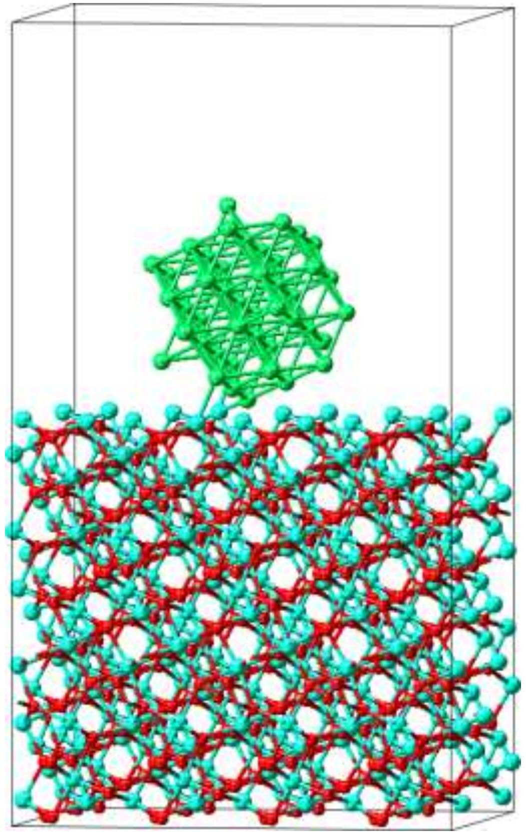
- Interface model

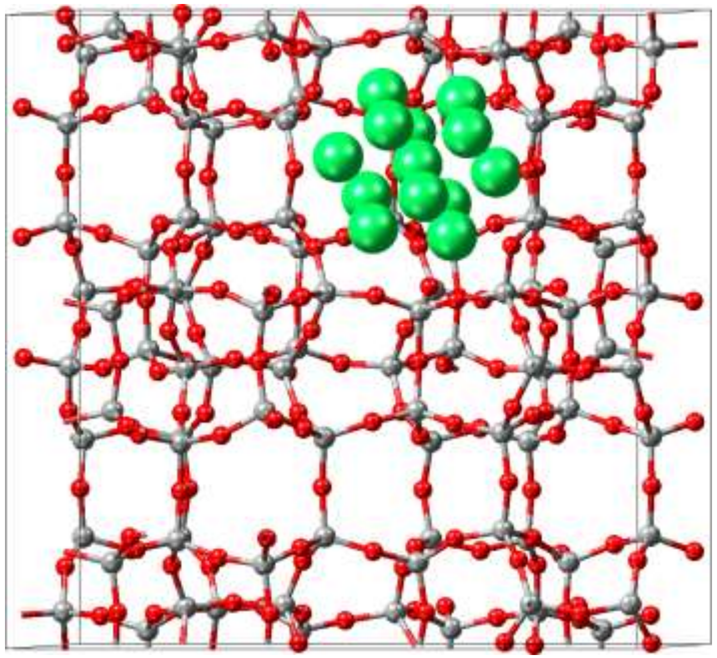


MedeA Nanobuilder: Build Particles, Tubes, Pipes, and Rods



MedeA Docking: Deposit Molecules and Particles on Surfaces or in Nanopores





Conclusion: What we have learned …

- Explore MSI Phase Diagrams and extract essential structural data with *MedeA InfoMaticA*
- Convert and transform less practical structures with various *MedeA Builders*
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Upcoming Webinar

Development of New Solvents for CO_2 Capture Using Molecular Simulations

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March 23rd, 2021

MedeA Modules Used in the Training

- *MedeA Environment*
- *MedeA MSI Phase Diagrams*
- *MedeA InfoMaticA & Databases*
- *MedeA Builders*
- *MedeA Interface Builder*
- *MedeA Morphology*
- *MedeA Docking*
- *MedeA HT Launchpad*

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Question and Answer Session

Dr. René Windiks

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Dr. David Reith

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Questions about Materials Design Trainings

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MedeA

Innovation by Simulation