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Training: Advanced Atomic Model Building Based on Comprehensive Databases

René Windiks
Materials Design



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 - Click on Related Resources

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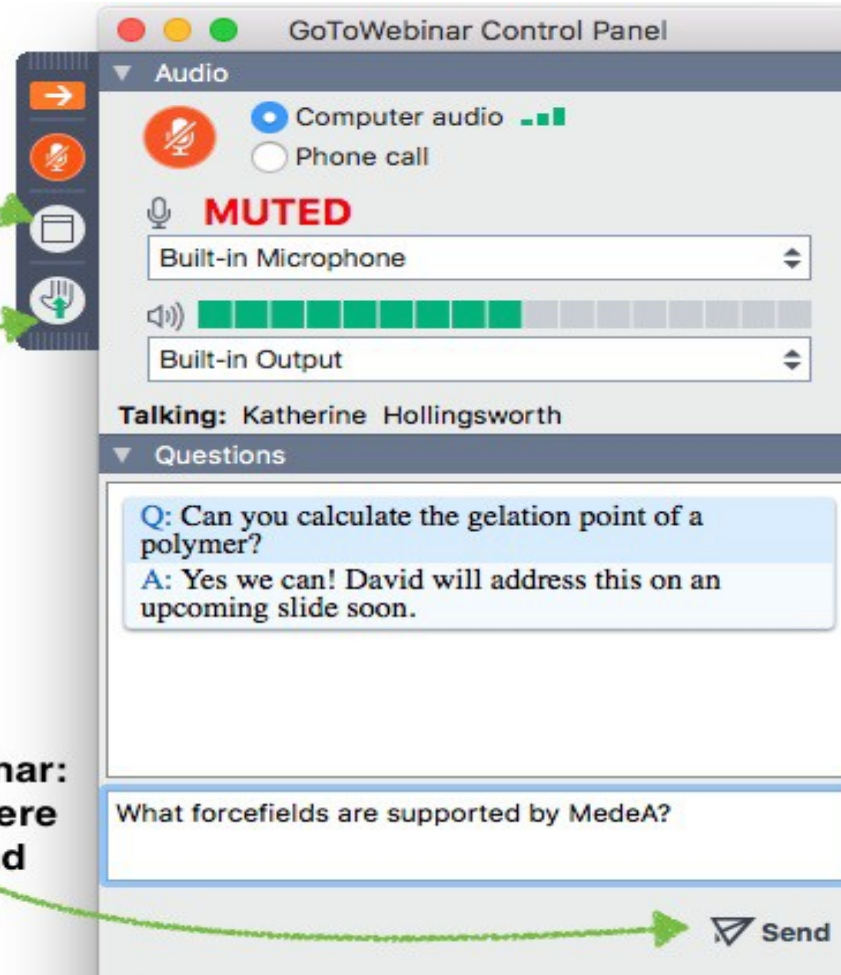
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Please Ask Questions!

Use the raise hand icon to bring attention to your question

full screen
during discussion:

**any time during webinar:
type your question here
and then press Send**



The screenshot shows the GoToWebinar Control Panel interface. It includes a sidebar with icons for full screen, mute, and raise hand. The main panel displays audio settings (Computer audio selected, muted), microphone and output device selection, and a 'Questions' section. A question is entered in the input field: 'What forcefields are supported by MedeA?'. A 'Send' button is visible at the bottom right.



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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

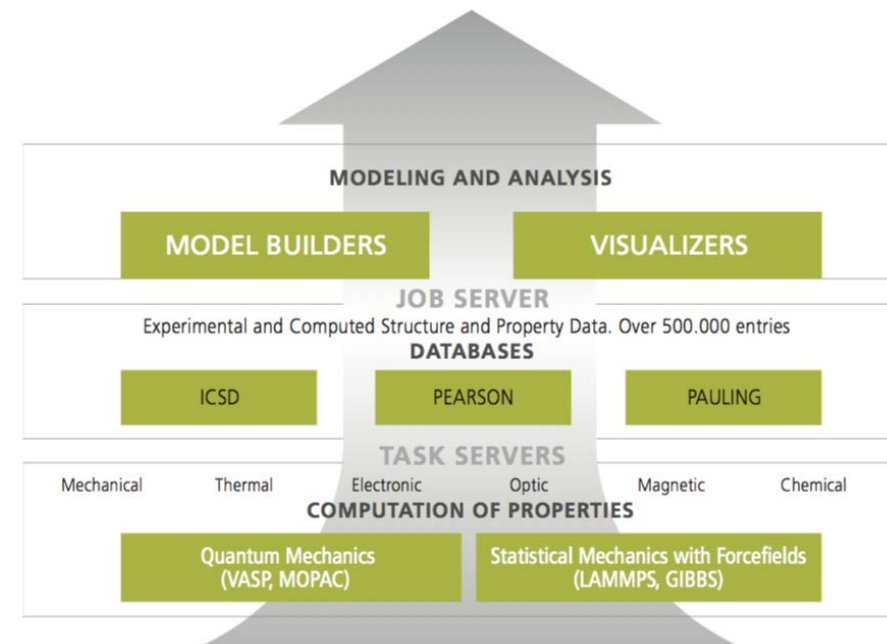
► High Throughput

- HT-Launchpad, HT-Descriptors, HT-Correlation

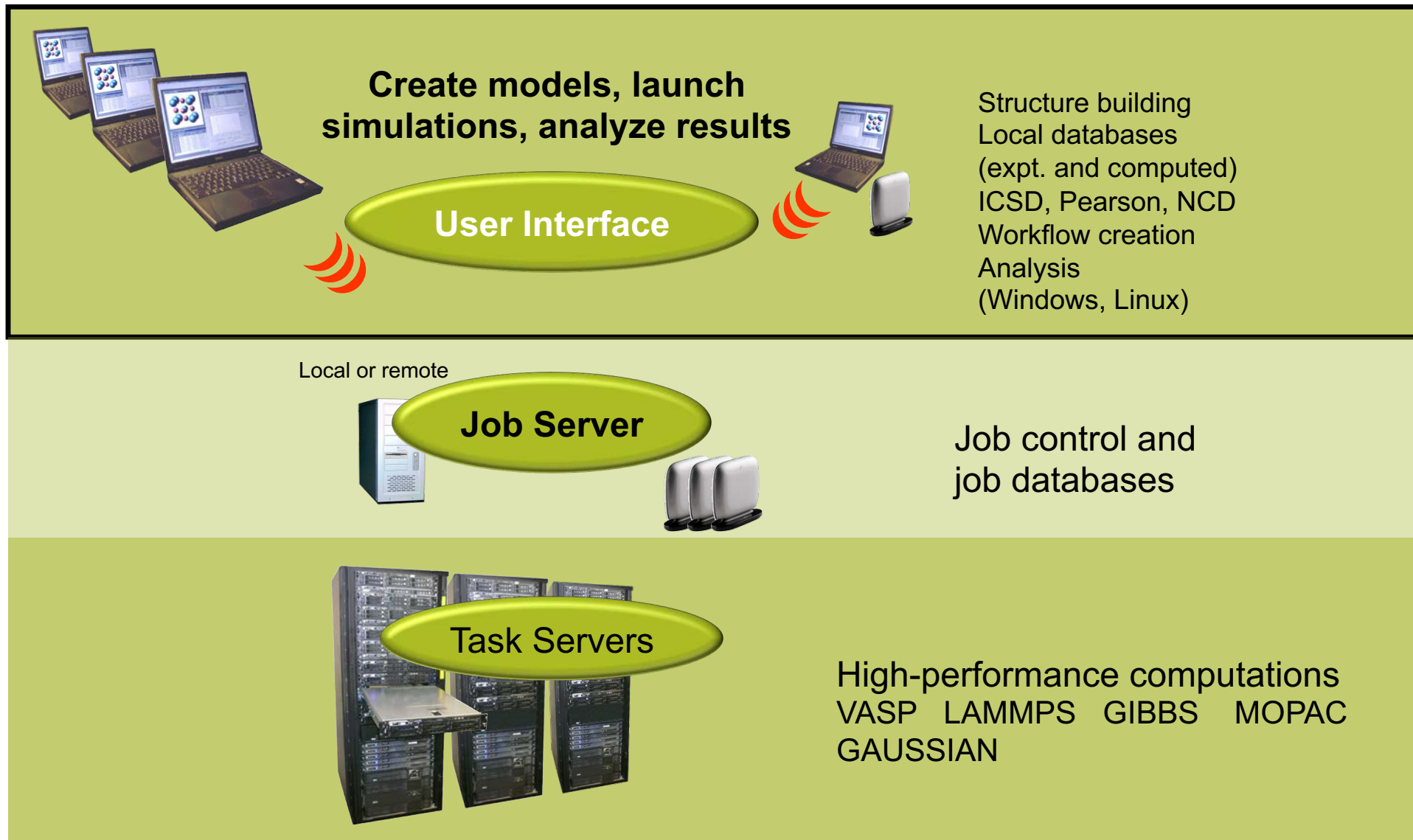
► Analysis

- 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

Search
Elements list: Ag Au As selected As selected + any other elements
Matching documents: 29
Matches to display: 15 Page 1 of 2

ID	Elements	Information
10.22558.1.8	Ag-Al-Au	Ternary Evaluations
10.49447.1.0	Ag-Au-Bi	Ternary Evaluations
10.23026.1.8	Ag-Au-Cd	Ternary Evaluations
10.23616.1.5	Ag-Au-Co	Ternary Evaluations
10.10255.1.6	Ag-Au-Cu	Ternary Evaluations
10.10255.2.5	Ag-Au-Cu	Ternary Evaluations
10.16923.1.2	Ag-Au-Gd	Ternary Evaluations
10.12130.1.5	Ag-Au-Ge	Ternary Evaluations
10.12130.2.9	Ag-Au-Ge	Ternary Evaluations
10.25524.1.9	Ag-Au-I	Ternary Evaluations
10.19479.1.5	Ag-Au-Ni	Ternary Evaluations
10.16966.1.6	Ag-Au-O	Ternary Evaluations
10.12131.1.0	Ag-Au-Pb	Ternary Evaluations
10.14545.1.7	Ag-Au-Pd	Ternary Evaluations

Files will be extracted in:
Phase diagram 30.21740.1.8
Phase diagram 10.14545.1.7

Text

- System Report
- Introduction
- Binary Systems
- Solid Phases
- Liquidus Surface
- Miscellaneous

Tables

- Table 1: Solid Phases
- Table 2: Analytical Representation Dependence of

References

Literature

Diagrams and images

- Fig. 1: Liquidus surface
- Fig. 2: Solidus surface
- Fig. 3: T-C-Section Ag-Au50Pd50
- Fig. 4: T-C-Section Au-Ag50Pd50
- Fig. 5: T-C-Section Pd-Ag50Au50
- Fig. 6: Lattice parameters of (Pd,Ag,Au) solid solu

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Authors Alan Prince and MSIT®
Title Ag-Au-Pd Ternary Phase Diagram Evaluation
Category Ternary Evaluations
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Editor Effenberg, G. (Ed.)
Publisher MSI, Materials Science International Services GmbH, Stuttgart
Publication year 1988
Version 1
Document ID 10.14545.1.7

Silver - Gold - Palladium

Alan Prince and Materials Science International Team MSIT®

Introduction

Ag, Au and Pd are completely soluble in each other in both the molten and solid states (>900°C). The Ag-Au-Pd ternary system shows only two-phase equilibrium, I+(Ag,Au,Pd), but the effect of Ag additions to



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

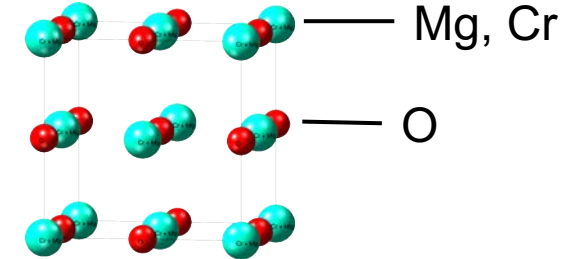
Crystal Structures With Partial Site Occupancies

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

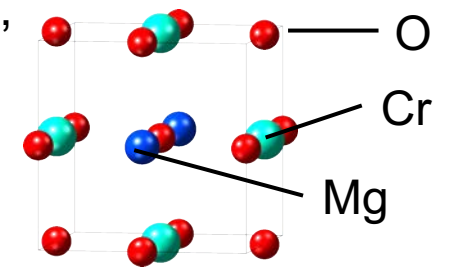
Site	Wyckoff Position	Element	X	Y	Z	Occupancy
O1	4b	O	0.50000	0.50000	0.50000	1.0
M	4a	Cr	0.00000	0.00000	0.00000	0.5025
M	4a	Mg	0.00000	0.00000	0.00000	0.2475

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

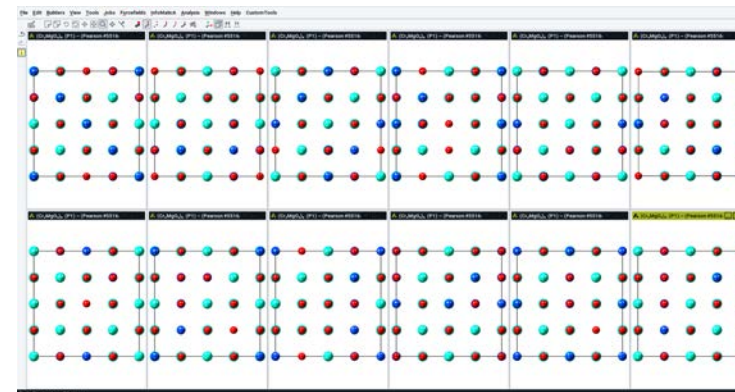
- ▶ $(\text{Mg,Cr})\text{O}$, s.g. Fm-3m



- ▶ $\text{Mg}_{0.25}\text{Cr}_{0.5}\text{O}$, i.e. MgCr_2O_4 , s.g. P4/mmm

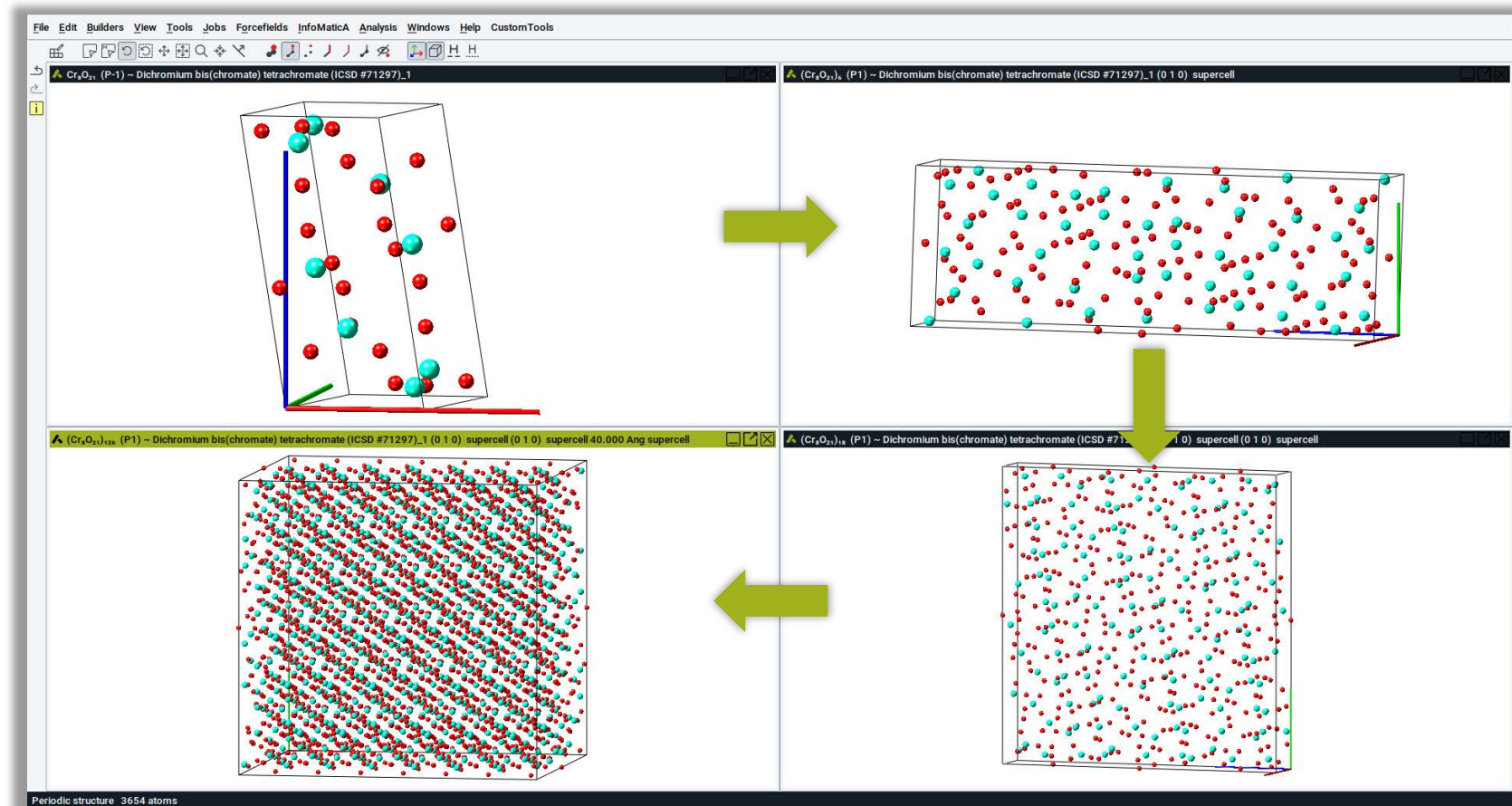
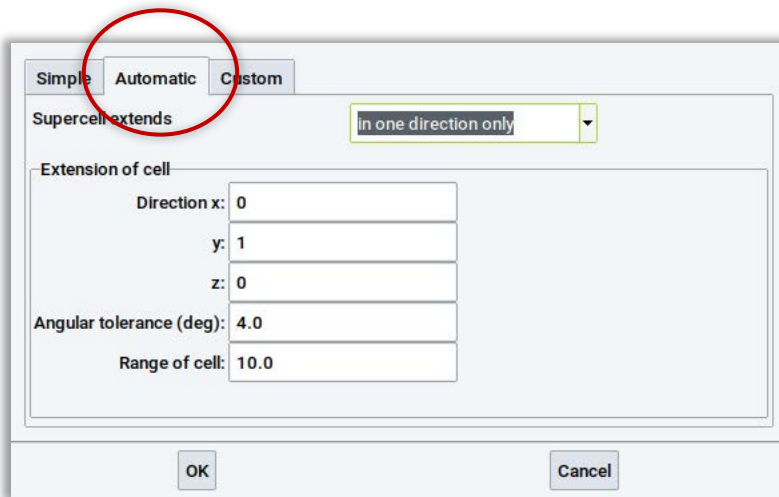


- ▶ $(\text{MgCr}_2\text{O}_4)_8$ with various symmetries



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*





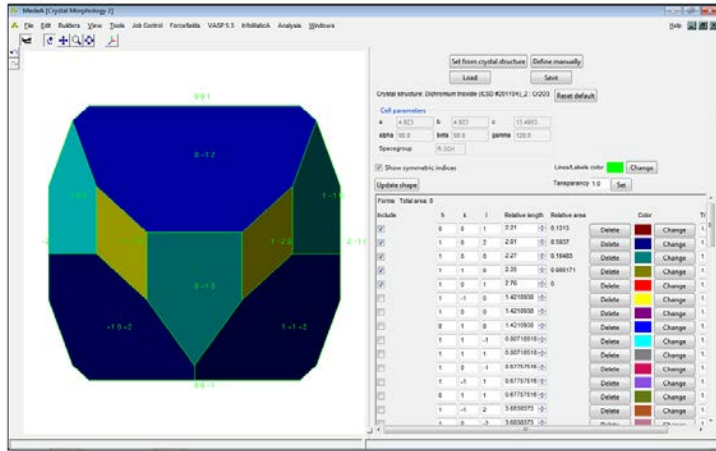
Visualize Facets of Macroscopic Crystals With *MedeA Morphology*



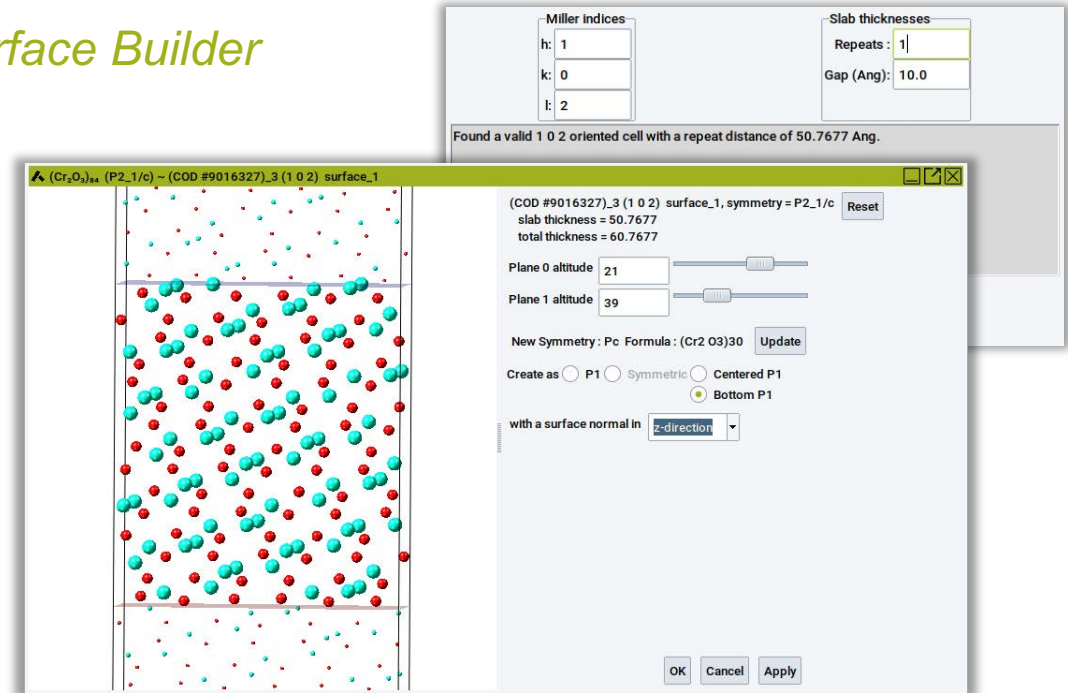
*MedeA Surface Builder: Create
Realistic Surface Models for Complex
Structures*

Model for (102) Surface of Cr_2O_3

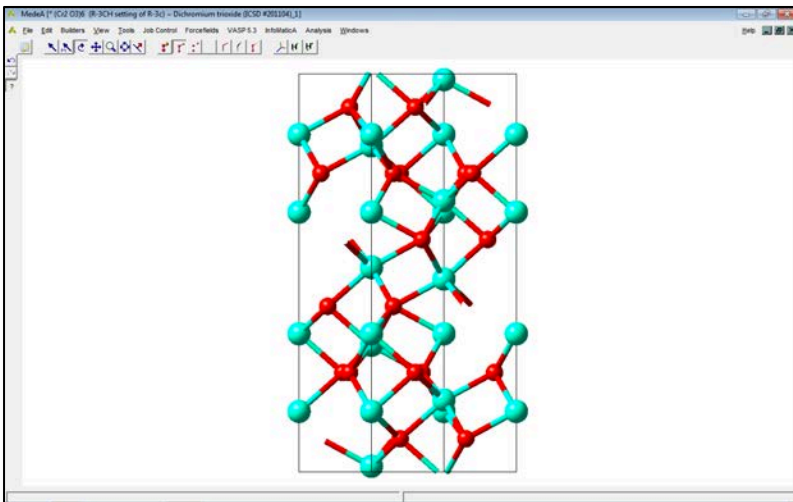
► MedeA Morphology



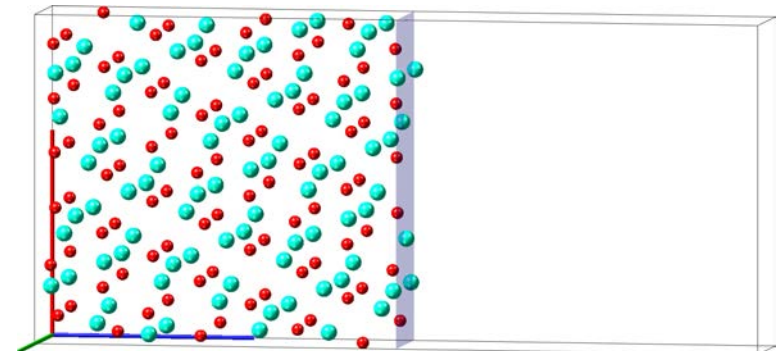
► MedeA Surface Builder



► Crystal structure



► (102) Surface model

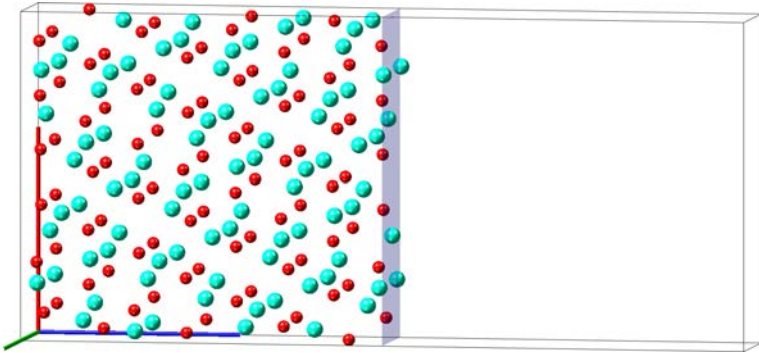




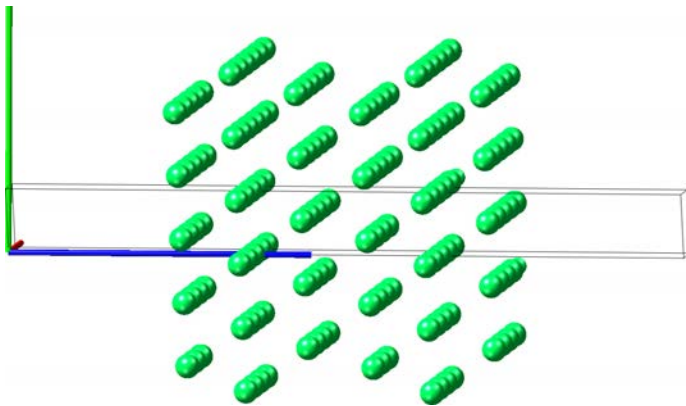
MedeA Interface Builder: Construct
Models With Minimal Strain & Lattice
Mismatch

Model Cr_2O_3 (102) / Fe(111) Interface

- ▶ Cr_2O_3 (102) Surface model



- ▶ Fe (111) surface model



- ▶ *MedeA Interface Builder*

Second System

Area tolerance (%)

Length tolerance (%)

Angle tolerance (%)

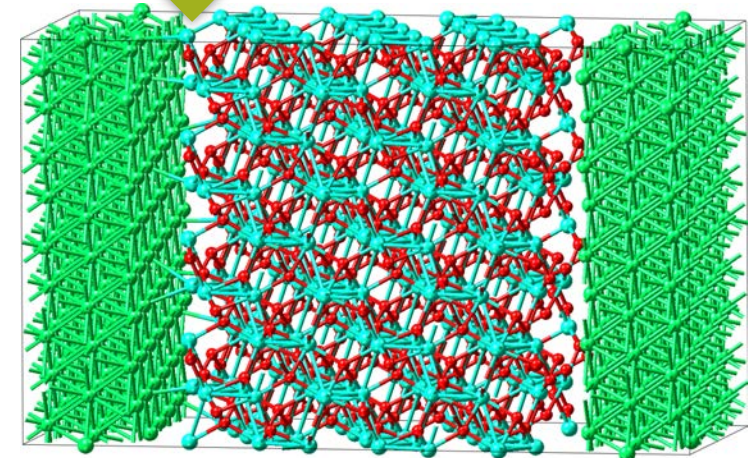
Cells to search

Weight of first system lattice parameters

0.5

Once the job is finished, you can retrieve the interfaces through the 'Interfaces->Retrieve' menu.

- ▶ Interface model





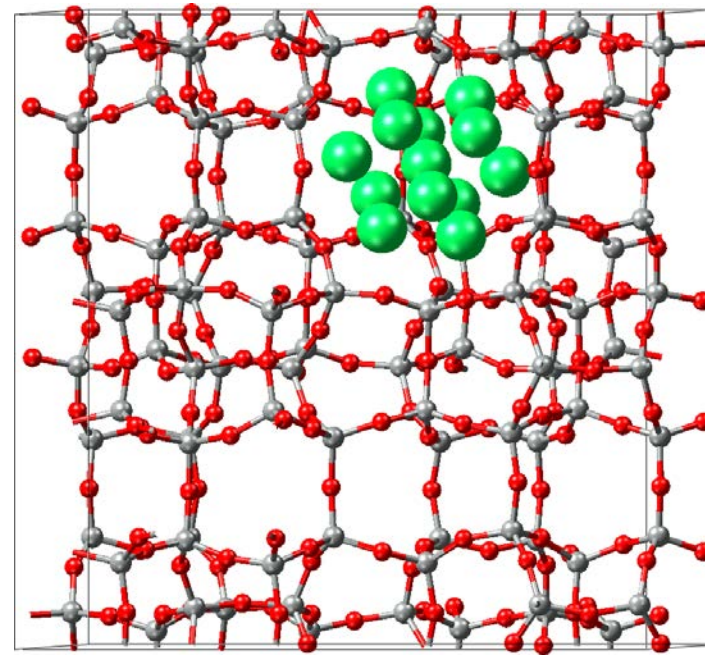
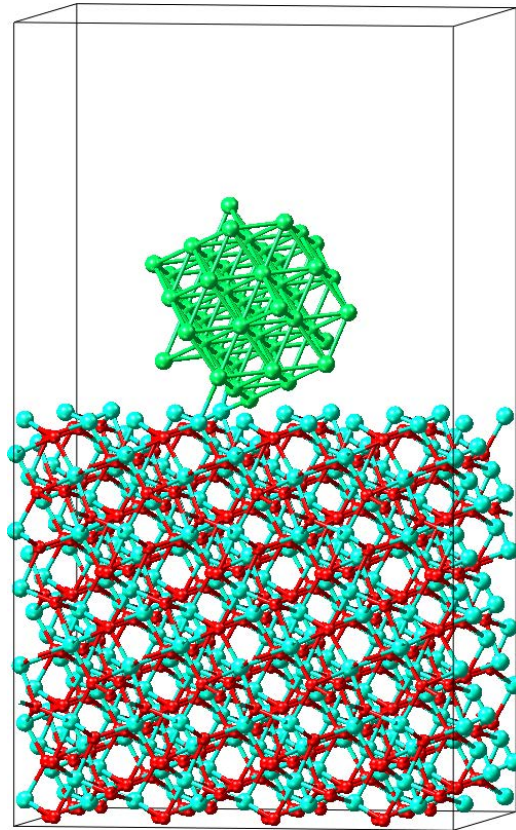
MedeA Nanobuilder: Build Particles, Tubes, Pipes, and Rods

The image displays the MedeA Nanobuilder software interface. On the left, there are three 3D molecular models: a cluster of red and yellow spheres, a long tube of blue and yellow spheres, and a yellow cylindrical shell. In the center, a 'Nanop...' dialog box is open, showing settings for 'Shape: sphere', 'Diameter: 10.0', and 'Dangling bonds: one'. To the right, another dialog box titled 'Build periodic system' is open, showing 'Packing: hexagonal', 'Packing distance: 3.4', and 'Type of nanotube: zigzag'. Below these, a 'Nested Nanotubes' table is visible, listing parameters for different nanotube configurations. To the right of the table, there are several concentric black circles representing nanotubes.

n, m	Radius	Gap	Repeat Length
10, 0	3.927	--	4.260
19, 0	7.444	3.517	4.260
28, 0	10.965	3.521	4.260
37, 0	14.487	3.522	4.260
46, 0	18.009	3.522	4.260



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*
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March 23rd, 2021

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- ▶ [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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- ▶ For questions or comments contact:

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khollingsworth@materialsdesign.com

Question and Answer Session



Dr. René Windiks

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Dr. David Reith

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Questions about Materials Design Trainings

Materials Design Support Team

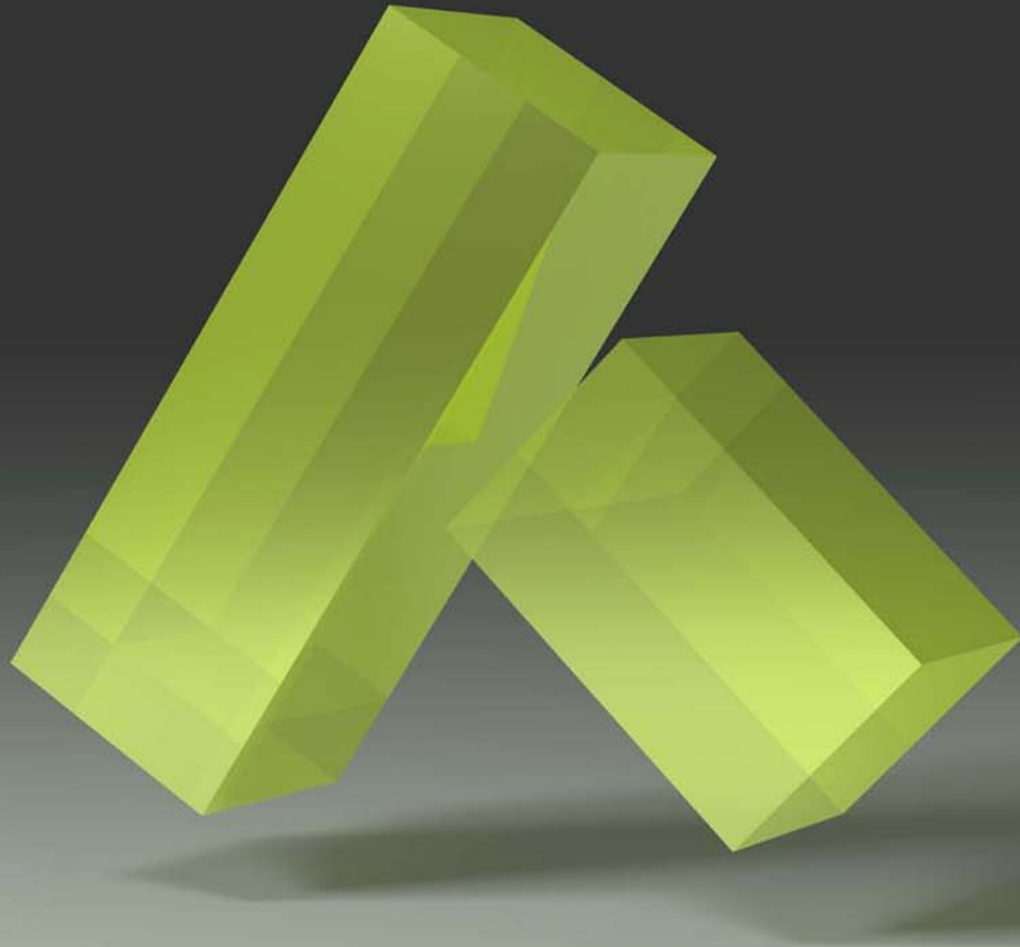
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Medea

Innovation by Simulation