



materials design®

# Training: Advanced Atomic Model Building Based on Comprehensive Databases

René Windiks  
Materials Design



# Materials Design Webinar Series

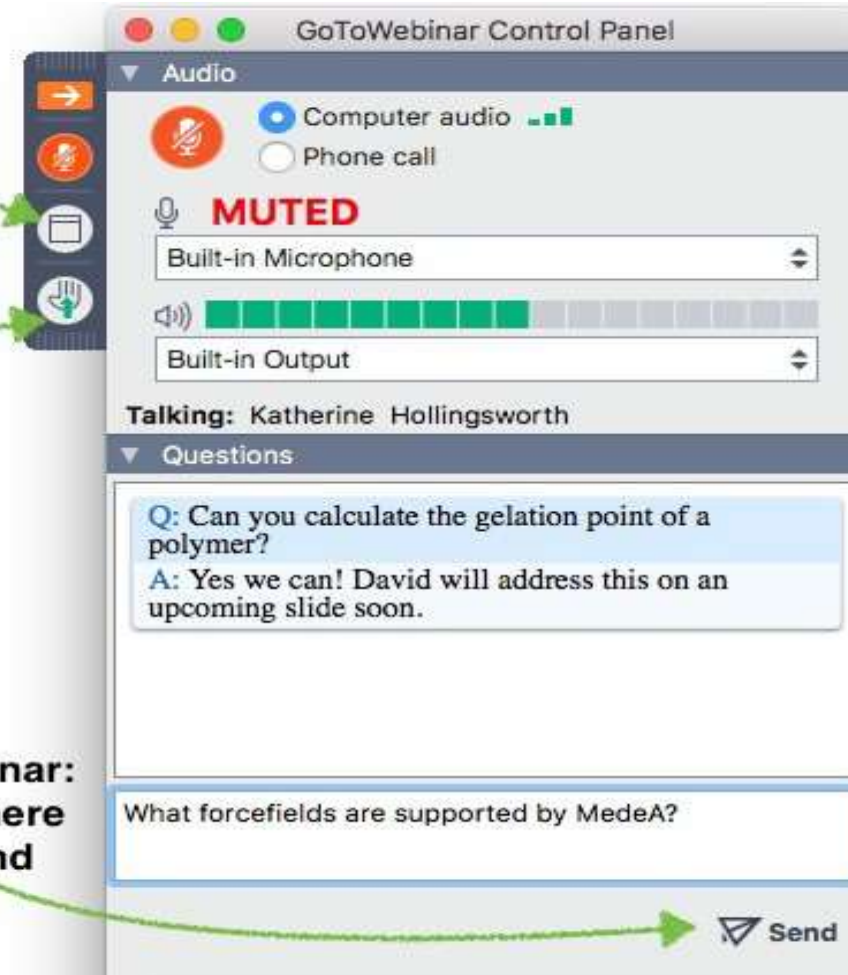
- ▶ We will be recording this training
  
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  - <http://www.materialsdesign.com/webinars/recorded>
  - The recording and training will be under the related webinar: Materials Constitution Data in MSI Eureka Fundamentals for Efficient R&D
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**Use 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**





# Speakers

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***Siwen Wang***

***René Windiks***

***Taylor Juran***

***Ray Shan***

# 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

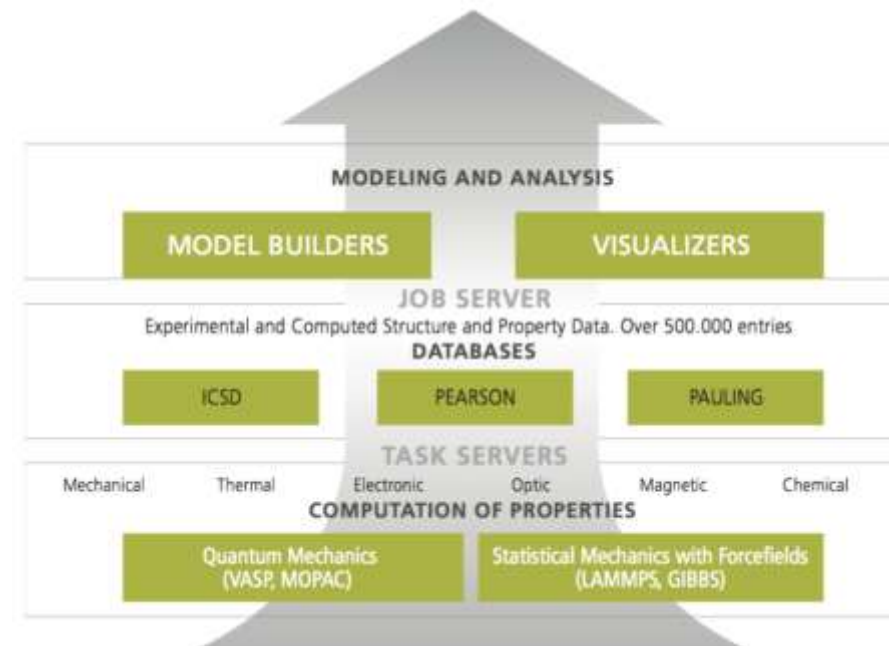
## ► High Throughput

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

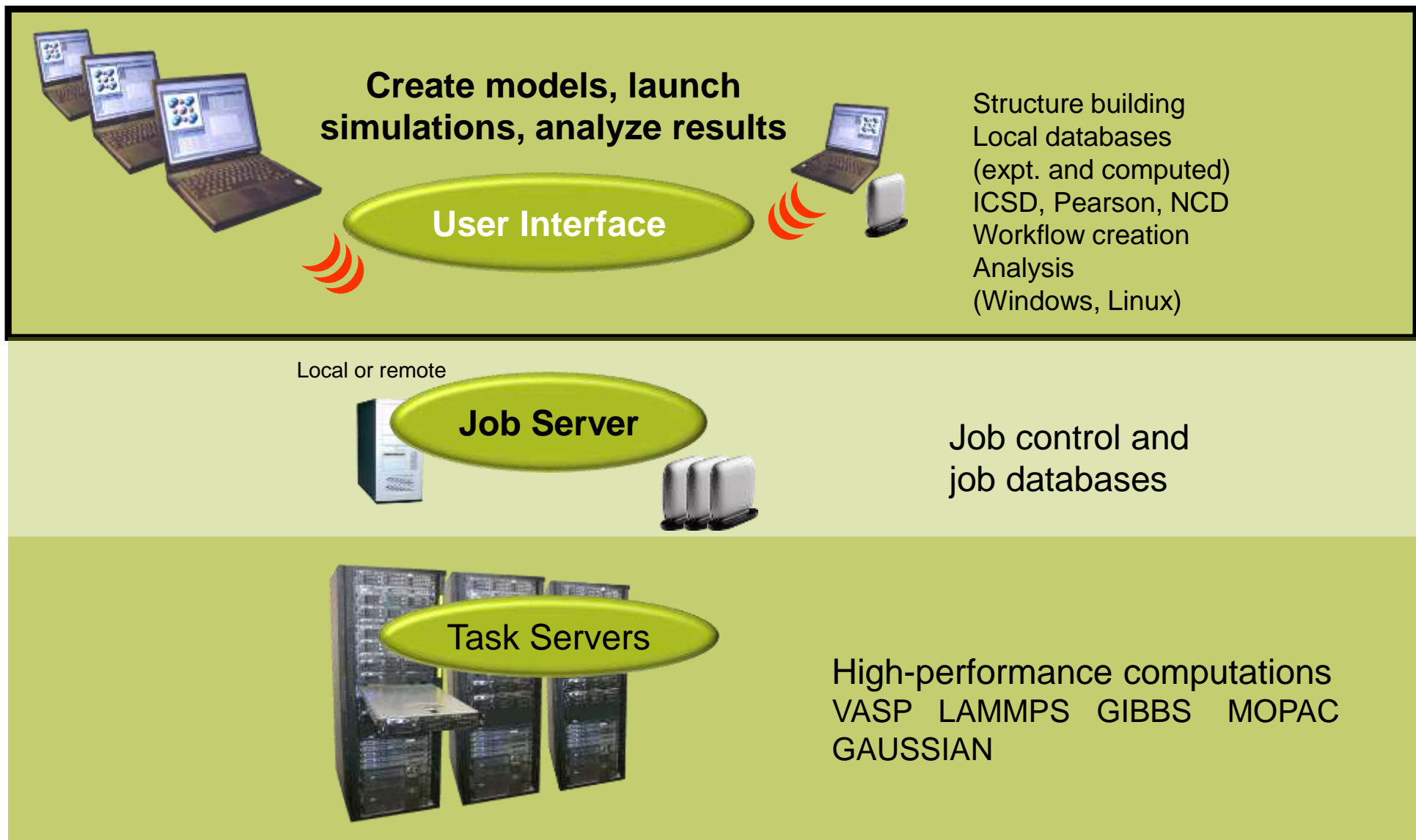
## ► Analysis

- 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

The screenshot displays the MedeA search interface. At the top, a search bar contains 'Ag Au' and options for 'As selected' and 'As selected + any other elements'. Below the search bar, it indicates 'Matching documents: 29' and 'Matches to display: 15'. A table lists search results with columns for ID, Elements, and Information. The selected document, 10.14545.1.7, is highlighted. A detailed factsheet for this document is shown, including a table of contents with sections like Text, Tables, References, and Diagrams and images. The factsheet also includes metadata such as Authors (Alan Prince and MSIT®), Title (Ag-Au-Pd Ternary Phase Diagram Evaluation), and Document ID (10.14545.1.7). The title 'Silver - Gold - Palladium' is prominently displayed in red.

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

**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

**Authors** Alan Prince and MSIT®  
**Title** Ag-Au-Pd Ternary Phase Diagram Evaluation  
**Category** Ternary Evaluations  
**Source** MSI Eureka  
**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, H-(Ag,Au,Pd), but the effect of Ag additions to



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

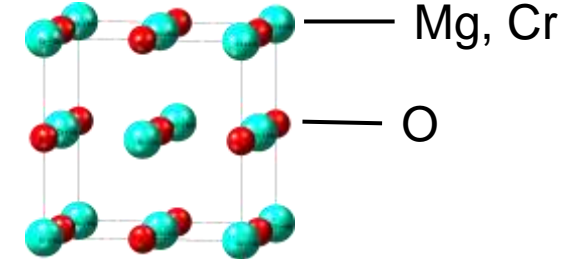
# Crystal Structures With Partial Site Occupancies

- ▶ 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

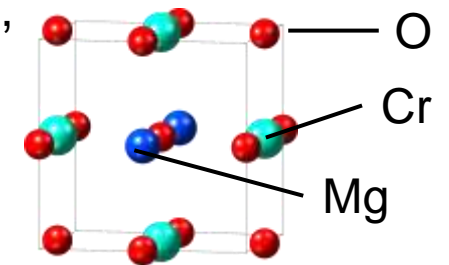
Site	Wyckoff Position	Element	X	Y	Z	Occupancy
O1	4b	O	0.50000	0.50000	0.50000	1.0
M	4a	Cr	0.00000	0.00000	0.00000	0.5025
M	4a	Mg	0.00000	0.00000	0.00000	0.2475

- ▶ 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

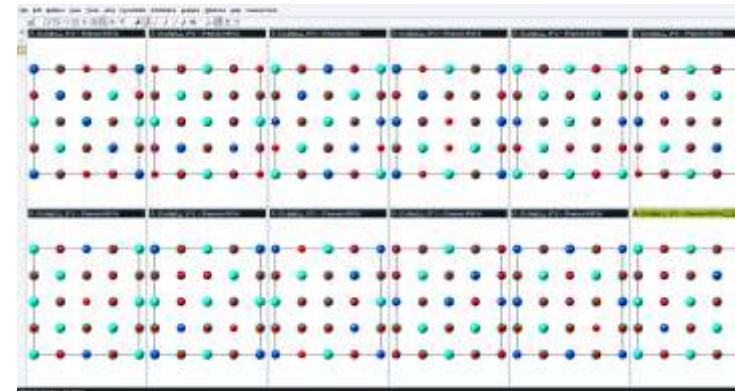
- ▶  $(\text{Mg,Cr})\text{O}$ , s.g. Fm-3m



- ▶  $\text{Mg}_{0.25}\text{Cr}_{0.5}\text{O}$ , i.e.  $\text{MgCr}_2\text{O}_4$ , s.g. P4/mmm

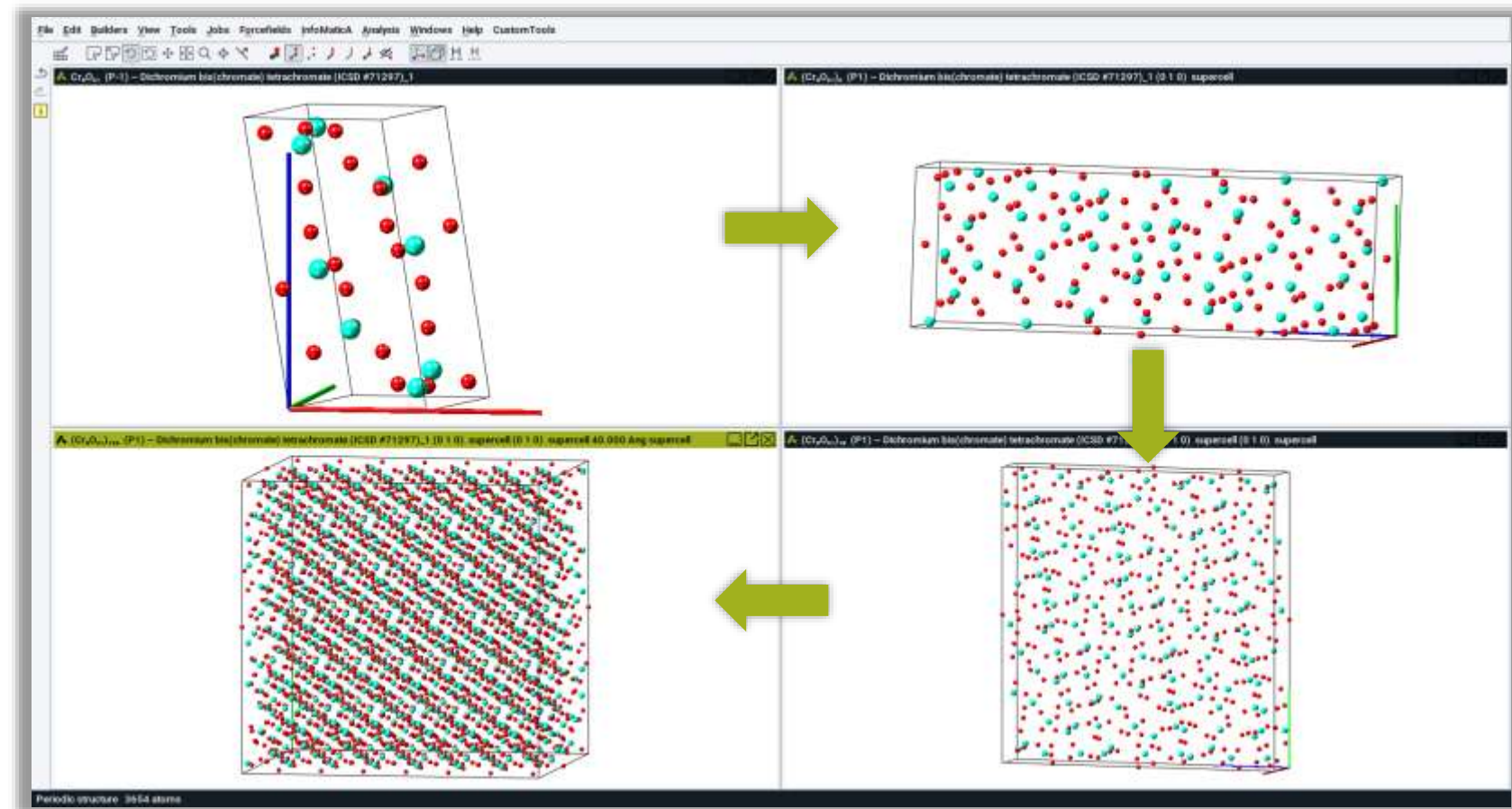
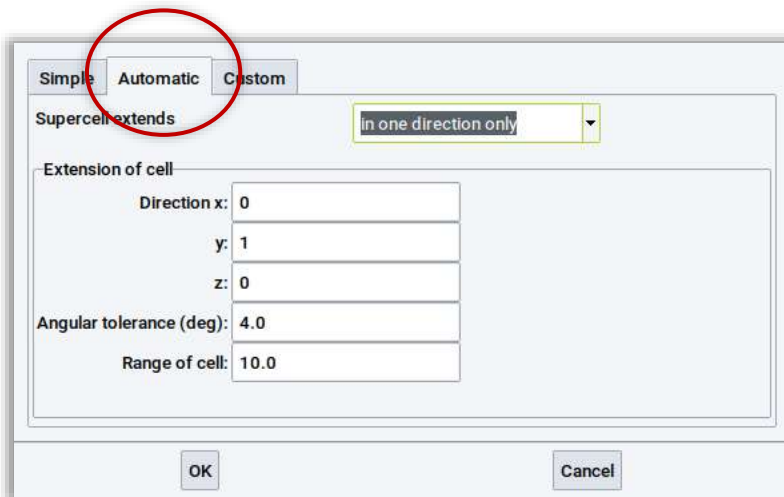


- ▶  $(\text{MgCr}_2\text{O}_4)_8$  with various symmetries



# 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*





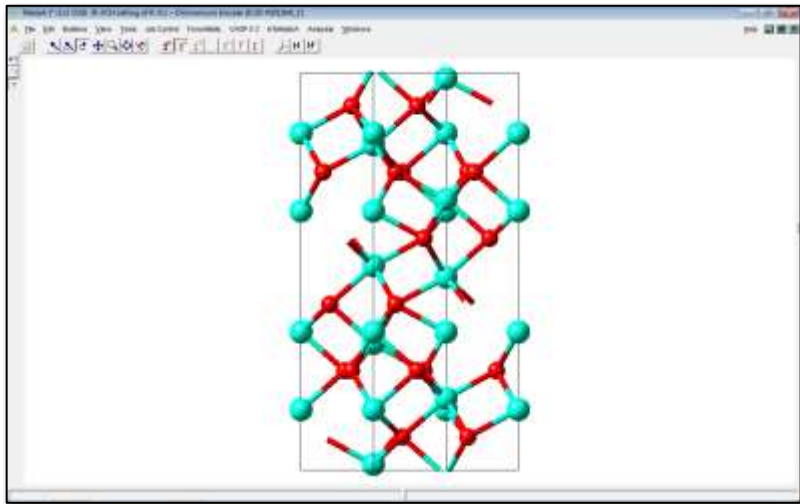
# Visualize Facets of Macroscopic Crystals With *MedeA Morphology*

# Morphology Simulation: $\text{Cr}_2\text{O}_3$

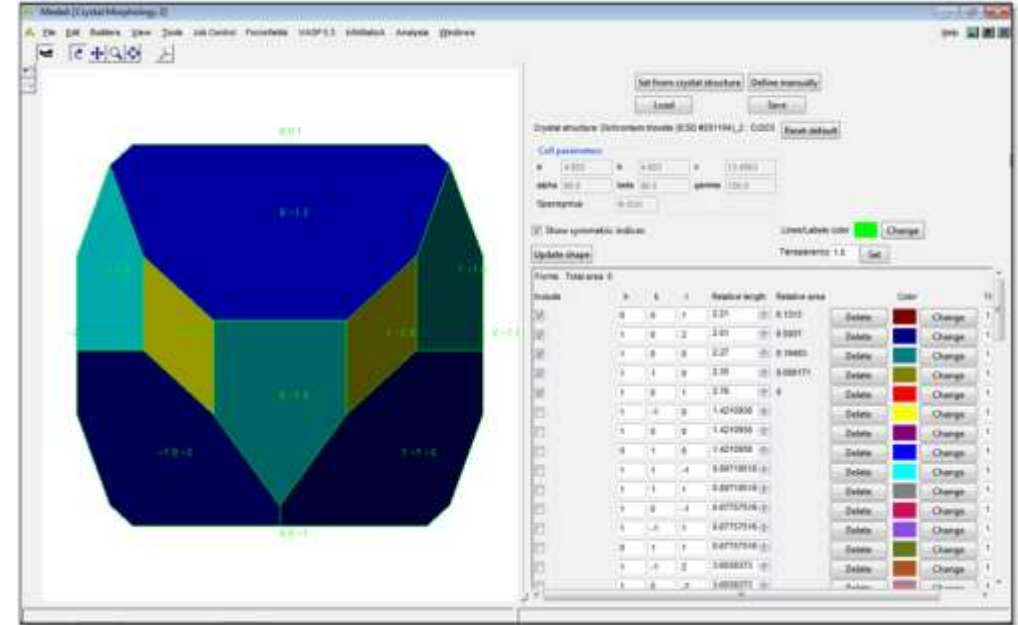
► Surface energies<sup>\*)</sup>

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

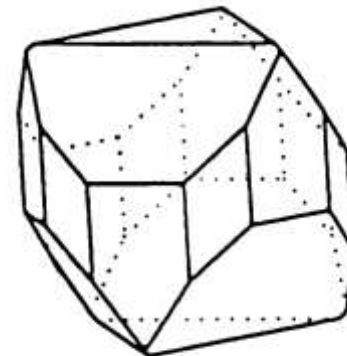
► Crystal structure



► Medea Morphology



► Morphology of Davies et al.<sup>\*)</sup>



(b)

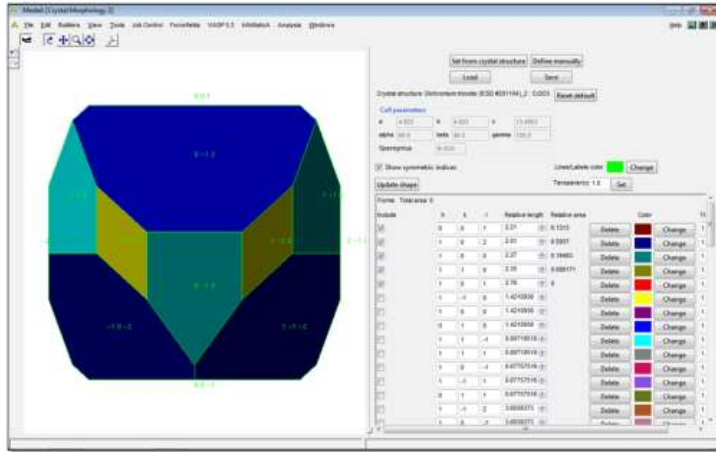
<sup>\*)</sup>Davies et al. J. Chem. Soc., Faraday Trans. 2: Mol. Chem. Phys., **85**(5), 555-563 (1989).



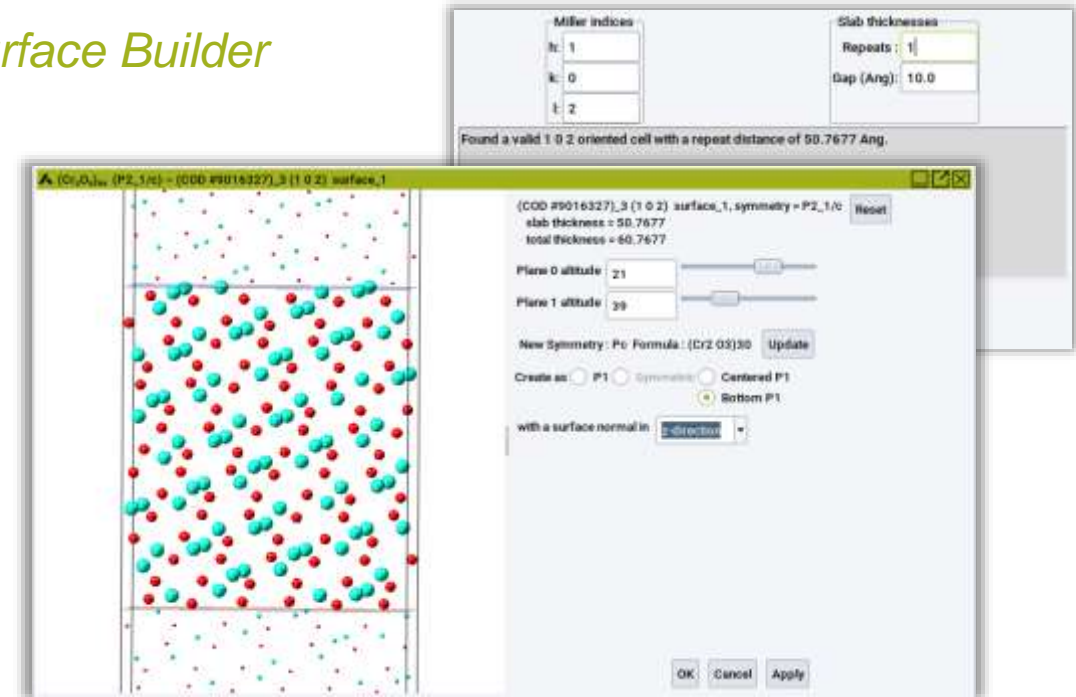
*MedeA Surface Builder. Create  
Realistic Surface Models for Complex  
Structures*

# Model for (102) Surface of $\text{Cr}_2\text{O}_3$

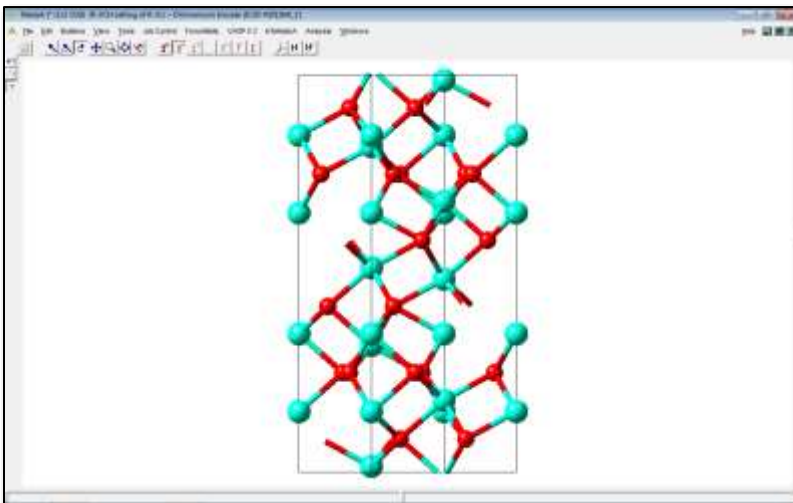
## ► MedeA Morphology



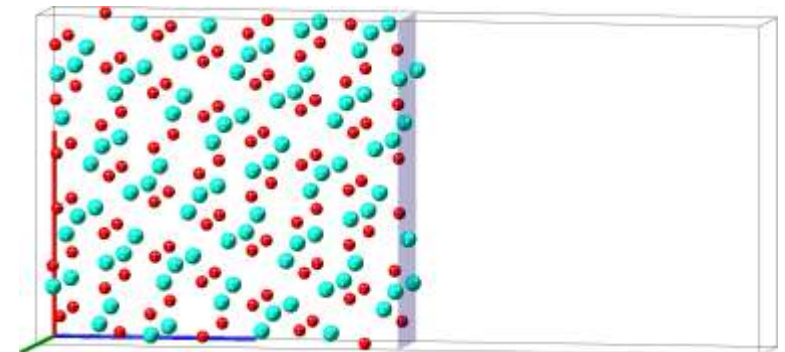
## ► MedeA Surface Builder



## ► Crystal structure



## ► (102) Surface model

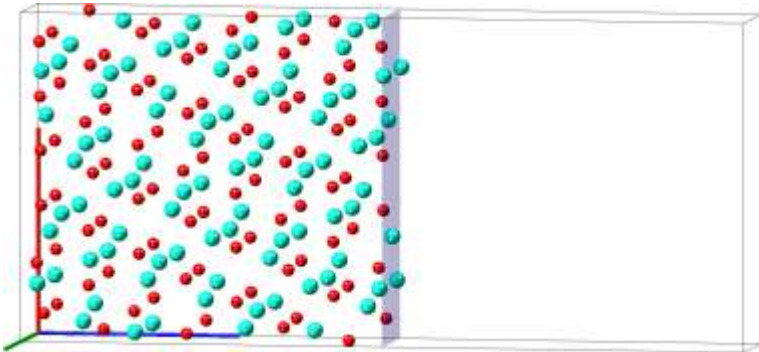




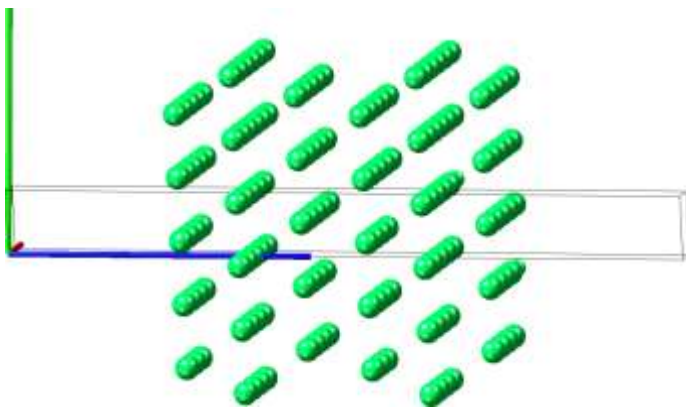
*MedeA Interface Builder*: Construct  
Models With Minimal Strain & Lattice  
Mismatch

# Model $\text{Cr}_2\text{O}_3$ (102) / Fe(111) Interface

- ▶  $\text{Cr}_2\text{O}_3$  (102) Surface model



- ▶ Fe (111) surface model



- ▶ *MedeA Interface Builder*

Second System:  $(\text{Fe})_s$  (P1) ~ Fe (111)

Area tolerance (%) 5

Length tolerance (%) 5

Angle tolerance (%) 5

# Cells to search 8

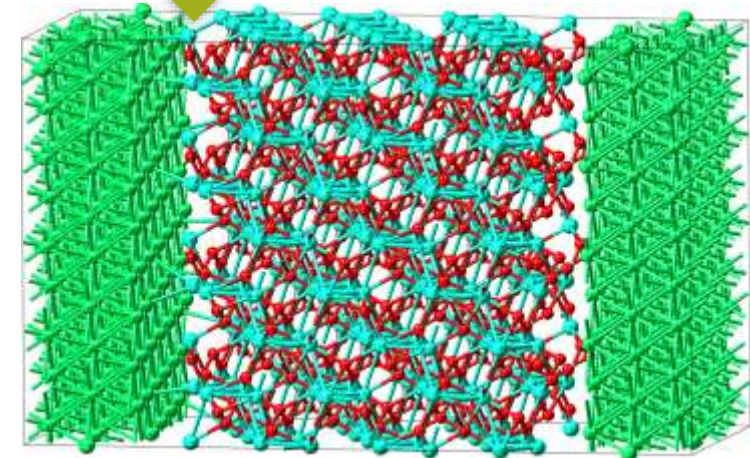
Weight of first system lattice parameters

0.5

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

Run Job Cancel

- ▶ Interface model





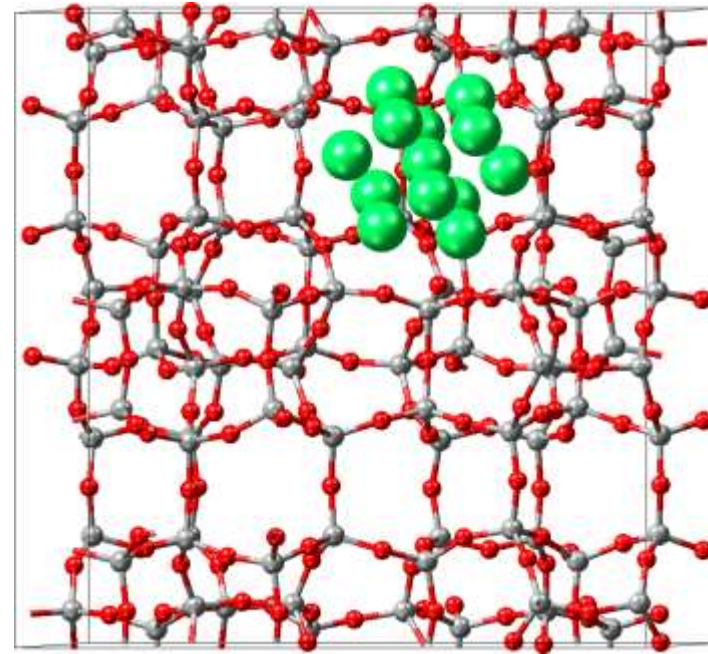
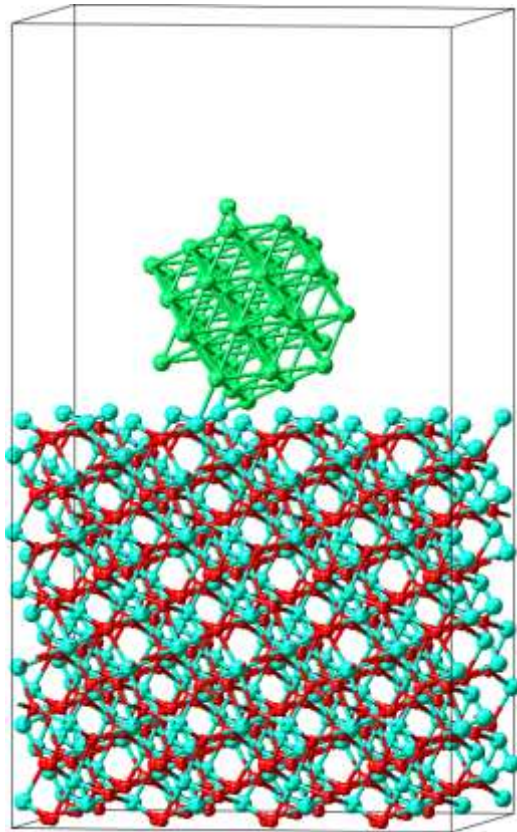
# MedeA Nanobuilder: Build Particles, Tubes, Pipes, and Rods

The image displays the MedeA Nanobuilder software interface. On the left, there are three 3D models: a cluster of red and yellow spheres, a long tube of white and blue spheres, and a yellow cylindrical shell. In the center, a 'Nanop...' dialog box is open, showing 'Shape: sphere', 'Diameter: 10.0', and 'Dangling bonds: one'. To the right, a 'Build periodic system' dialog box 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.

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*
- Convert and transform less practical structures with various *MedeA Builders*
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- *MedeA Surface Builder*: Create realistic surface models for complex structures
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- *MedeA Docking*: Deposit molecules on surfaces or in nanopores



# Upcoming Webinar

## Development of New Solvents for CO<sub>2</sub> Capture Using Molecular Simulations

Register:

[www.materialsdesign.com/webinars](http://www.materialsdesign.com/webinars)

March 23<sup>rd</sup>, 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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- ▶ For questions or comments contact:  
  
Katherine Hollingsworth  
[khollingsworth@materialsdesign.com](mailto:khollingsworth@materialsdesign.com)

# Question and Answer Session



***Dr. René Windiks***

*Materials Design*



***Dr. David Reith***

*Materials Design*

# Questions about Materials Design Trainings

***Materials Design Support Team***

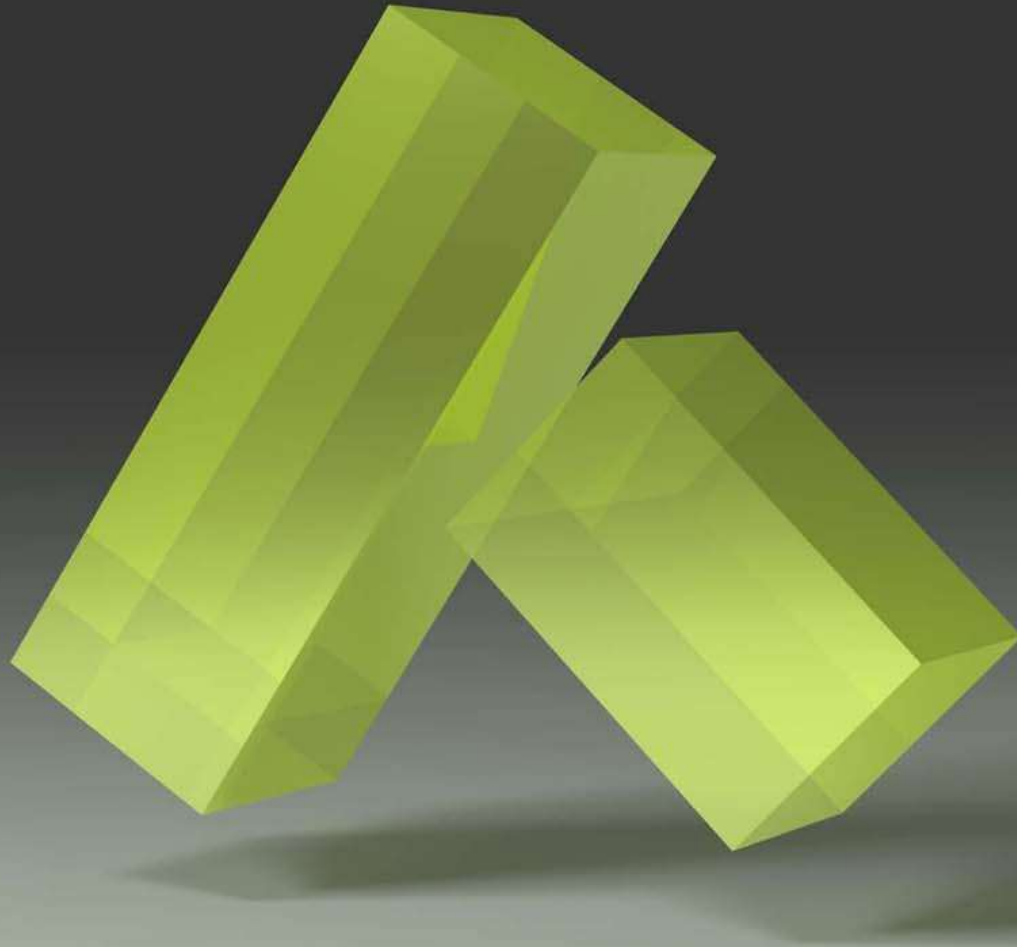
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# *Medea*

Innovation by Simulation