



materials design

UGM 2020 Training Series

MedeA LAMMPS: Robust Gateway to Molecular Dynamics

Materials Design

October 13th, 2020

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Materials Design UGM

Training & Support Team



Ray Shan
presenter



David Reith
moderator



Taylor Juran



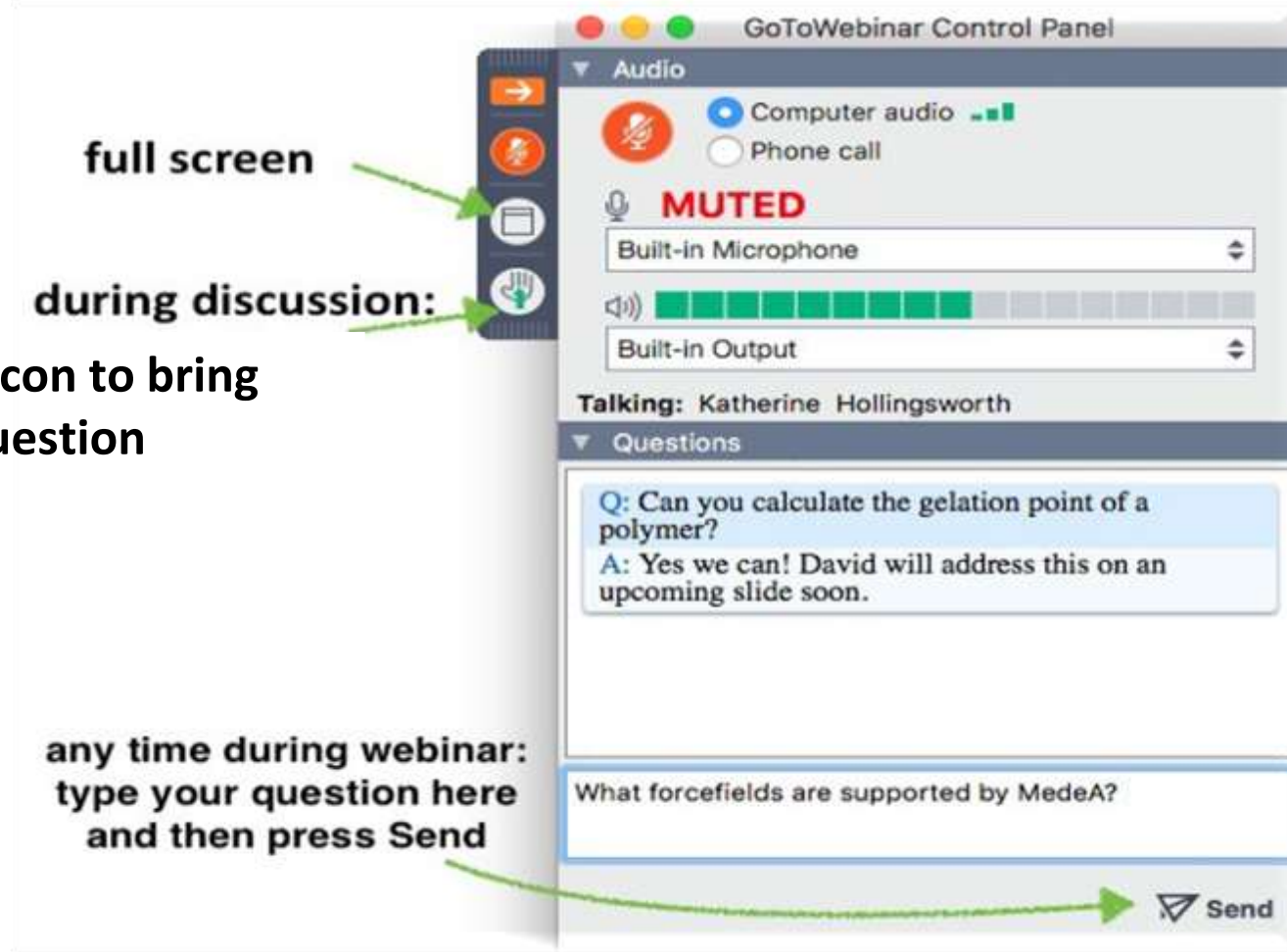
René Windiks



Siwen Wang

Please Ask Questions!

Use the raise hand icon to bring attention to your question



The screenshot shows the 'GoToWebinar Control Panel' window. On the left, a vertical toolbar contains icons for full screen, mute, and raise hand. Green arrows point from text labels to these icons: 'full screen' points to the full screen icon, 'during discussion:' points to the raise hand icon, and 'any time during webinar: type your question here and then press Send' points to the 'Send' button at the bottom right. The main panel shows audio settings with 'Computer audio' selected and the microphone muted. Below the audio settings, the 'Talking' section shows 'Katherine Hollingsworth' is speaking. The 'Questions' section displays a question: 'Q: Can you calculate the gelation point of a polymer?' and an answer: 'A: Yes we can! David will address this on an upcoming slide soon.' At the bottom, a text input field contains the question 'What forcefields are supported by Medea?' and a 'Send' button with a paper plane icon.



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UGM 2020 Training Series

MedeA LAMMPS: Robust Gateway to Molecular Dynamics

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Outline



- ▶ MedeA LAMMPS
- ▶ MedeA Forcefields Bundle
- ▶ MedeA Mesoscale Simulations
- ▶ MedeA Deformation
- ▶ MedeA Deposition
- ▶ Conclusions



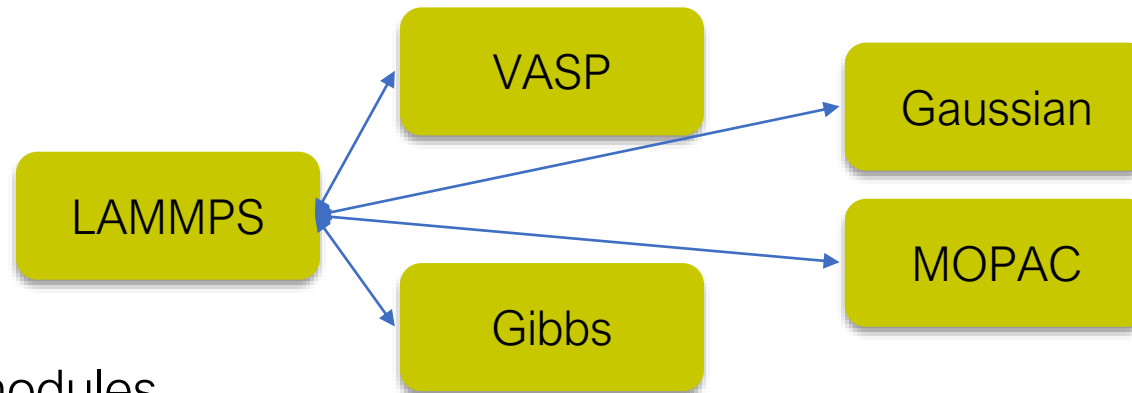
MedeA LAMMPS



MedeA LAMMPS

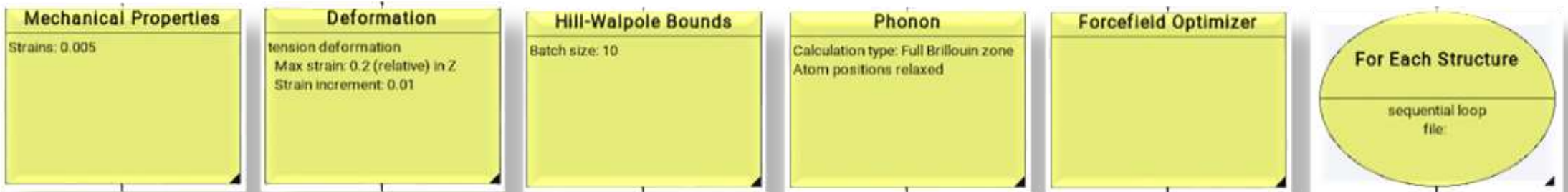
► Integrated with other simulation engines

- Quantum Methods (VASP, MOPAC, Gaussian) and Monte-Carlo (Gibbs)



► Integrated with other modules

- Mechanical Properties, Deformation, Hill-Walpole Analysis, Forcefield Optimizer, and High-throughput Launchpad






MedeA LAMMPS

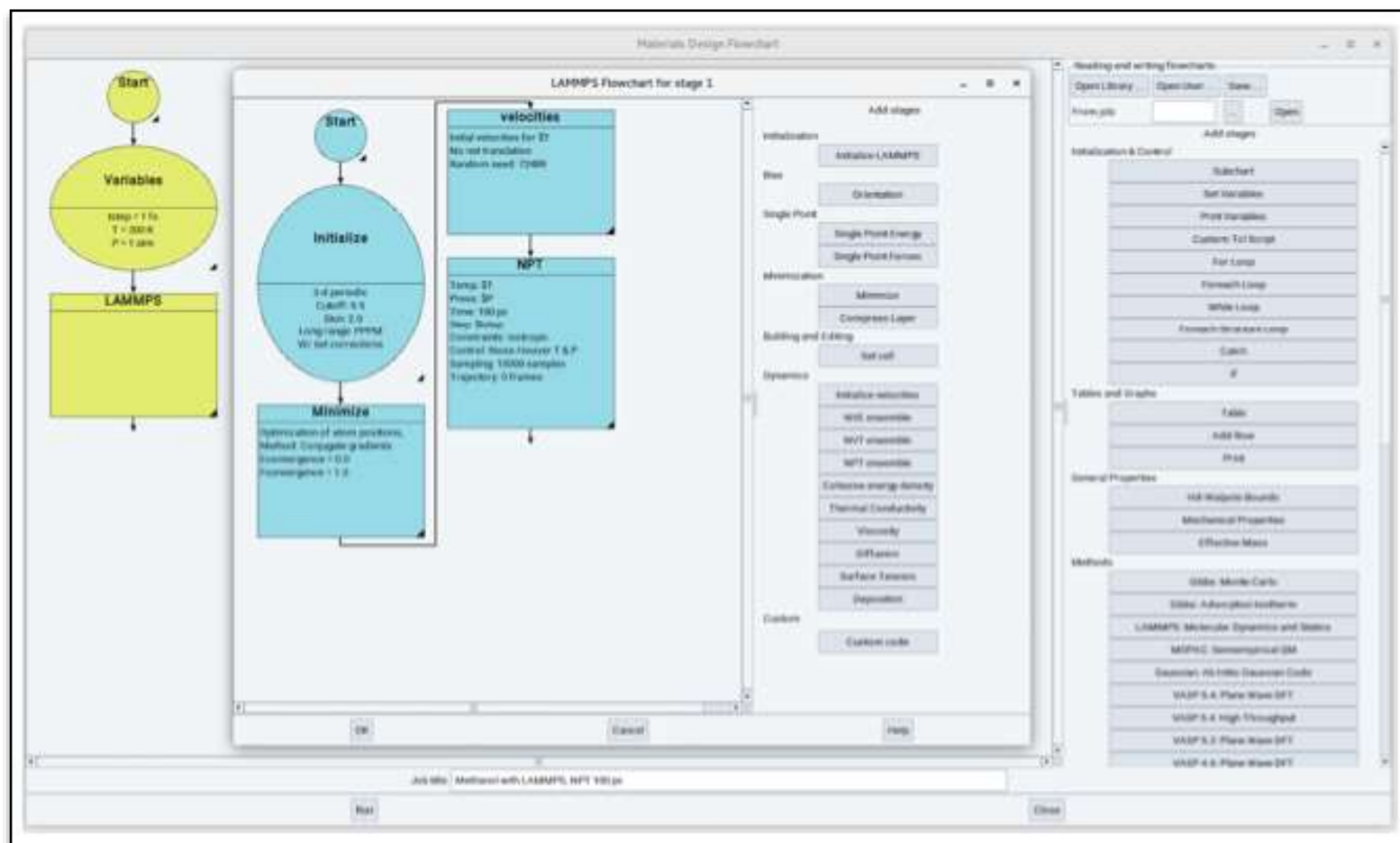


Introduction to MedeA LAMMPS

Release 3.1.0

- **Objective:** Learn how to set up and run LAMMPS simulations with MedeA
- **Modules:** MedeA LAMMPS, Supercell Builder, Amorphous Materials Builder

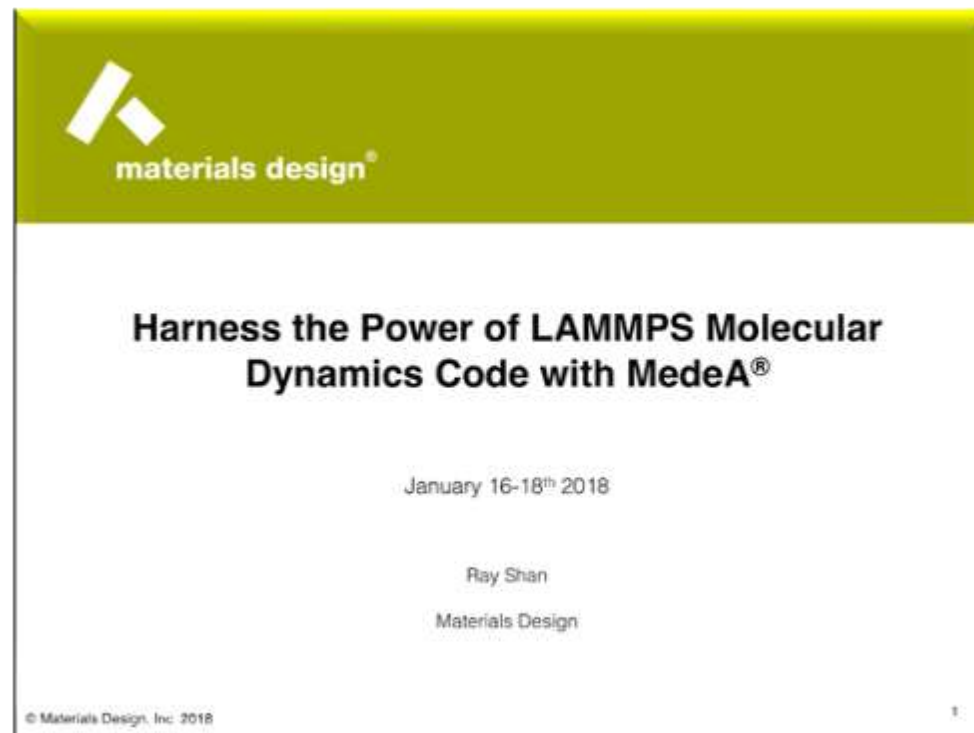
		
Preparation time	Run time (2 Intel cores)	Level
10 minutes	5 minutes	Beginner



MedeA LAMMPS



- ▶ Watch the webinar
 - ▶ *Harness the Power of LAMMPS Molecular Dynamics Code with MedeA*
 - ▶ <http://my.materialsdesign.com/webinar-12>





MedeA Forcefield Bundle



Interatomic Potentials in MedeA



▶ Metallic

- EAM *
- All LAMMPS `eam`, `eam/fs`, and `eam/alloy` variants
- MEAM

▶ Inorganic

- Buckingham (`buck`)
- BKS (`buck/coul`)
- Clay-FF (`harmonic + lj + coul`)
- CVFF_aug (`class2`)
- Morse/`coul`

▶ Semiconductor

- Tersoff
- Stlinger-Weber
- REBO

▶ Organic (valence):

- PCFF/PCFF+ *
- Compass/Compass+
- OPLS-AA/OPLS-AA+ *
- AUA/AUA+ *
- Trappe+ *

▶ Mesoscale

- SPICA
- Martini

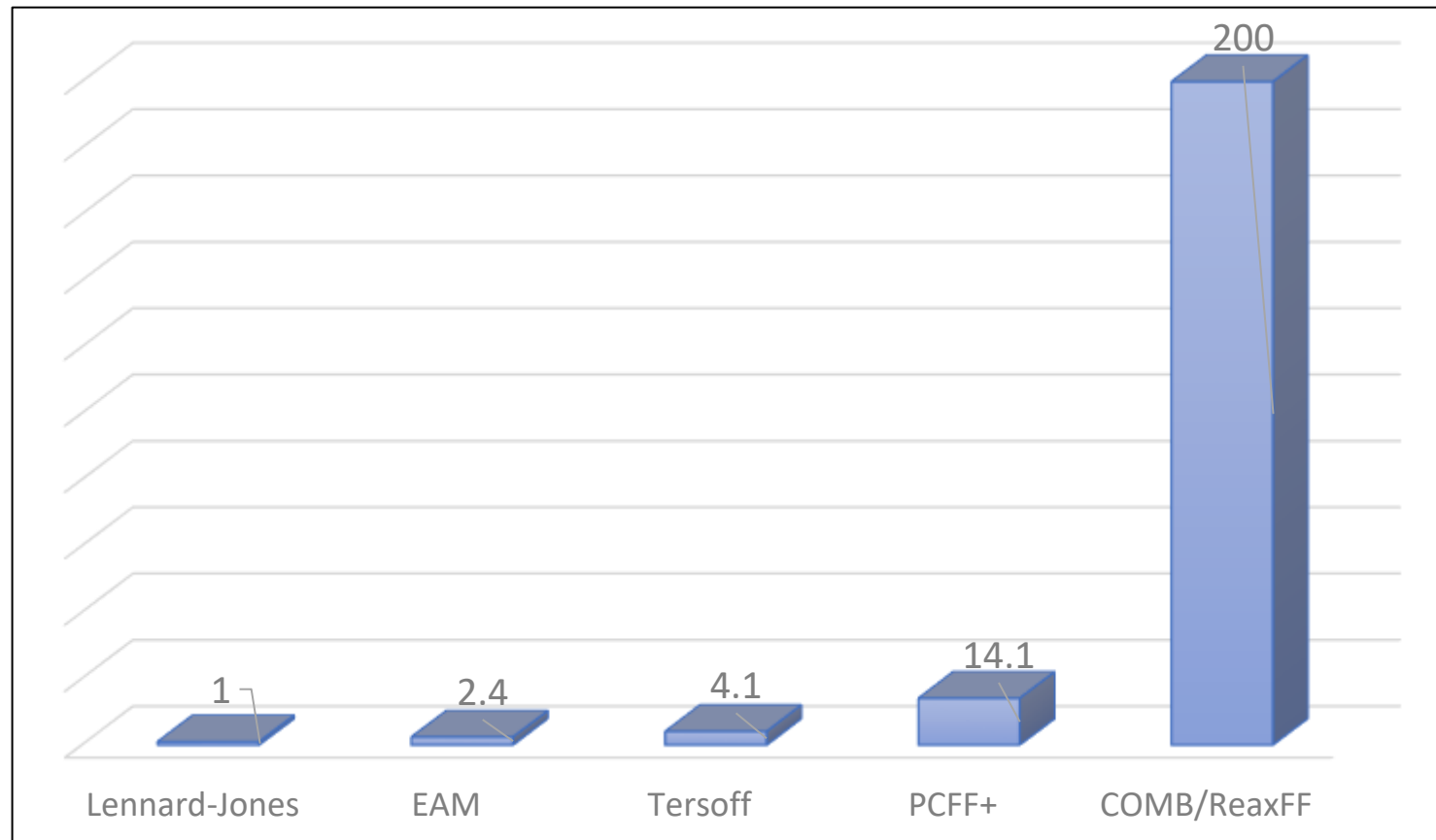
▶ Variable charge

- Streitz-Mintmire (`eam + coul + qeq`)
- COMB3
- ReaxFF

* Also available in MedeA®-GIBBS

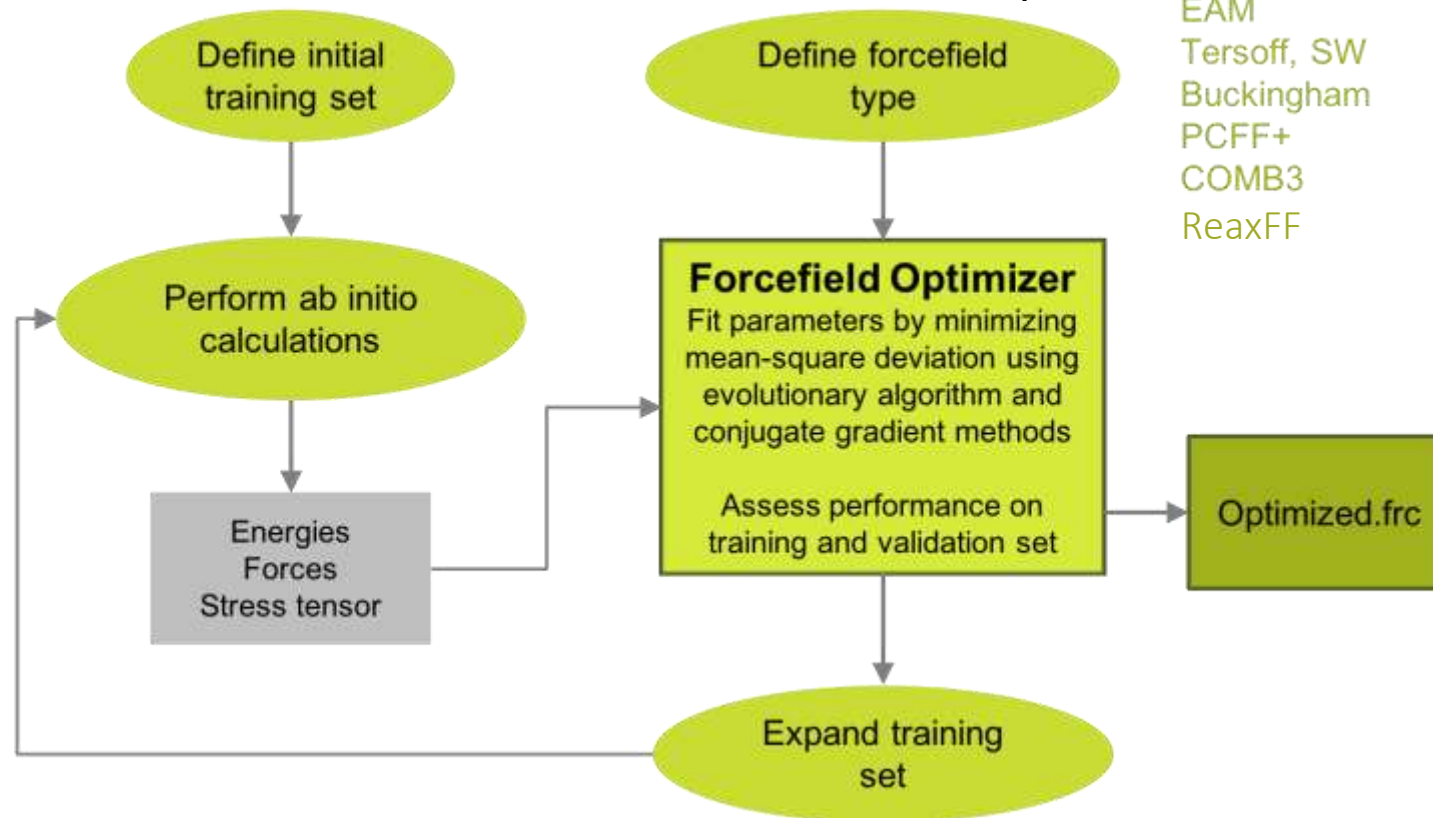
Cost of Classical Forcefields

- ▶ Long-range electrostatics: 10x more expensive than LJ
- ▶ Variable charge equilibration: ~100x more expensive than LJ



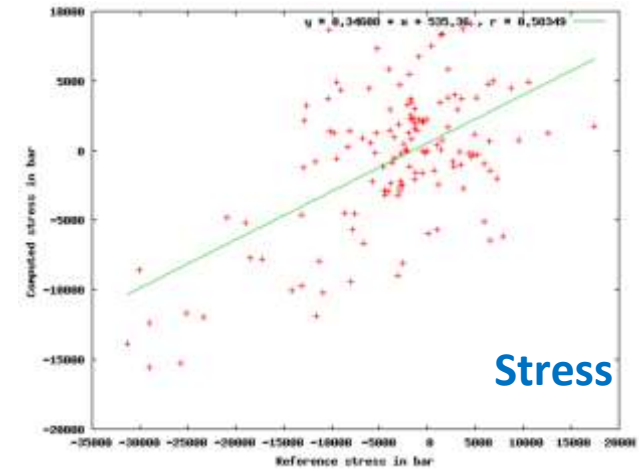
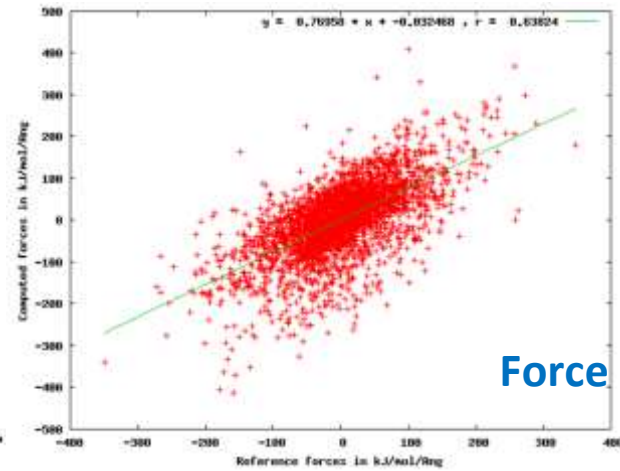
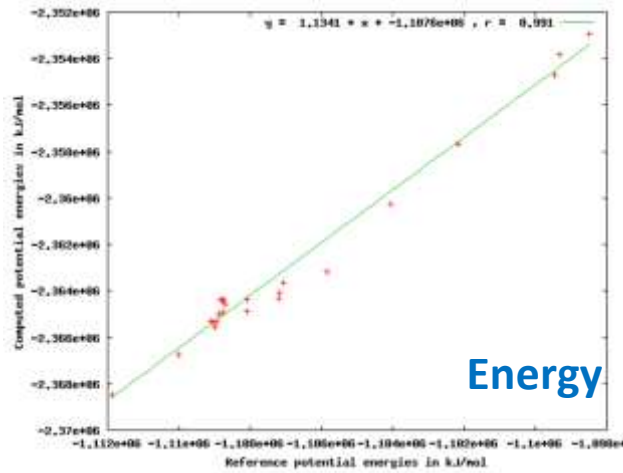
Flexibility with MedeA Forcefields

- ▶ Import external forcefield parameters
- ▶ Import external forcefield parameter files
- ▶ Develop new forcefields with MedeA Forcefield Optimizer

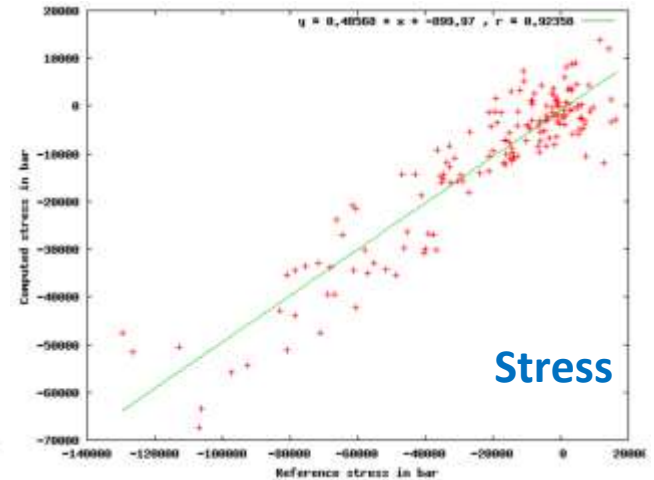
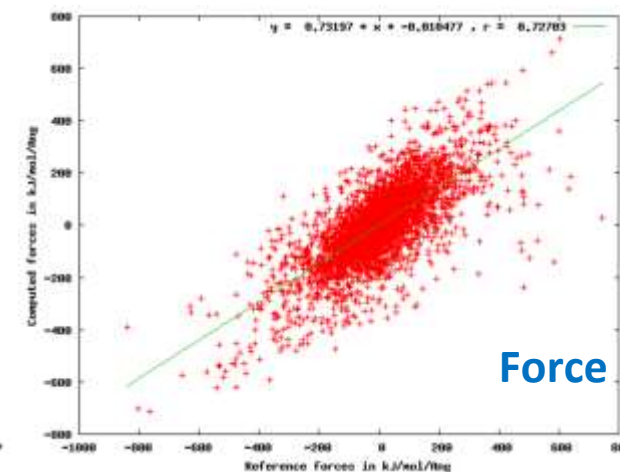
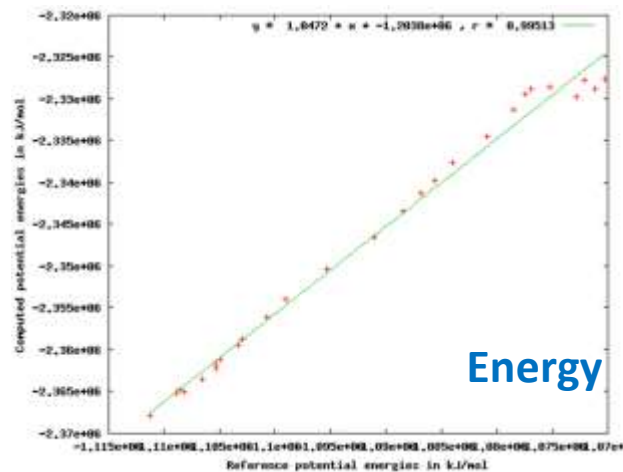


Visualize the Optimization

Training



Validation



Interatomic Potentials in MedeA

- ▶ Watch the webinar:
 - ▶ *Classical Forcefields for Modeling Materials on Atomic Scale*
 - ▶ <http://my.materialsdesign.com/webinar-10>

$$\begin{aligned}
 E_{pot} &= \sum_{\text{atoms}} [K_2(r-r_0)^2 + K_3(r-r_0)^3 + K_4(r-r_0)^4] & U_{ij}(r) &= \frac{q_i q_j}{r_{ij}} + A_{ij} e^{-r_{ij}/\rho_{ij}} - \frac{C_{ij}}{r^6} \\
 &+ \sum_{\text{angles}} [H_2(\theta-\theta_0)^2 + H_3(\theta-\theta_0)^3 + H_4(\theta-\theta_0)^4] \\
 &+ \sum_{\text{torsions}} [V_1 \{1 - \cos(\phi - \phi_0^0)\} + V_2 \{1 - \cos(2\phi - \phi_0^0)\} + V_3 \{1 - \cos(3\phi - \phi_0^0)\}] & X_i &= -\mu_i = -\frac{\partial E(\rho)}{\partial \rho} = e \frac{\partial E(q_i)}{\partial q_i} \\
 &+ \sum_{\text{planes}} K_x \chi^2 & \mathbf{F}_i &= -\frac{\partial E}{\partial \mathbf{r}_i} = m_i \mathbf{a}_i, \\
 &+ \sum_{\text{charges}} \frac{q_i q_j}{r_{ij}} E = \frac{1}{2} \sum_i \sum_{j \neq i} V_{ij}(r_{ij}) + F_i \left(\sum_{j \neq i} \rho_j(r_{ij}) \right) & &+ \sum_{\text{torsions}} \sum_{\text{angles}} K_{\omega} (\theta - \theta_0) (\theta' - \theta'_0) \\
 &+ \sum_{\text{charges}} \left[2 \left(\frac{r_{ij}^0}{r_{ij}} \right)^6 - 3 \left(\frac{r_{ij}^0}{r_{ij}} \right)^3 \right] = \frac{1}{2} \sum_i \sum_{j \neq i} [V^{\text{ext}}(R_{ij}, q_i, q_j)] & &+ \sum_{\text{torsions}} \sum_{\text{angles}} K_{\omega} (r - r_0) (\theta - \theta_0) \\
 &E = \frac{1}{2} \sum_i \sum_{j \neq i} V_{ij}(r_{ij}) - (b^{\text{angle}} + b^{\text{coord}} + b^{\text{torsion}} + b^{\text{conformation}}) \sum_{\text{atoms}} \left[\sum_{\text{torsions}} \sum_{\text{angles}} (r' - r'_0) [V_1 \cos(\phi) + V_2 \cos(\phi) + V_3 \cos(\phi)] \right. \\
 &V_{ij}(r_{ij}) = V_{ij}^R(r_{ij}) + b_{ij} V_{ij}^A(r_{ij}) & &+ \sum_{\text{torsions}} \sum_{\text{angles}} (\theta - \theta_0) [V_1 \cos(\phi) + V_2 \cos(\phi) + V_3 \cos(\phi)] \\
 &E = \frac{1}{2} \sum_i \sum_{j \neq i} \Phi_2(r_{ij}) + \sum_i \sum_{j \neq i} \sum_{k > j} \Phi_3(r_{ij}, r_{ik}, \theta_{ijk}) & \mathbf{a}_i &= d^2 \mathbf{r}_i / dt^2
 \end{aligned}$$



MedeA Mesoscale Simulations

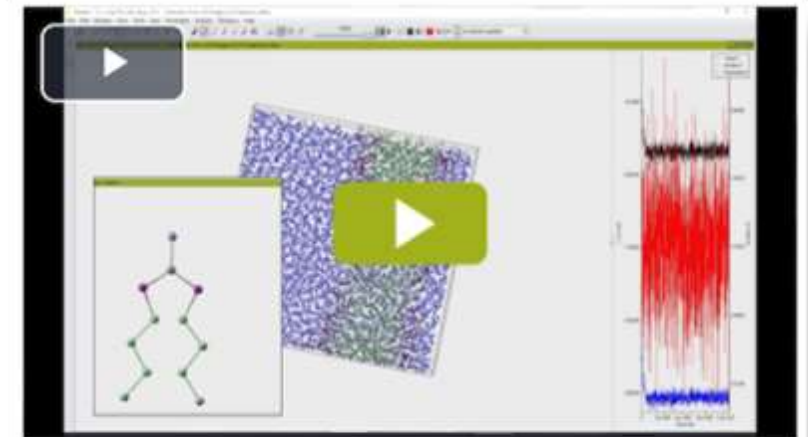


MedeA Mesoscale Simulations

- ▶ Watch the webinar
 - ▶ *Extending Time- and Length-Scales with Mesoscale Simulations*
 - ▶ <http://my.materialsdesign.com/webinar-36>

- ▶ Demo: DPPC in water, bi-layer self assembly

Watch the Webinar



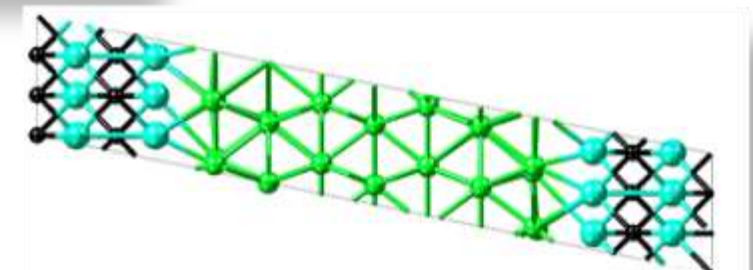
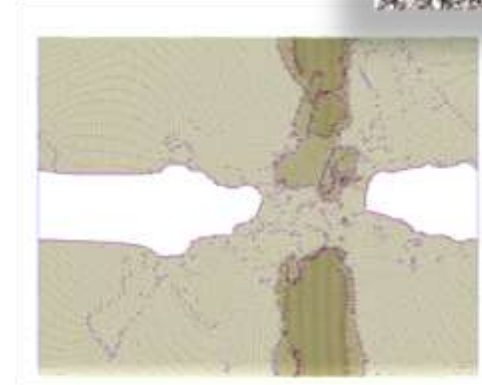
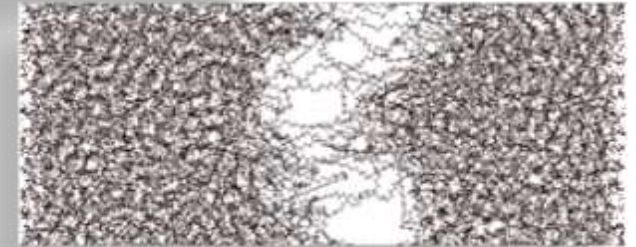
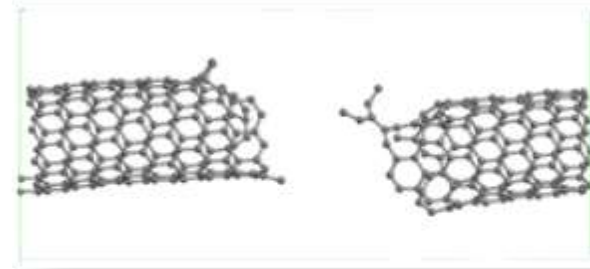


MedeA Deformation



Deformation Simulations

- ▶ Tensile deformation of CNT with Tersoff
- ▶ Tensile deformation of PE with PCFF+
- ▶ Crack propagation of Zr with EAM
- ▶ Shear deformation of Co/WC interface

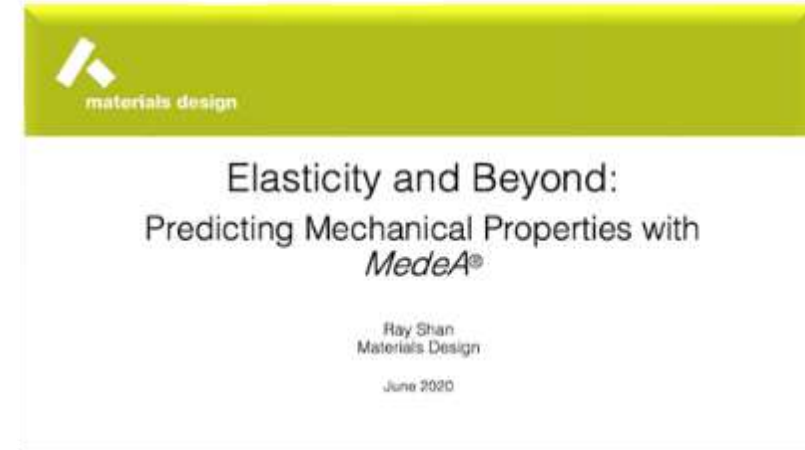


MedeA Deformation



- ▶ Watch the webinar
 - ▶ *Elasticity and Beyond: Predicting Mechanical Properties with MedeA*
 - ▶ <http://my.materialsdesign.com/webinar-33>

- ▶ Demo:
 - ▶ <http://my.materialsdesign.com/webinar-38>





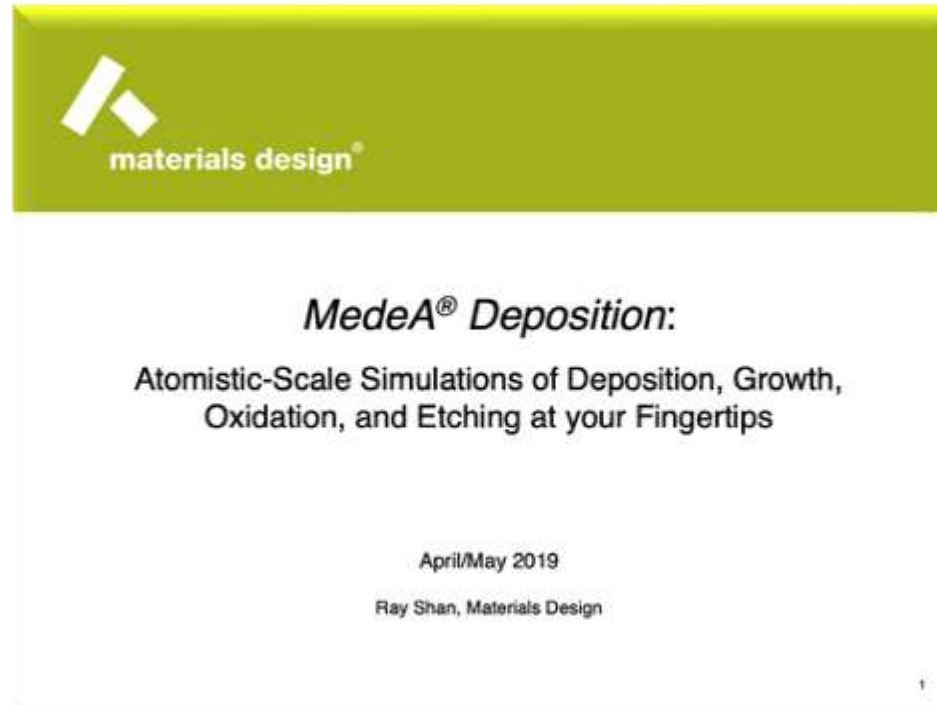
MedeA Deposition



MedeA Deposition

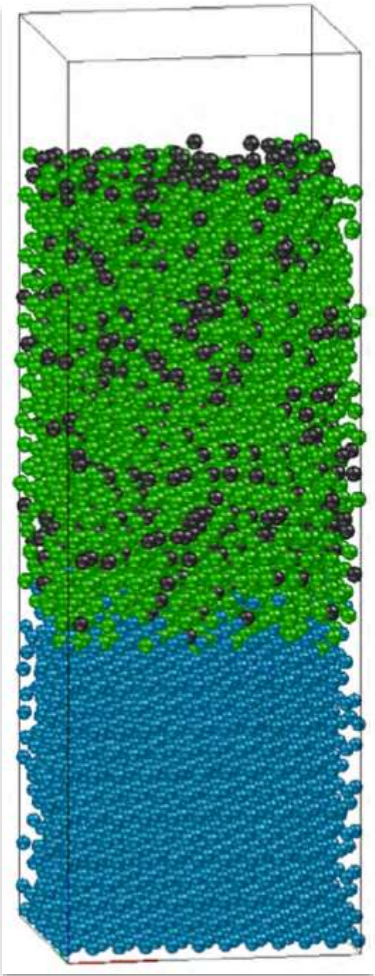


- ▶ Watch the webinar
 - ▶ *MedeA Deposition: Atomistic-Scale Simulations of Deposition, Growth, Oxidation, and Etching at your Fingertips*
 - ▶ <http://my.materialsdesign.com/webinar-26>

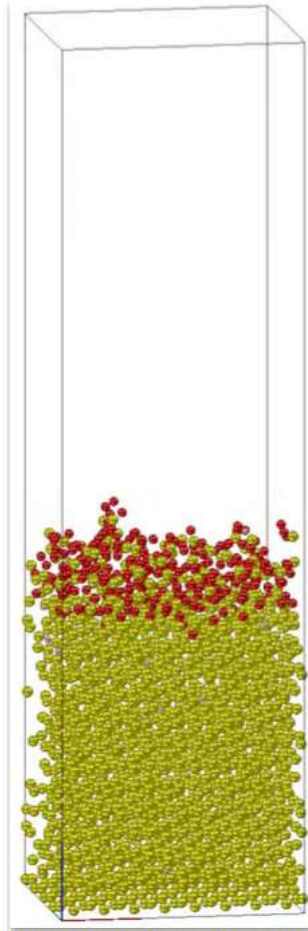


MedeA Deposition Examples

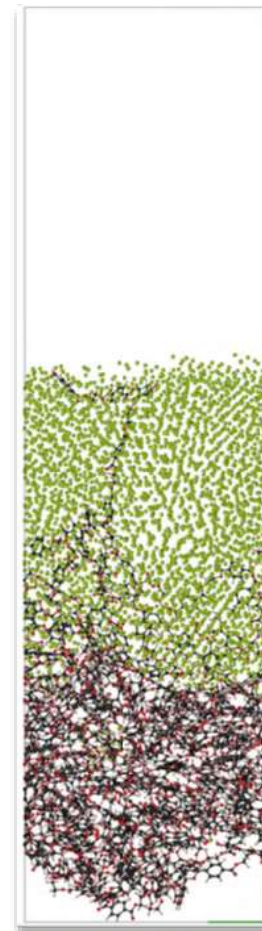
Sputtering of Pd/Ag on Ti



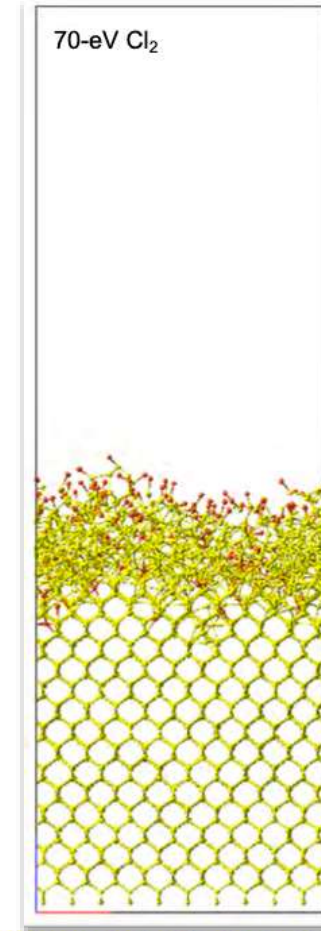
CVD of O₂ on Si



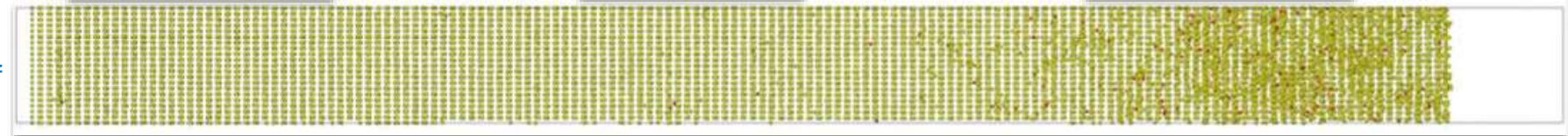
Sputtering of Al on PET



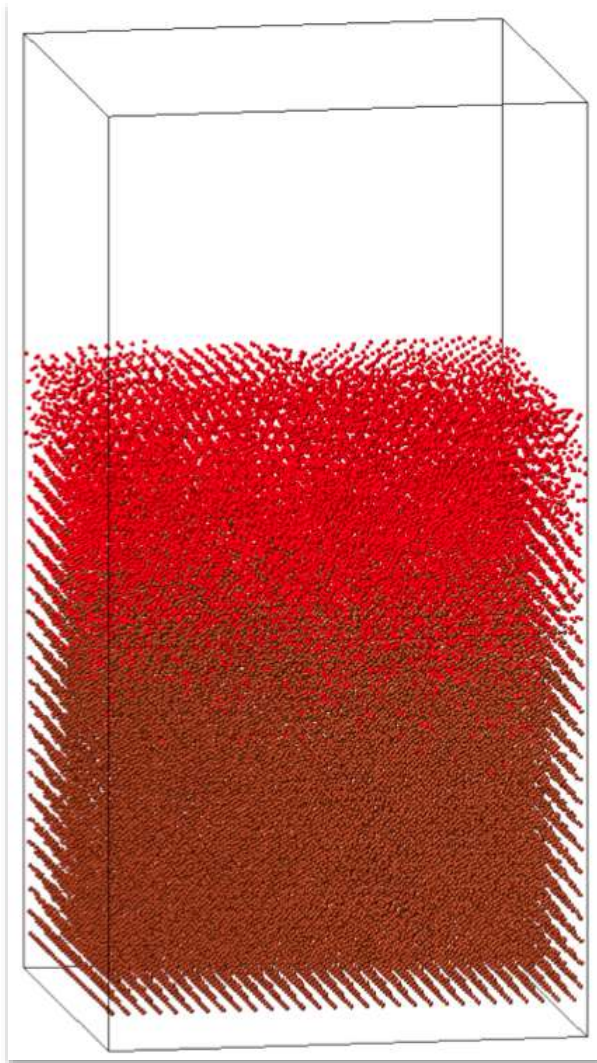
Etching of Si with Cl₂



Ion implantation of O in Si






MedeA Deposition



Cold Spray of Cu Nanoparticles on the Cu Surface

Release 3.1.0

- **Objective:** Learn how to simulate the cold spray of metal nanoparticles onto metal surfaces
- **Modules:** *MedeA Deposition, MedeA EAM, MedeA LAMMPS*

		
Preparation time	Run time (4 Intel cores)	Level
30 minutes	2 hours	Intermediate

Conclusions



In this live demonstration, we looked at:

- ▶ *MedeA LAMMPS*, the robust gateway to classical molecular dynamics simulations
- ▶ The collection of interatomic potentials in *MedeA*, including those for metals and alloys, semiconductors, ionic systems, and organic systems, as well as the variable charge potentials
- ▶ The steps to export and edit an existing potential (frc) file, and that for importing any external potential parameters into *MedeA*
- ▶ The *MedeA Mesoscale*, *Deformation*, *Deposition* modules that employ interatomic potentials for simulating a wide variety of materials processes and properties

List of Resources




► Tutorials:

- Introduction to MedeA LAMMPS: Learn how to set up and run LAMMPS molecular dynamics simulations with MedeA
- Importing External Potential Parameters into MedeA: Learn how to import external potential parameters and files into MedeA
- Deposition of O2 on a Si Surface with Reactive Potentials: Learn how to perform deposition simulation with reactive potentials using MedeA Deposition
- Cold Spray of Cu Nanoparticles on the Cu Surface: Learn how to simulate the cold spray of metal nanoparticles onto metal surfaces with MedeA Deposition
- Plastic Deformation and Fracture of Single-walled Carbon Nanotube: Learn how to set up and run plastic deformation and fracture simulations with MedeA Deformation
- Mesoscale Simulations of Water and Octane: Learn how to set up and run a mesoscale simulation of a mixture with MedeA
- Self-assembly of Lipid Bilayer: Learn how to run a mesoscale molecular dynamics simulation of self-assembly on a time-scale of a microsecond with MedeA
- Mechanical Properties of a Thermoset Through Mesoscale Simulations: Learn how to predict mechanical properties of a thermoset through mesoscale simulations

► Webinars:

- MedeA 3.1: <http://my.materialsdesign.com/webinar-38>
- MedeA Mesoscale: <http://my.materialsdesign.com/webinar-36>
- MedeA Elastic Properties and Deformation: <http://my.materialsdesign.com/webinar-33>
- MedeA Deposition: <http://my.materialsdesign.com/webinar-26>
- MedeA ReaxFF: <http://my.materialsdesign.com/webinar-17>
- MedeA LAMMPS: <http://my.materialsdesign.com/webinar-12>
- MedeA Forcefields: <http://my.materialsdesign.com/webinar-10>

A world map with a dark blue background and glowing yellow city lights. A network of glowing blue lines connects various nodes across the globe, representing a global network. The text is centered over the map.

**Materials Design UGM
GOING GLOBAL
October
ugm.materialsdesign.com**

Announcements

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Professor Georg Kresse

University of Wien



Dr. David Reith

Materials Design

Tomorrow's Plenary Speaker

October 14th

Next Week's MedeA Training

October 20th

UGM 2020 Discussion Forum

Get help. Contribute ideas. Ask questions. Join the discussion.

General Discussions

Share your UGM experience, ideas, pictures and more!

4

1

Follow



Plenary Sessions

Discuss the sessions, ask questions, post comments

12

3

Follow



Training

Follow the training sessions, ask questions, post comments

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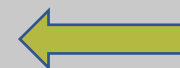
Follow



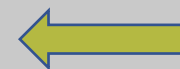
Announcements

Visit the UGM Forum page

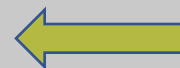
<https://www.ugm.materialsdesign.com/forum>



- Get help on training



- Contribute your ideas



- Discuss the posters and plenary presentations

- Ask questions

Technical Sessions

Additional resources, posters, and video presentations of scientific and technical research in the *MedeA* community.

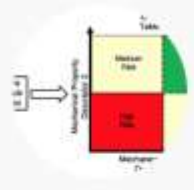


Announcements

Visit the Technical Session page Submitted Talks and Posters

<https://www.ugm.materialsdesign.com/posters>

- There is still time to submit
- Open to customers under maintenance
- Easily upload on the contributor's page
- Interested? Do you have questions?
 - Contact Volker Eyert
 - UGM@materialsdesign.com



poster

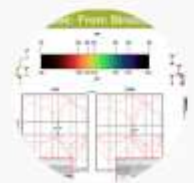
Risk Assessment of Drug Substance Tabletability using Quantum Mechanical Methods

View

In this work, periodic density functional theory as implemented in MedeA-VASP MT module was used to predict the mechanical properties of the single crystal structures of Vertex compounds along with other literature and small organic molecules in an automated manner



Contributor
Satish Iyemperumal



poster

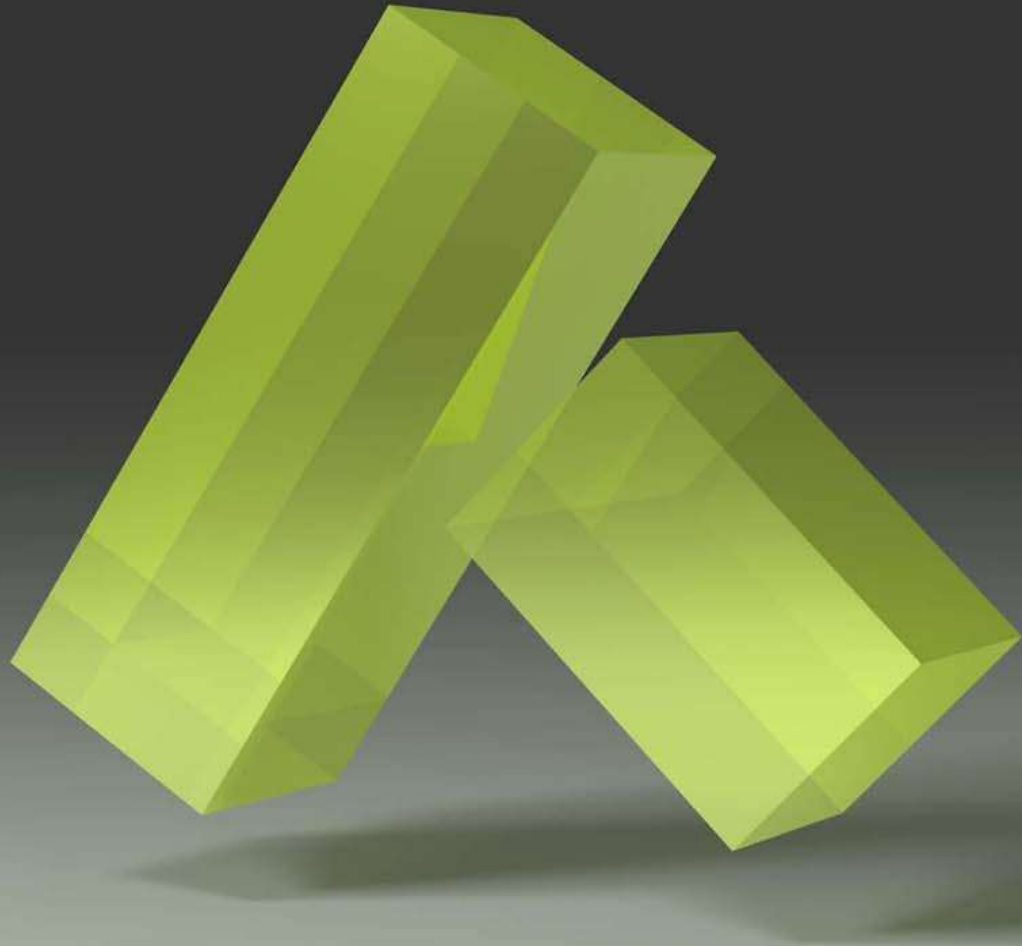
The Color of Materials: Value from Computed Optical Properties

View

This poster provides guidelines for the calculation of the color of materials within the MedeA computational environment and illustrates the steps leading from the structure of



Contributor
Volker Eyert



Medea

Innovation by Simulation