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WEBINAR

MedeA 3.1

Marianna Yiannourakou, Walter Wolf, Jörg-Rüdiger Hill

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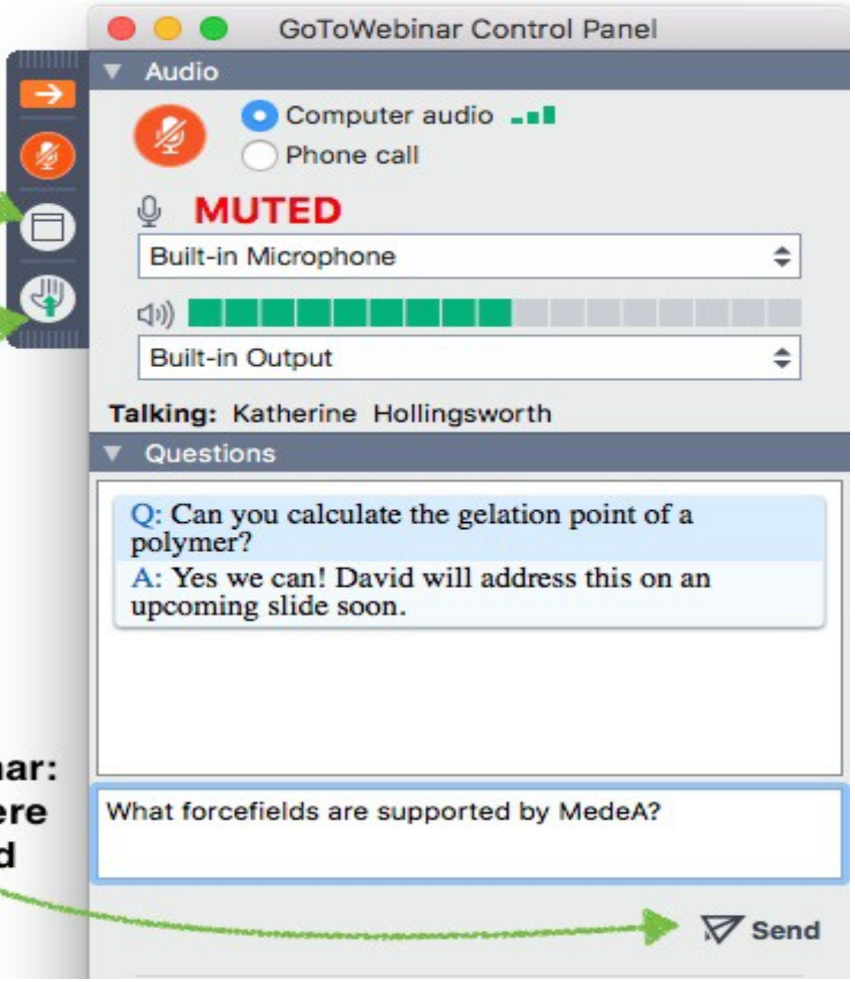

Webinar Speakers

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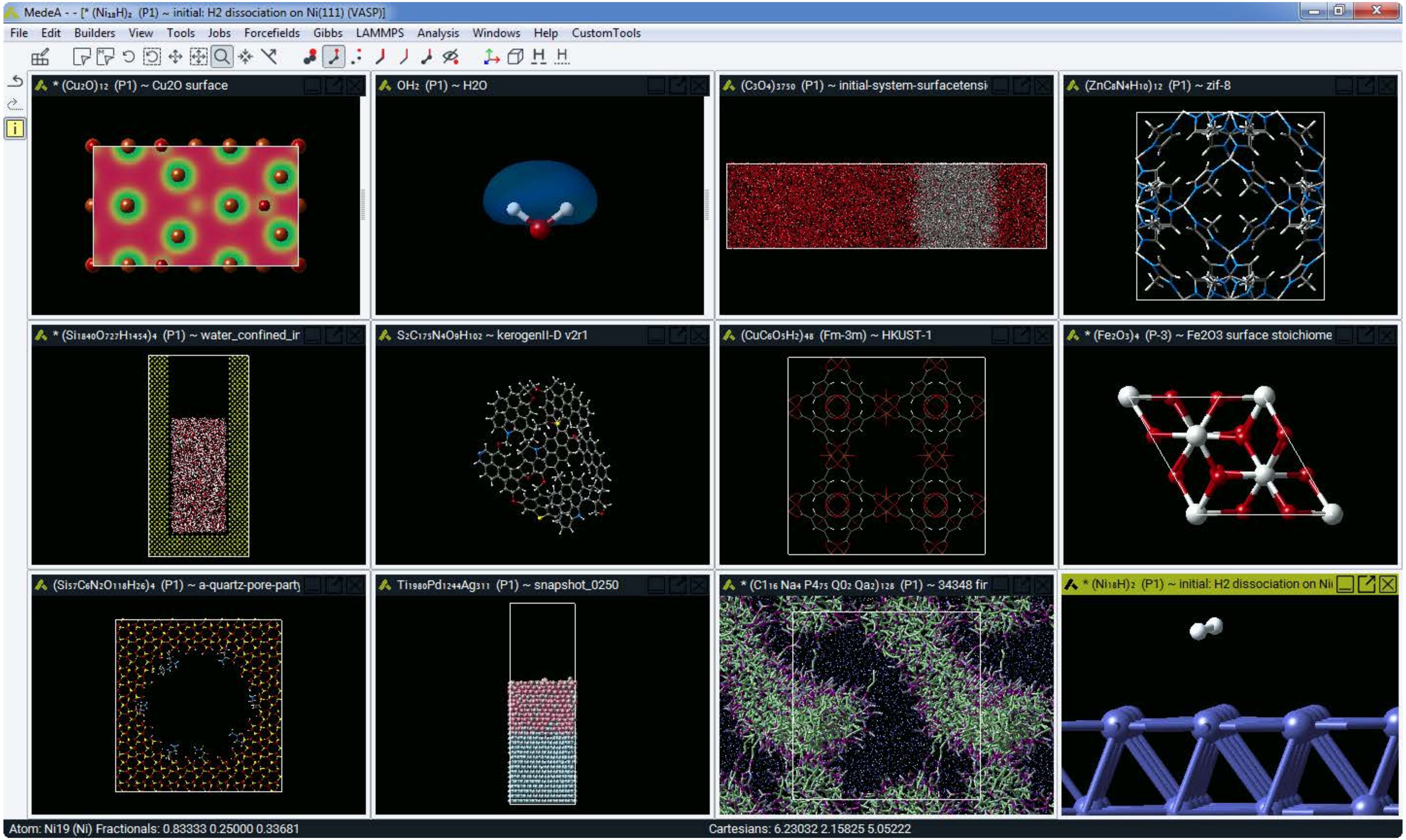
MedeA 3.1: Precision at Scale -The New Normal



Outline

01 Overview of *MedeA*® 3.1 – Precision at Scale -The New Normal

A brief overview of *MedeA* and the new features and enhancements of *MedeA* 3.1

02 VASP 6

More details on new features available from VASP 6 made easily accessible by *MedeA 3.1*

03 Mesoscale Simulations

A practical application for performing mesoscale simulations with *MedeA 3.1*

Databases

Direct access to experimental and calculated structure data gathered over decades – more than 1,1 million structures

Builders

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

Compute Engines

VASP, GAUSSIAN, MOPAC, LAMMPS, GIBBS

Forcefields + Forcefield Optimizer

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

Property Modules

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

High Throughput

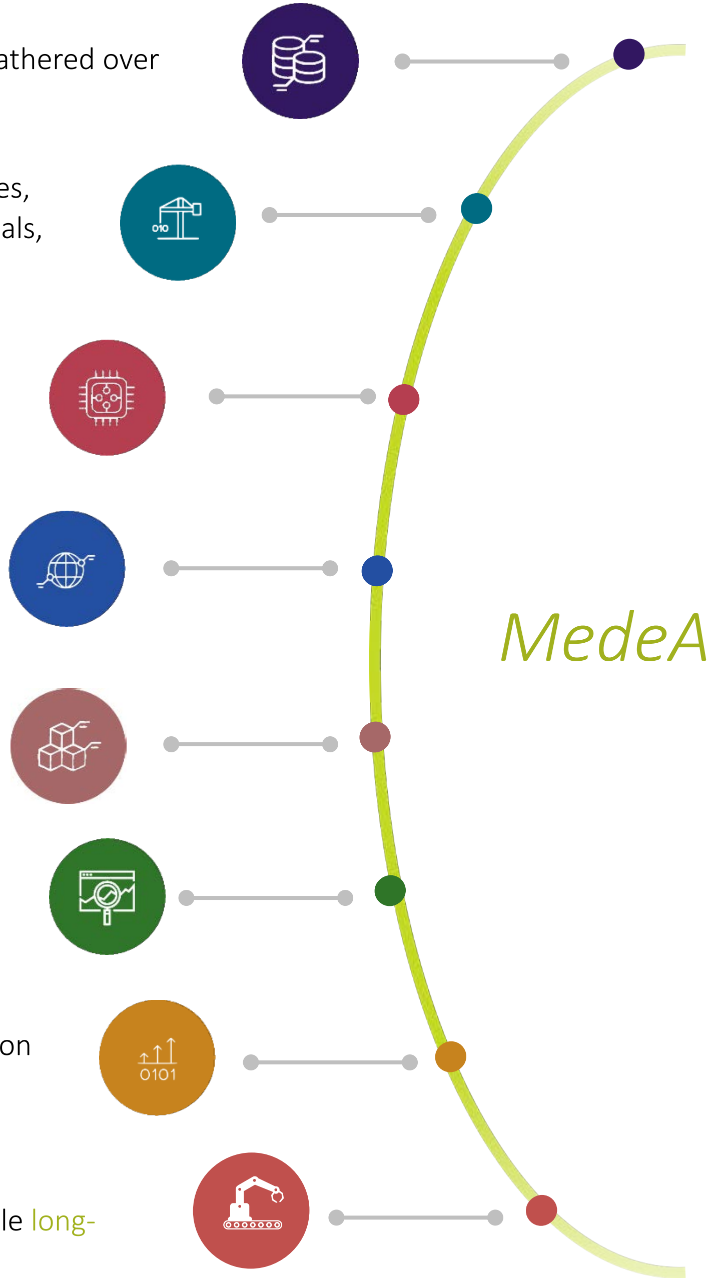
Generation of large and consistent sets of computed data & descriptors

Analysis Tools

Analysis and post-processing tools, for system characterization, visualization and analysis of calculated properties

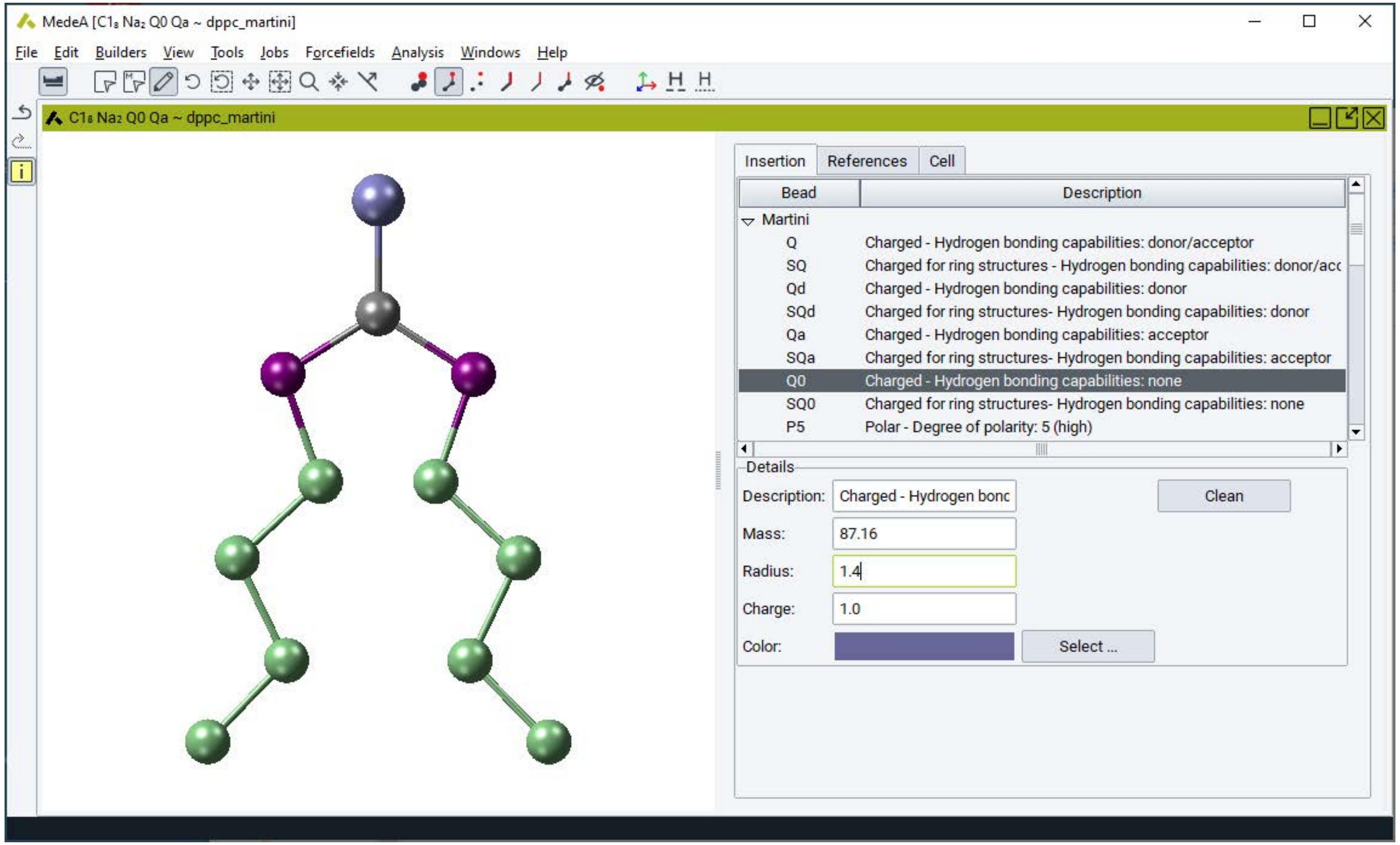
JobServer & TaskServer

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



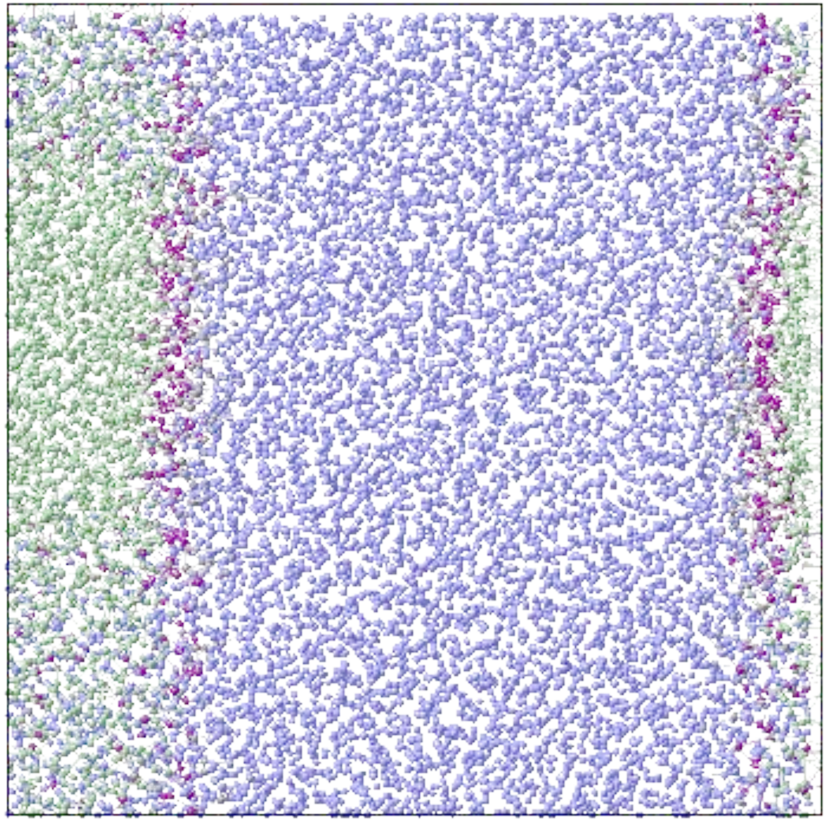
Mesoscale builder and coarse-grained systems

- *MedeA* 3.1 can be used to create and simulate coarse-grained (mesoscale) systems
- Mesoscale systems can be used in **polymer builder**, **amorphous builder** and **thermoset builder**
- Simulations can be performed with **LAMMPS**, properties can be predicted as for atomistic systems
- Mesoscale simulations can be performed on **microseconds** and **tens of nanometers**



Mesoscale Simulations With *MedeA* 3.1

- *MedeA* 3.1 supports
  - Sketching of mesoscale systems
  - MARTINI and SPICA forcefields
  - Creation of user defined bead libraries and forcefields
  - Building of polymers, amorphous systems and thermosets for mesoscale systems
  - LAMMPS simulations including Diffusion, Viscosity, Thermal conductivity, Surface tension
  - Hill-Walpole bounds
  - Mechanical properties
  - Deformation



What's new in *MedeA VASP 6*

- *Dedicated GUI for accessing VASP 6*
- *ScaLAPACK, Hybrid OpenMP/MPI support*
- *Adiabatic Connection ACFDT/RPA*
  - Low scaling algorithm for large systems
  - Accurate energy combining Hartree-Fock exact exchange and accurate correlation
  - Finite temperature (also for metals)
  - Forces and Γ-point phonons
  - Automatic optimization of atom positions
- *Møller-Plesset Perturbation Theory (MP2)*
  - Accurate energy combining Hartree-Fock exact exchange and accurate correlation
- *Low Scaling GW*
  - Quasiparticle spectra from low scaling GW algorithms for large systems
  - Finite temperature (also for metals)
- *Electron-Phonon Coupling (Displacements)*
  - Single configuration (Zacharias-Giustino)
  - Full Monte Carlo sampling of finite temperature configurations
- *Core-Level Spectroscopy (XAS, XANES)*
- *Dielectric-dependent Hybrid Functionals*
- *Numerous Enhancements*

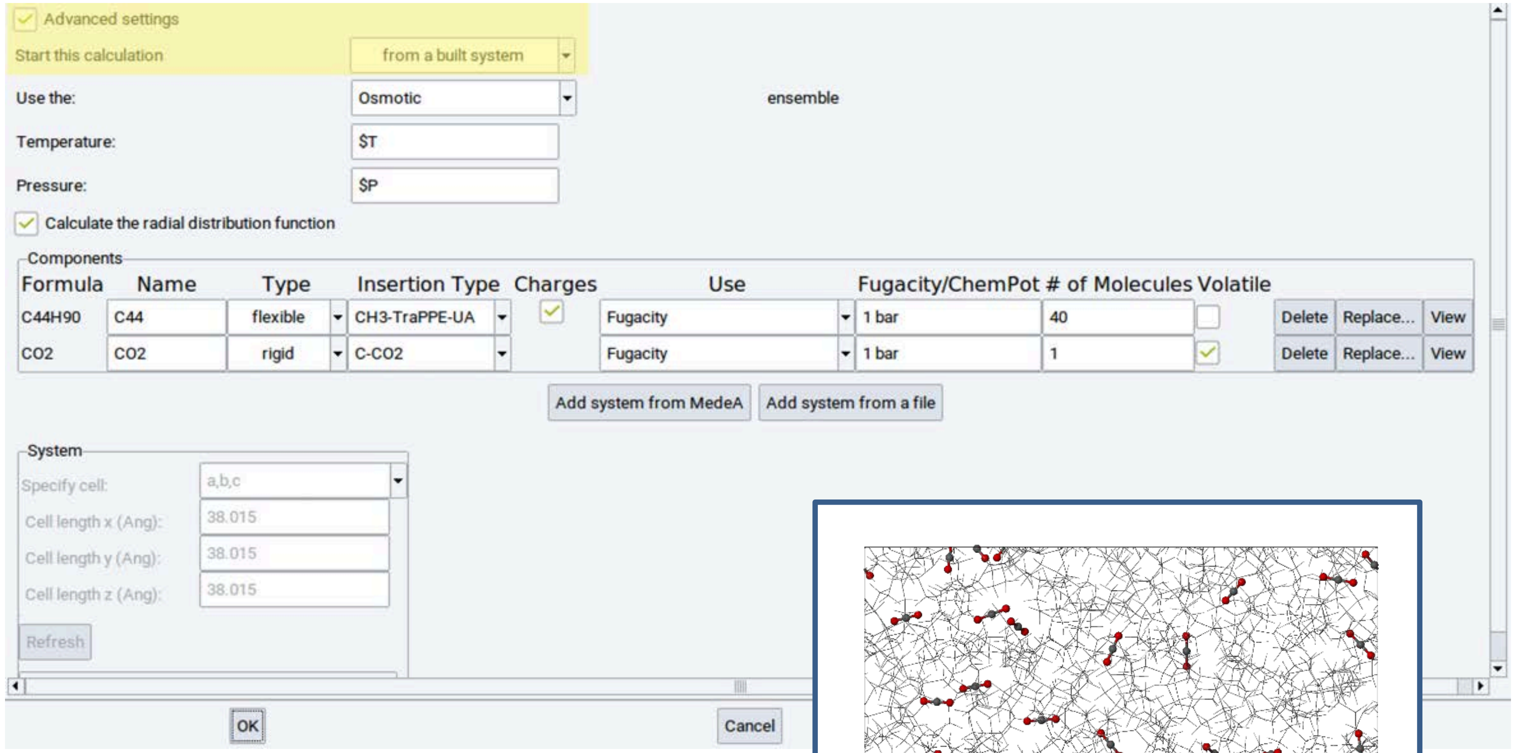
What's new in *MedeA LAMMPS*

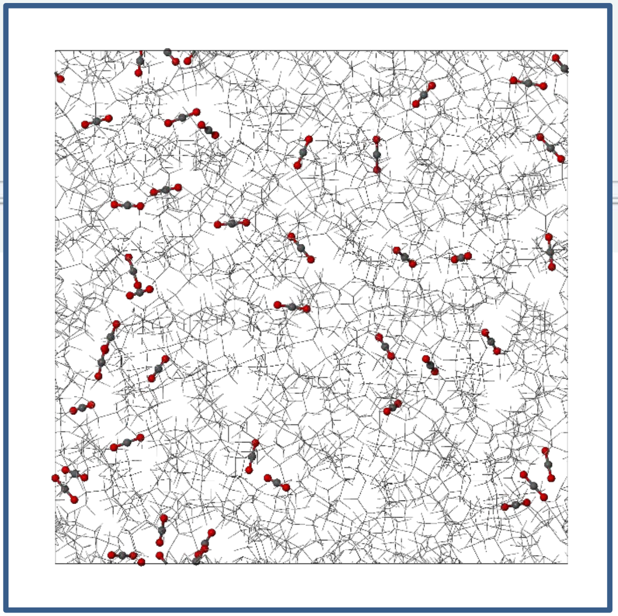
- Updated *MedeA LAMMPS* to the most recent stable version: 3 Mar 2020
  - Supported in the Deformation stage
  - New capabilities available via the Custom stage:
    - LATTE package for LANL density functional tight binding (DFTB) code (available on Linux)
    - USER-COLVARS package for simulations with collective variables (available on Linux and Windows)

- Supports NVIDIA GPUs on Linux up to compute capabilities of 7.5
  - Supported by CUDA Toolkit 10.0
  - Tesla K, P, V, and T series, Quadro K, P, GV, and RTX series, GeForce GTX/RTX series, and Titan X, V, and RTX series
  - Added support for minimization on GPUs

What's new in *MedeA GIBBS*

- GIBBS 9.7.3
- Start single-phase simulations from a pre-built system
  - Perform simulations on **crystalline solids**
  - Expedite simulations by **starting from a configuration built by the amorphous builder**
  - Carry out **osmotic ensemble simulations on (more) complex systems** that have been pre-equilibrated using LAMMPS

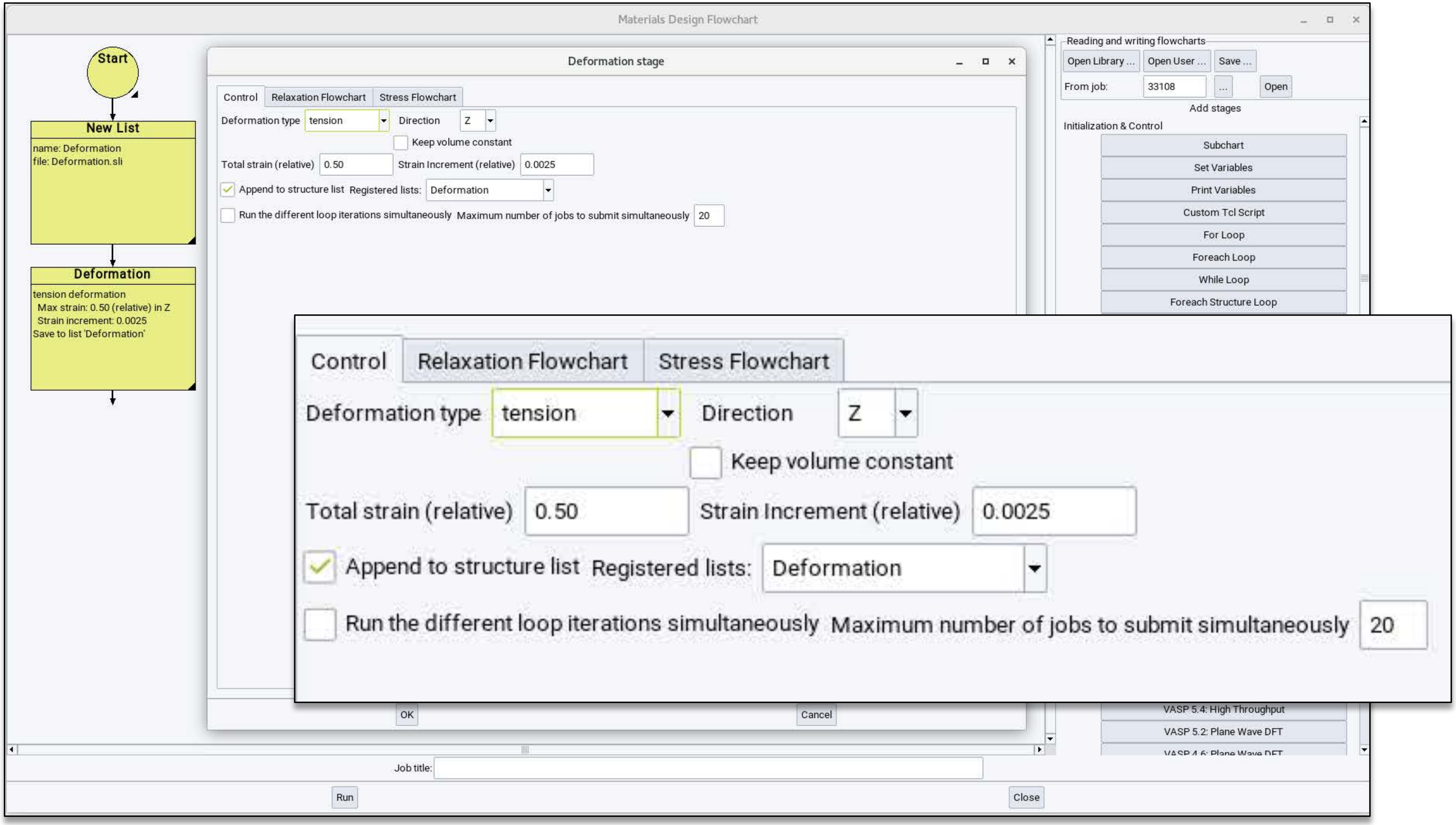




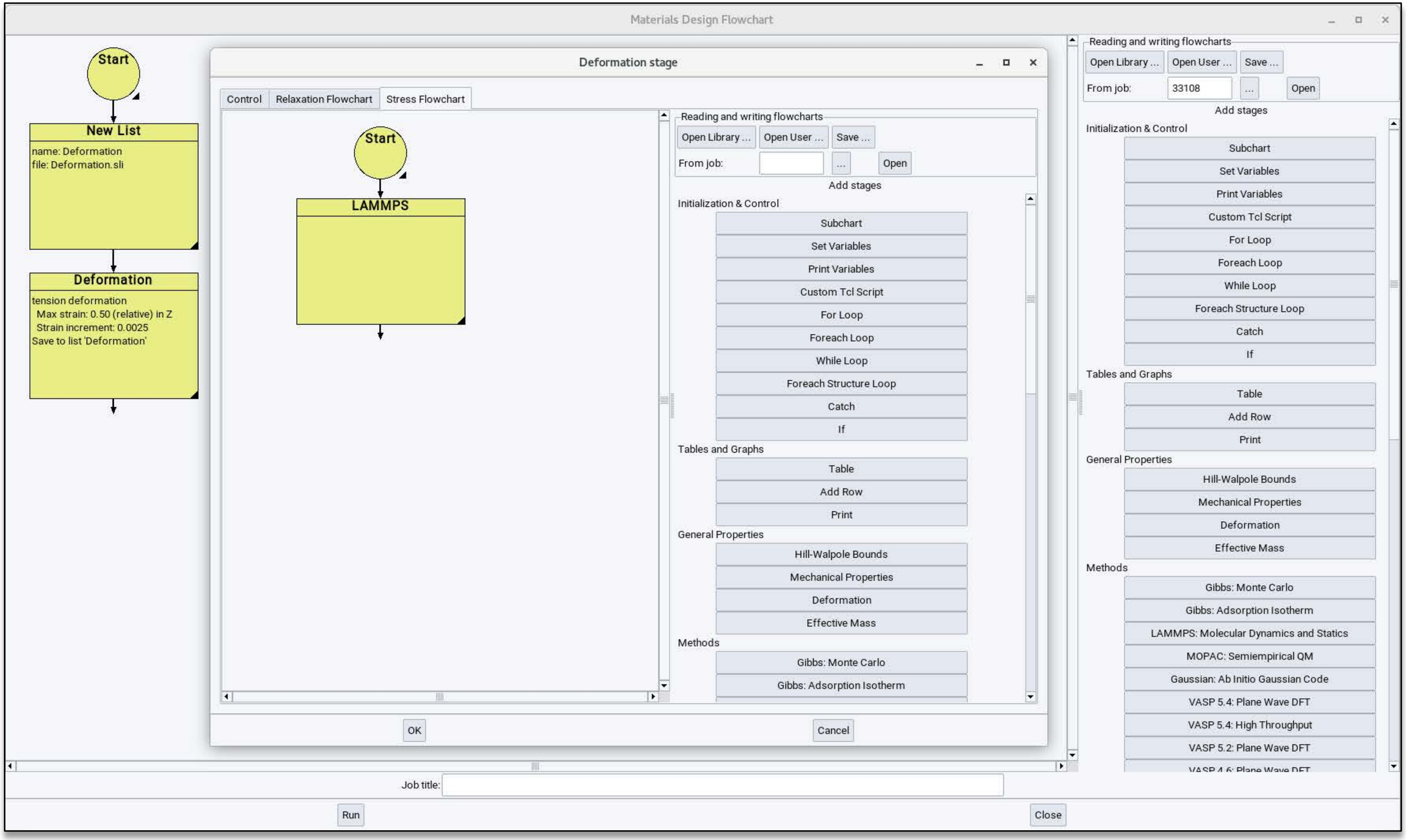
MedeA Deformation

- **Deformation** module *NEW*
  - Working with *MedeA LAMMPS* & *MedeA VASP*
- *MedeA Deformation* evaluates the stress-strain relationships of structures **beyond** the elastic regime, which can be used to extract mechanical properties of idealized structures including yield strength, ultimate strength, fracture strength, and shear strength.
- Performs tension, compression, and shear deformations
- Fully automated and robust computational procedure designed to achieve utmost efficiency for the mechanical properties ***beyond*** the elastic regime
- Automated stress-strain curves for results validation

MedeA Deformation

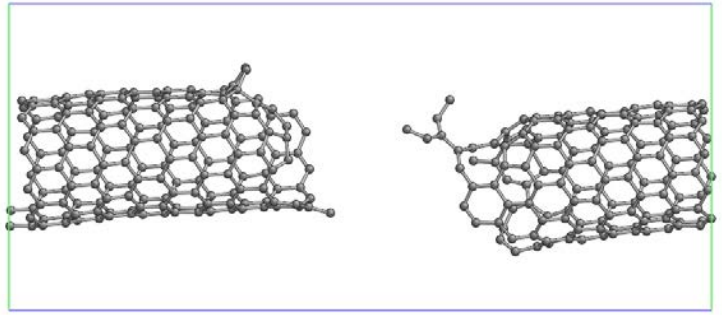


MedeA Deformation

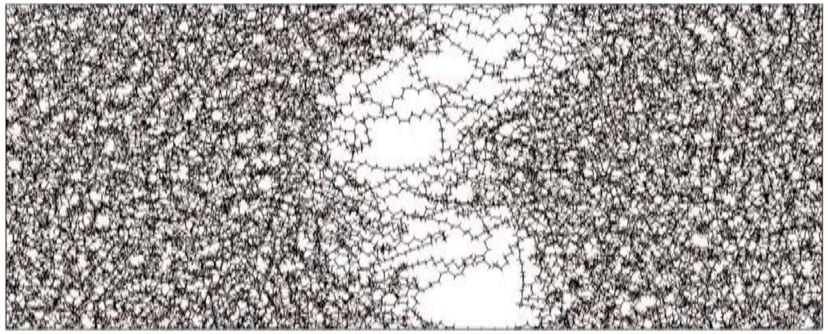


Deformation Simulations

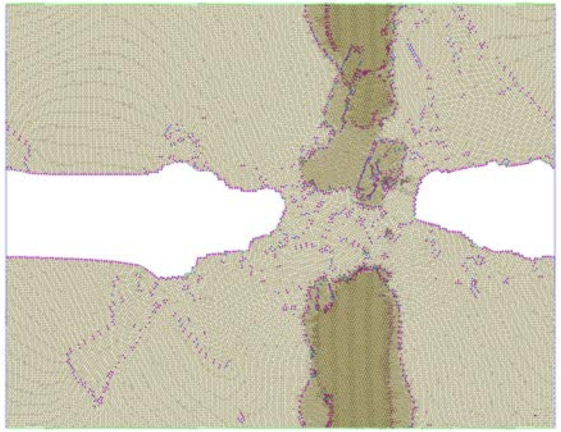
- Tensile deformation of CNT with Tersoff



- Tensile deformation of PE with PCFF+



- Crack propagation of Zr with EAM



see Webinar "Elasticity and Beyond:Predicting Mechanical Properties with MedeA" by Ray Shan

UNIFAC

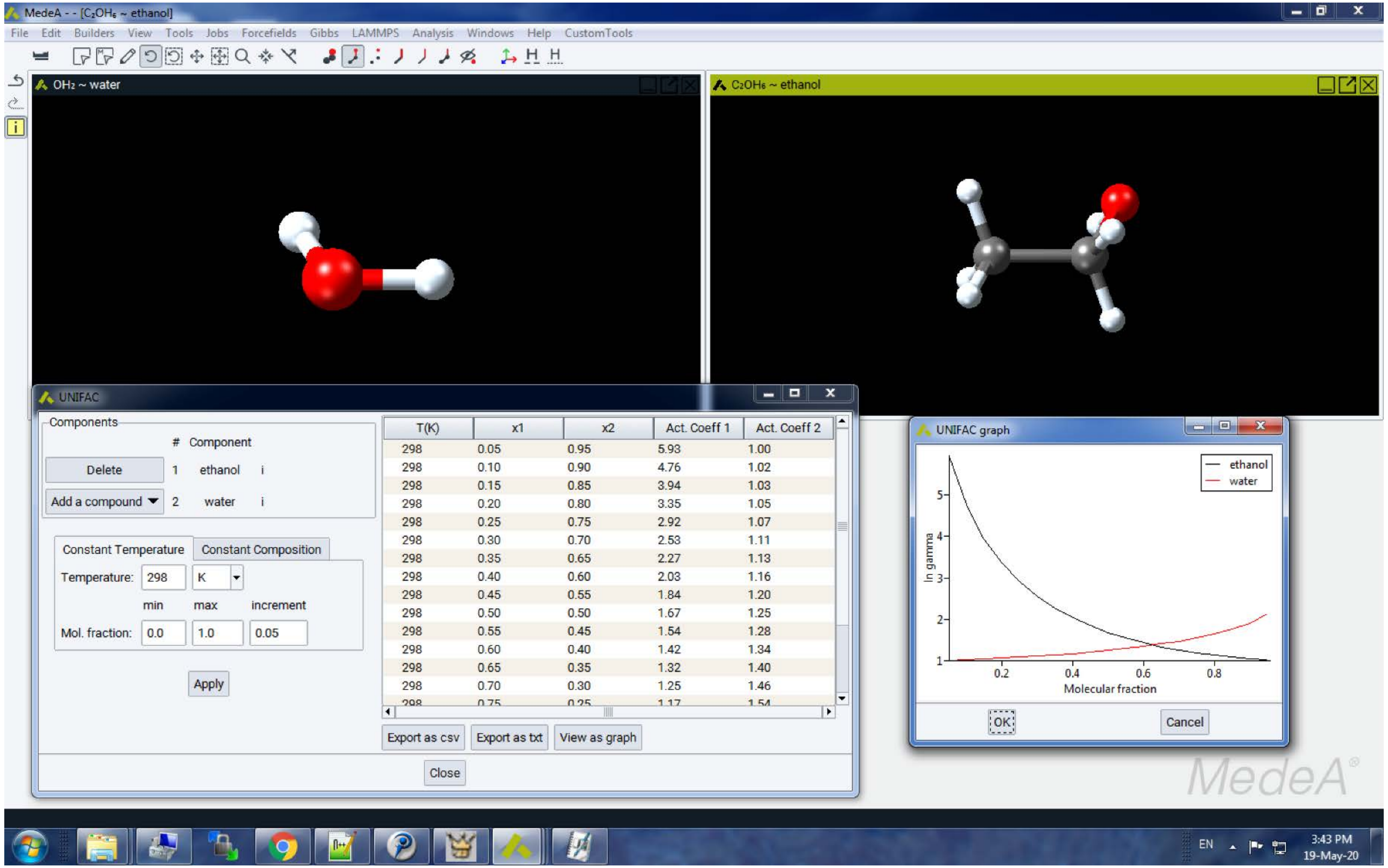
- UNIFAC *NEW*
  - The **UNIFAC** method (**UNI**QUAC **F**unctional-group **A**ctivity **C**oefficients) is a semi-empirical method for the prediction of non-electrolyte activity in non-ideal mixtures. UNIFAC uses the functional groups present on the molecules that make up the liquid mixture to calculate activity coefficients. By using interactions for each of the functional groups present on the molecules, as well as some binary interaction coefficients, the activity of each of the solutions can be calculated. This information can be used to obtain information on liquid equilibria, which is useful in many thermodynamic calculations, such as chemical reactor design, and distillation calculations.
  - The UNIFAC model was first published in 1975 by Fredenslund, Jones and Prausnitz.
  - The output of a UNIFAC calculation can be used to create close-to-equilibrium input for MC or MD simulations.

UNIFAC

- Partial Pressure of compound i in a mixture, P_i:

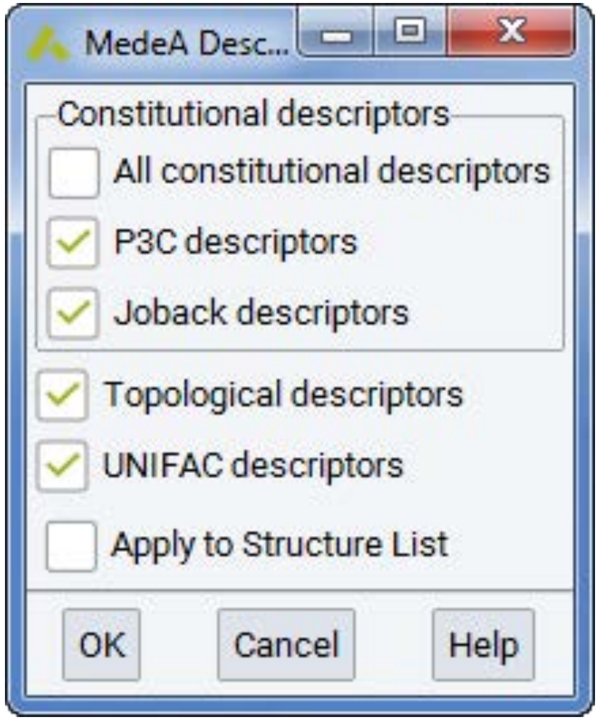
$$P_i = x_i \cdot \gamma_i \cdot P_i^{sat}$$

  - x_i is the molar fraction of i in the mixture
  - γ_i is the activity coefficient of compound i in a mixture
  - P_i^{sat} is the saturation pressure or pure compound i at the same T



Molecular Descriptors

- Types:
  - Topological (16) *NEW*
  - Joback groups (41)
  - P3C (35)
  - UNIFAC (104) *NEW*
- All can be added in a structure list from the Molecular Descriptors stage

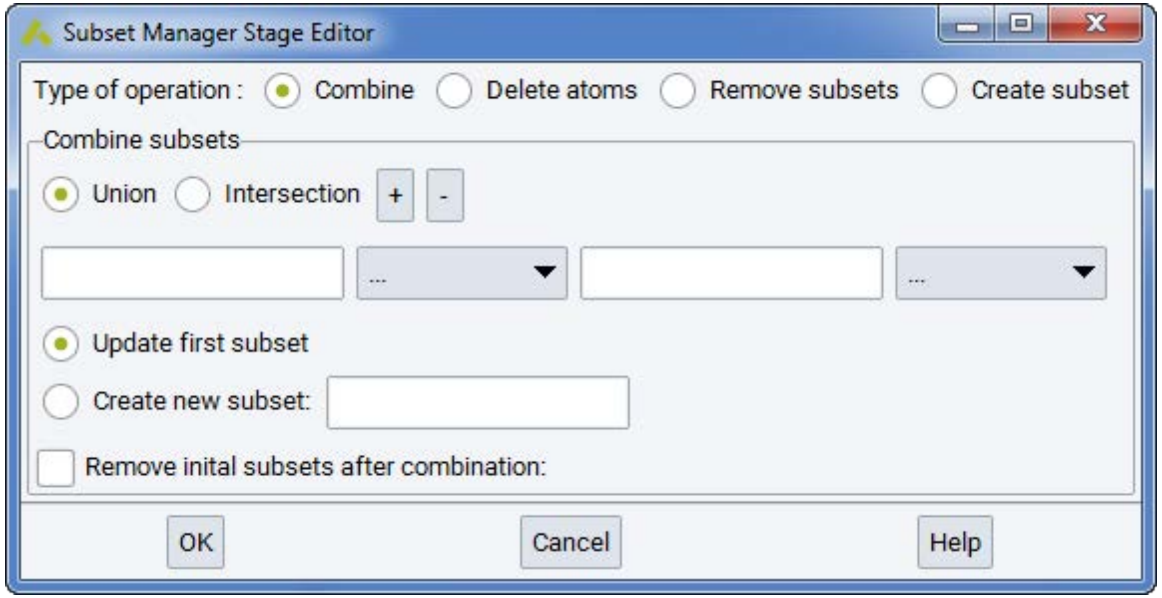


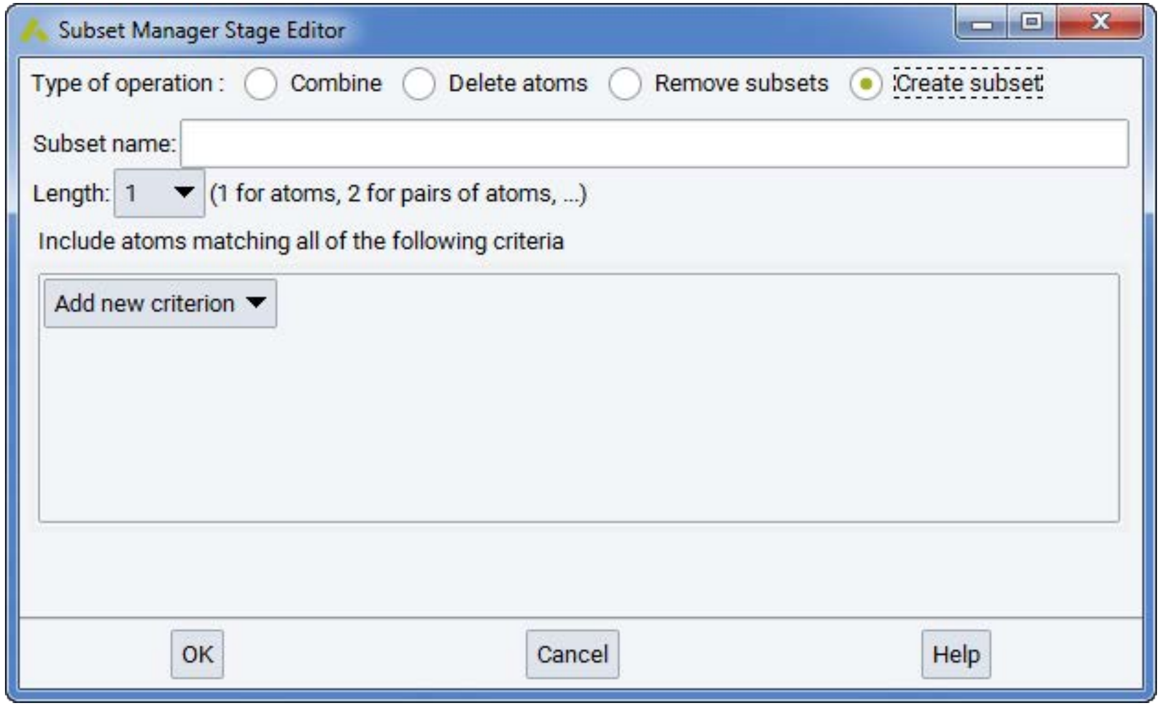
Forcefields

- **Mesoscale FFs**
  - MARTINI *NEW*
  - SPICA (old Shinoda, De Vane, Klein) *NEW*
- **pcff+**
  - Extensions for –OCH_3 terminated oligo-ethyleneglycols
  - Improved parametrization for urea
  - New parameters for divalent Mg and Sr cations
  - Optimized parameters for type Ba^+ (based on $BaCO_3$)
- **EAM**
  - Combination of morse FF with Streitz-Mintrmire charge equilibration
- Added explicit pair interactions handling in *MedeA LAMMPS*

Extension of “Subset Manager” stage

- Added ability to create subsets in a flowchart stage, i.e. completing the control of managing subsets in flowcharts, aiding:
  - Applying changes to a system before or after a simulation run,
  - Preparing a system for analysis



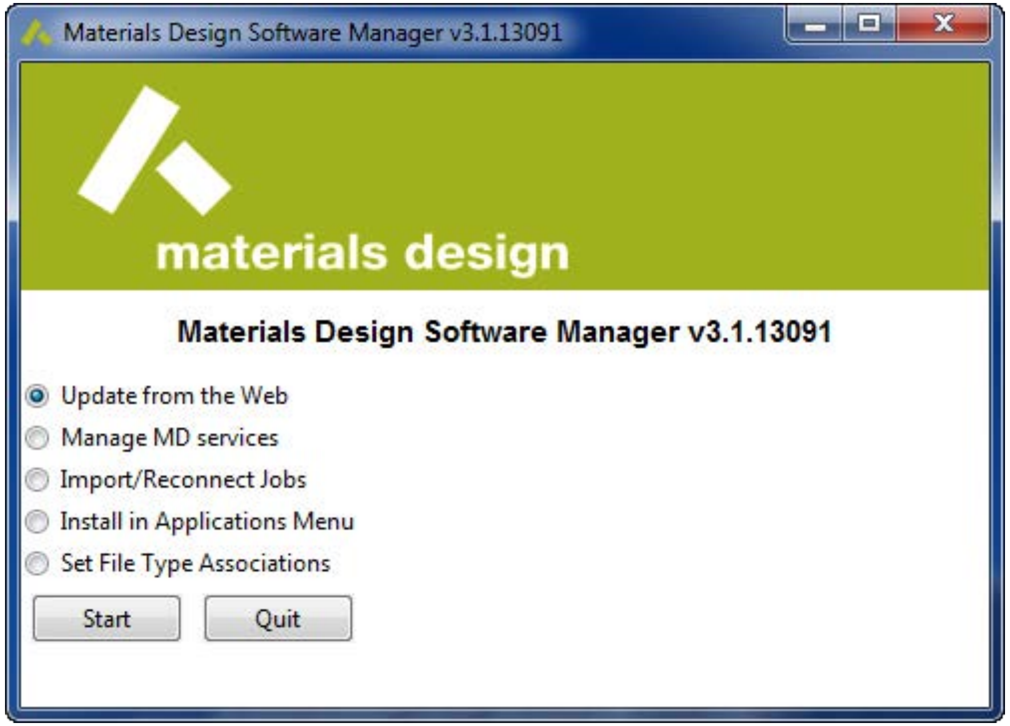


Flowchart Library

- Extensive updates and extensions to existing flowchart library
  - Building
  - GIBBS
  - VASP
  - MOPAC
  - LAMMPS
  - Mechanical Properties
  - UNCLE
  - Gaussian
  - Descriptors
  - Other

Maintenance

- Update of Maintenance program
  - Improved efficiency, speed and robustness
  - GUI update
- Full installation from terminal available



VASP 6

VASP 6 in *MedeA* 3.1

Research Objective

- Accurate energy by combining exact non-local exchange and accurate treatment of electronic correlation

- Accurate energy and forces for larger systems, and
- for metals, semiconductors and insulators

- Accurate quasiparticles and optical spectra for larger systems

- Electron-phonon coupling for temperature dependent properties

- XAS, XANES, core excitation spectroscopy

Solution Provided by VASP 6

- Adiabatic connection fluctuation dissipation theorem within the random phase approximation (ACFDT-RPA)
- Møller-Plesset perturbation theory

- Low scaling ACFDT-RPA (space-time method)
- ACFDT-RPA for finite temperatures based on Fermi smearing

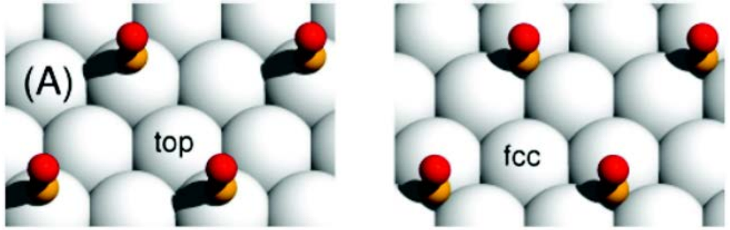
- Low scaling GW approach (space-time method)

- Single displacement approach (Zacharias-Giustino) or full Monte Carlo sampling

- Supercell core-hole approach

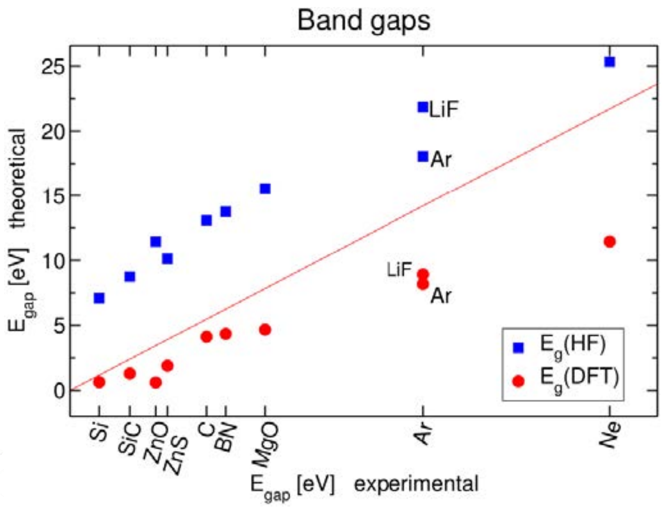
Need for Accurate Methods Beyond DFT and Hybrid

Adsorption of CO on Cu, Rh, Pt (111)



Incorrect site preference predictions (eV):

	Cu(111)	Rh(111)	Pt(111)
PBE	-0.165	-0.099	-0.157
PBE0	0.027	0.005	-0.056
HSE03	0.006	0.016	-0.069



Lattice constant

	MRE	MARE
PBE	0.8	1.0
PBE0	0.1	0.5
HSE	0.2	0.5
B3LYP	1.0	1.2

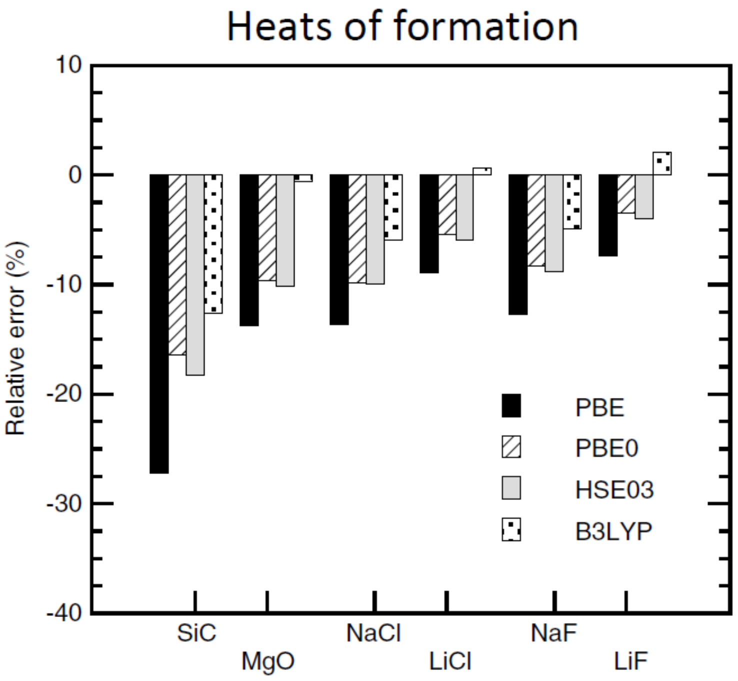
Bulk modulus

	MRE	MARE
PBE	-9.8	9.4
PBE0	-1.2	5.7
HSE	-3.1	6.4
B3LYP	-10.2	11.4

Atomization energy

	MRE	MARE
PBE	-1.9	3.4
PBE0	-6.5	7.4
HSE	-5.1	6.3
B3LYP	-17.6	17.6

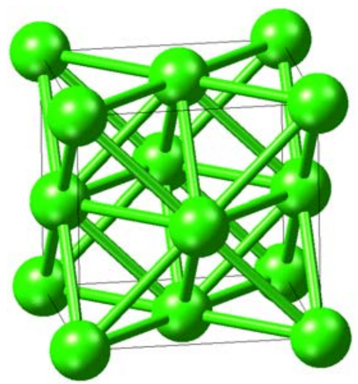
see Webinar "VASP 6: Total energies beyond DFT" by Martijn Marsman



ΔH (kJ/mol)	PBE	EXP
$Al+N_2 \rightarrow AlN$	262	350
$Mg+H_2 \rightarrow MgH_2$	52	78
$Si+C \rightarrow SiC$	51	69
CO→CO@Rh	183	144

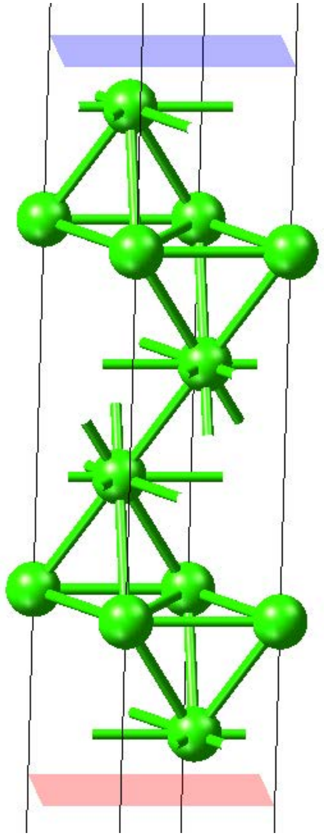
Build Model for CO Adsorbed on Pt(111) in *MedeA*

Retrieve fcc Pt from structural databases
MedeA InfoMaticA

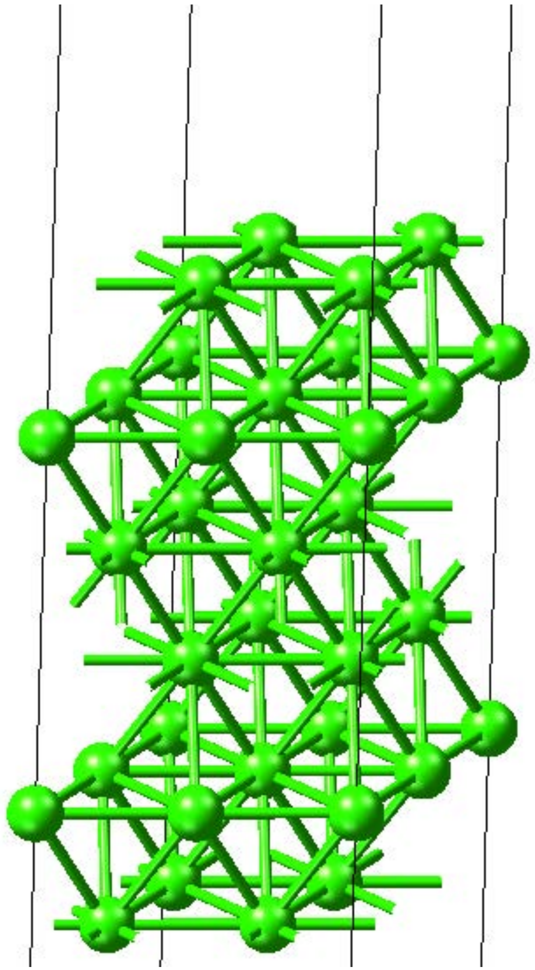


Optimize the lattice
MedeA VASP 6

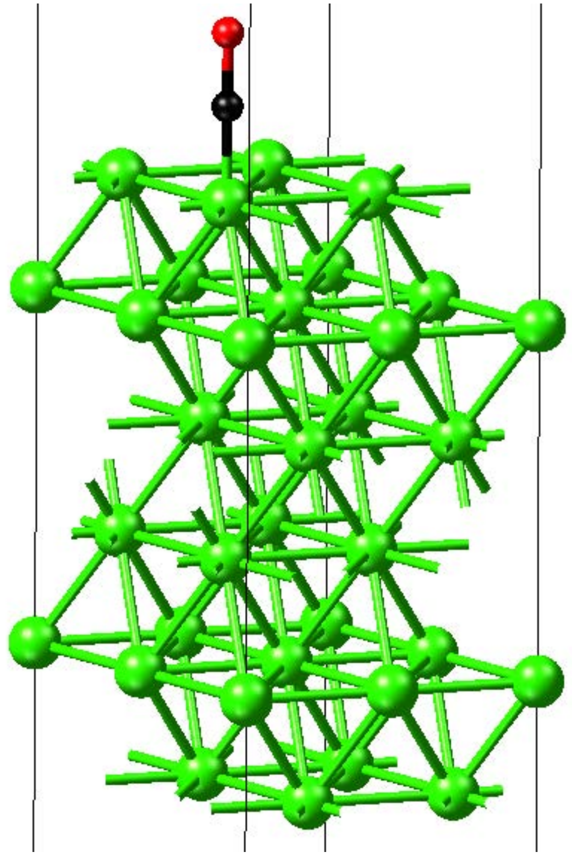
Build Pt(111) surface
MedeA Surface Builder



Build 2x2 Pt(111) supercell
MedeA Supercell Builder

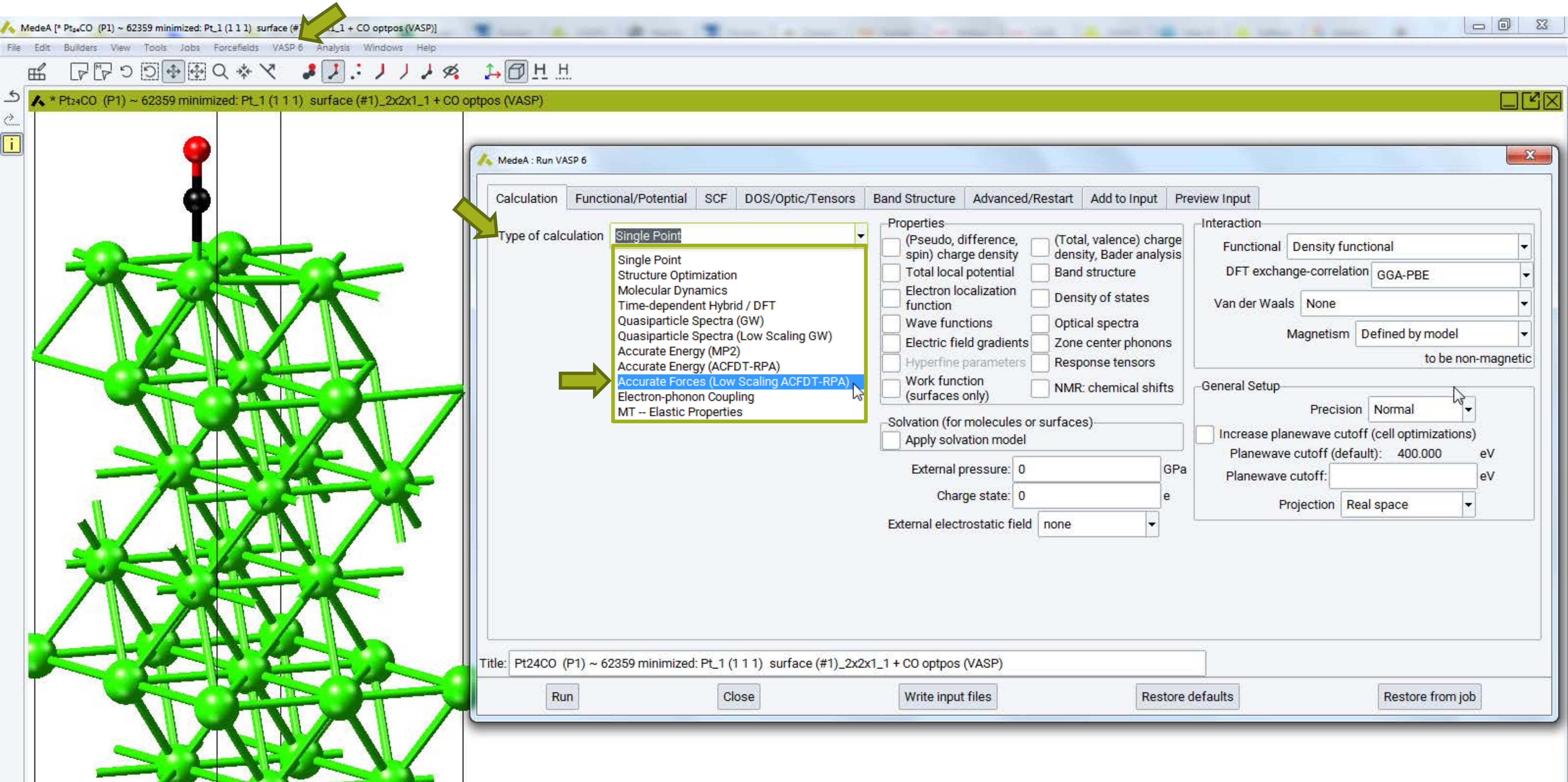


Place CO on Pt(111)
Freeze lower Pt atoms
MedeA Structure Editor

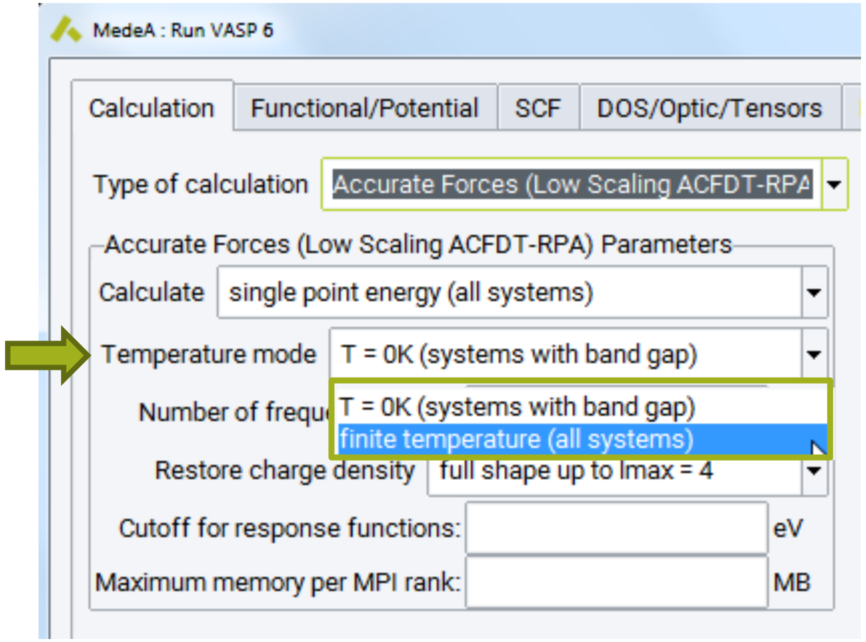


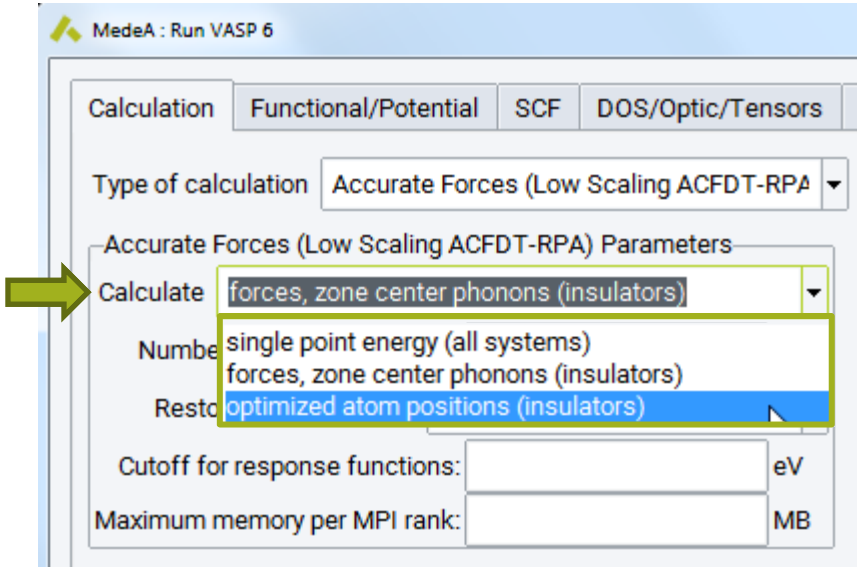
Optimize atom positions
MedeA VASP 6

Low Scaling ACFDT-RPA in *MedeA VASP 6*



Low Scaling ACFDT-RPA in *MedeA VASP 6*





- Single point energy for all systems
  - Semiconductors and insulators
    - T = 0K temperature mode
  - Metals
    - finite temperature mode

- Forces and zone center phonons
- Optimization of atom positions
  - for semiconductors and insulators only
    - Finite temperature mode for metals under development

Standard vs. Low Scaling ACFDT-RPA

Results for Pt24CO in Job.out:

```
VASP 6 CALCULATION PROTOCOL:
============================
1. Single point low scaling ACFDT-RPA calculation of the energy

Low scaling ACFDT-RPA calculation for accurate total energy
==============================================================

VASP parameters
===============


……


 ACFDT-RPA correlation energy:            -423.475687 eV for Pt24CO
       Hartree-Fock total energy:            -242.317531 eV for Pt24CO
Correction for partial occupancy:             -11.292225 eV for Pt24CO
----------------------------------------------------------------------------
          ACFDT-RPA total energy:            -665.793218 eV for Pt24CO

Electronic contributions:
                          Empirical Formula          Cell
                                Pt24CO          Pt24CO
                          --------------- ---------------
         ACFDT-RPA Energy      -64239.264      -64239.264 kJ/mol

Job completed on Fri 28 August 2020 at 12:42:54 CEST after 7923 s (2:12:03)
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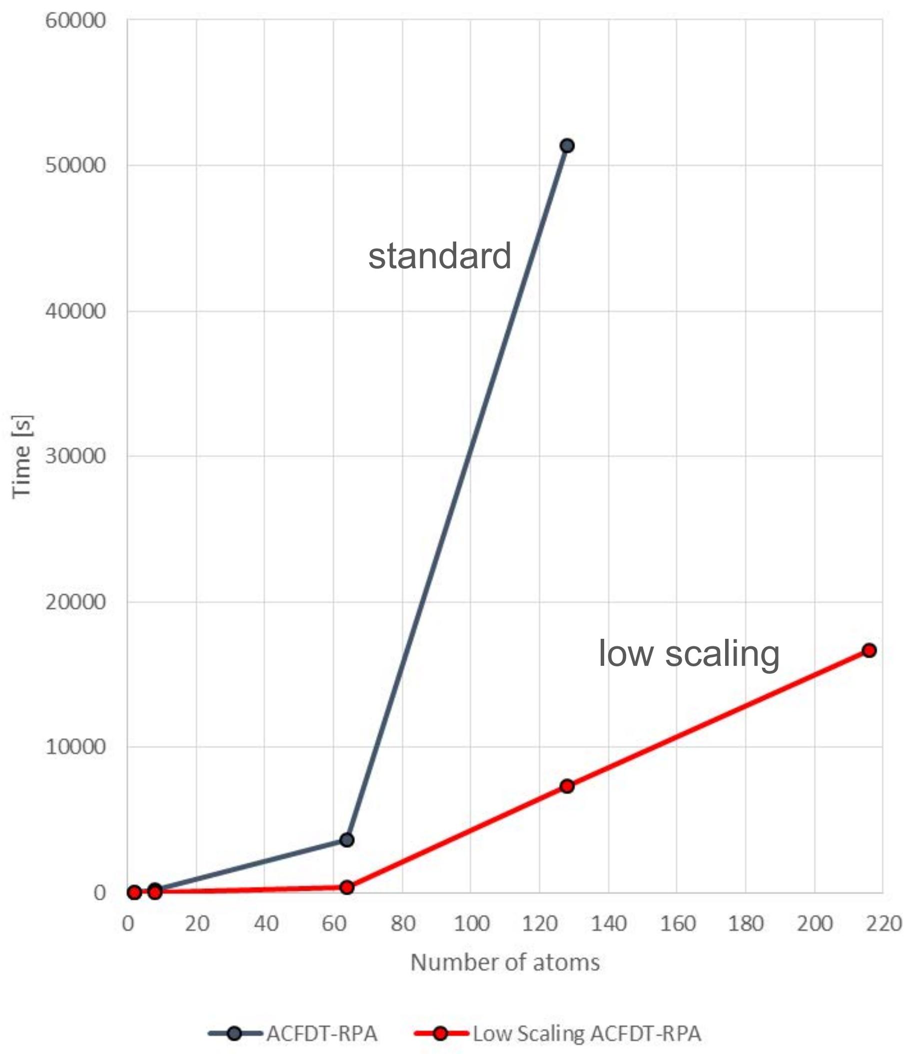
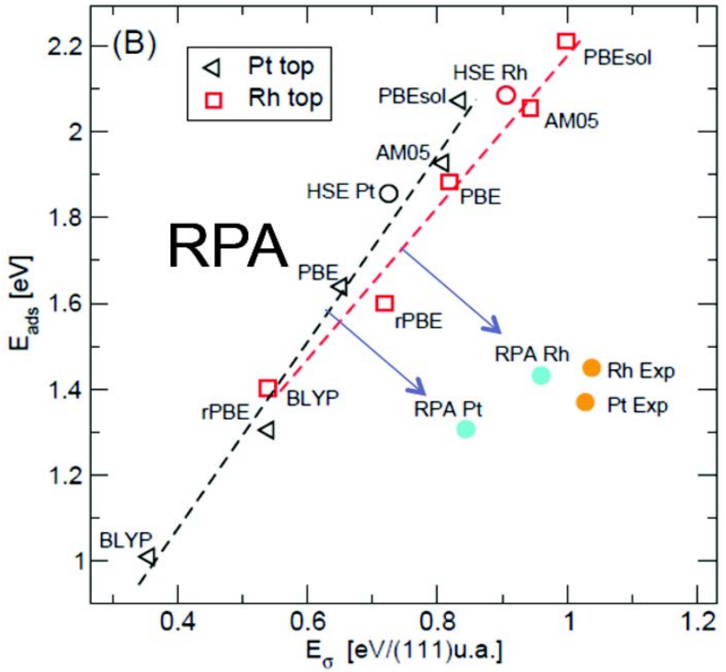
Compute time vs. supercell size for Si:



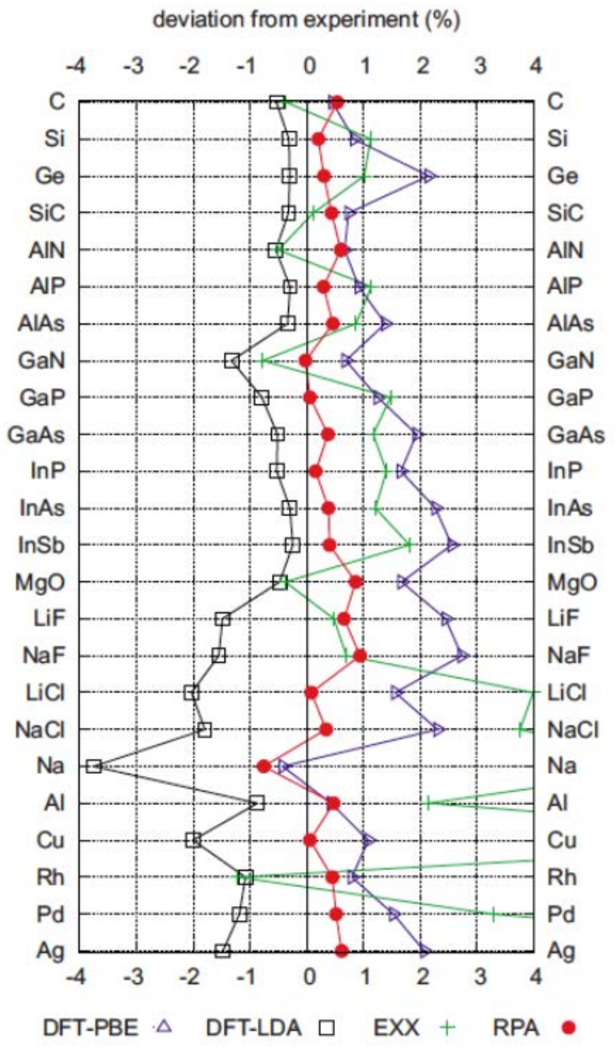
Benefit of Accurate Energies and Forces from ACFDT-RPA

Adsorption of CO on Rh, Pt (111)



- ACFDT-RPA delivers
  - Correct site preference
  - Good adsorption energies
  - Excellent lattice constants
  - Good surface energies

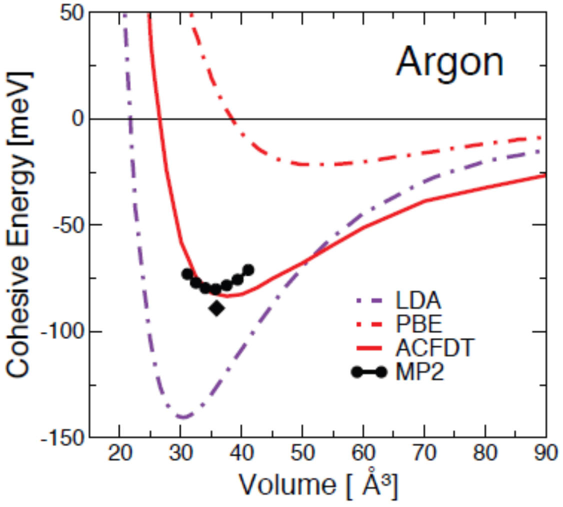
Lattice parameters



Heats of formation

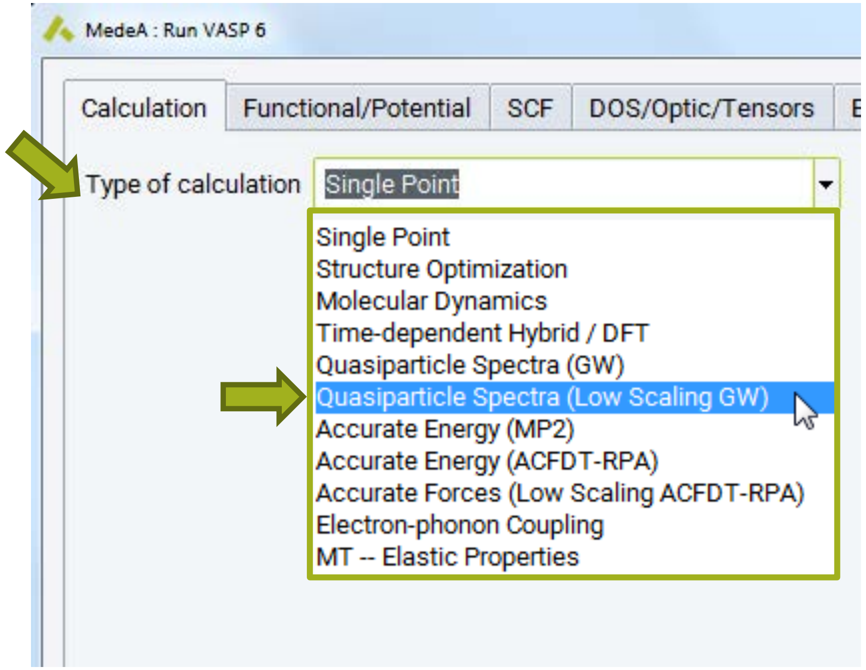
	PBE	Hartree-Fock	RPA	EXP
LiF	570	664	609	621
NaF	522	607	567	576
NaCl	355	433	405	413
MgO	516	587	577	603
MgH_2	52	113	72	78
AlN	262	350	291	321
SiC	51	69	64	69

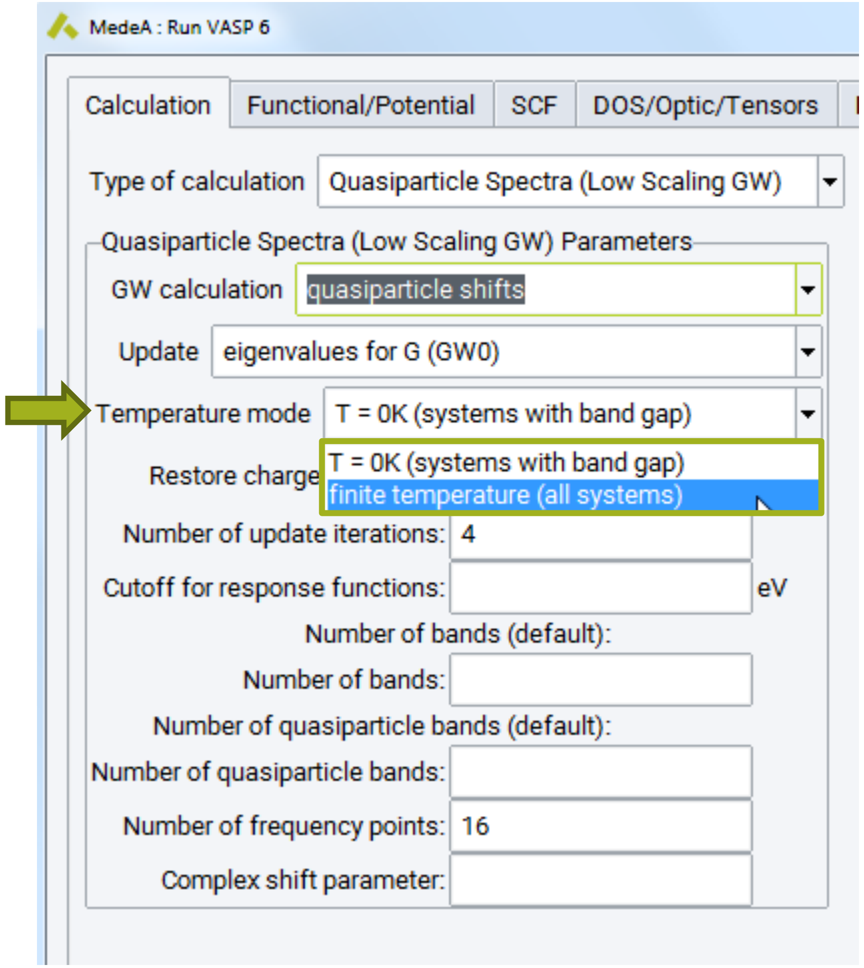
Van der Waals interactions



see Webinar "VASP 6: Total energies beyond DFT" by Martijn Marsman

Low Scaling GW for Quasiparticles and Optical Spectra



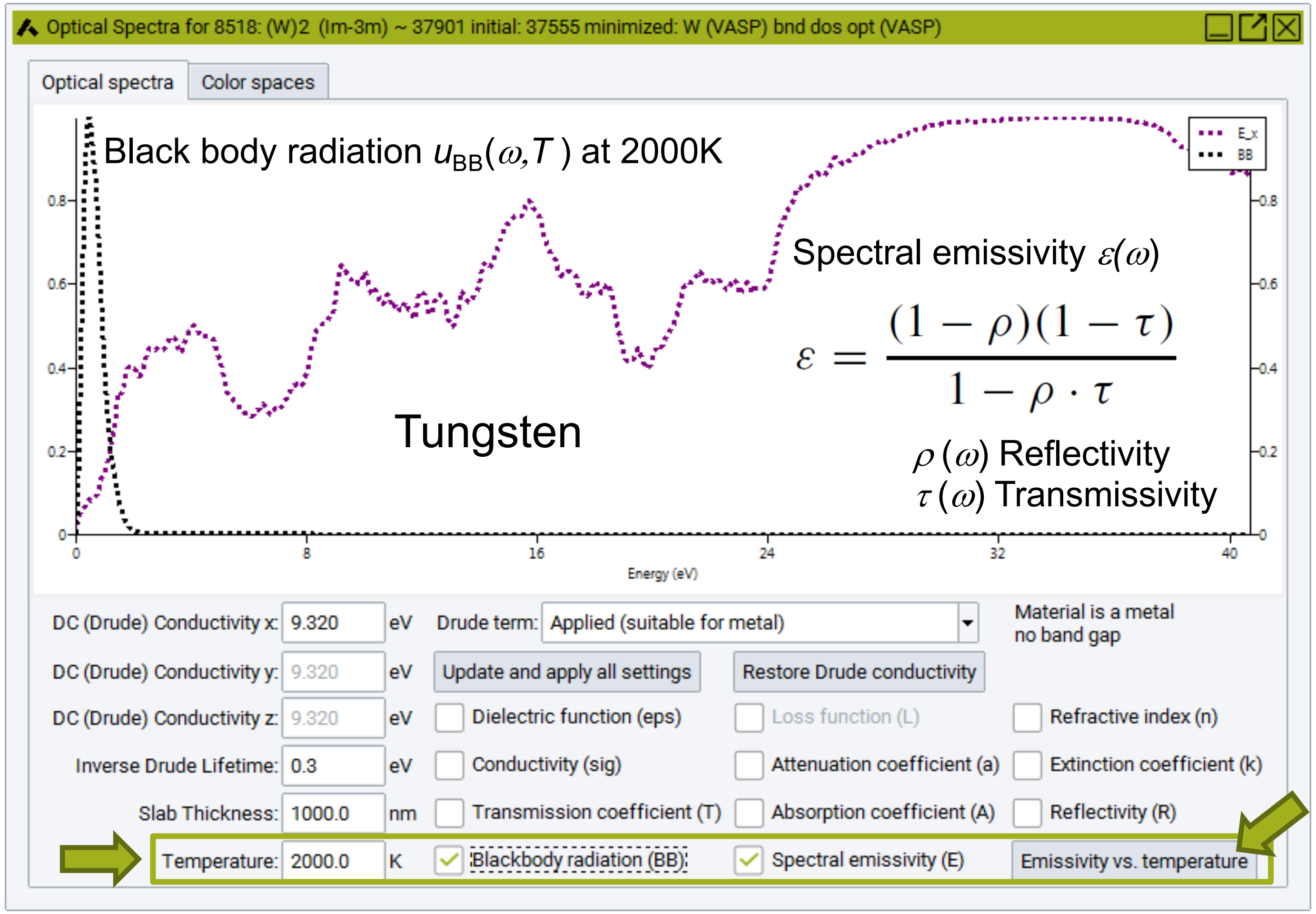


- Optical spectra are available from
  - the Optical Spectra checkbox in the Properties subpanel of the Calculation Tab for local, semi-local, van der Waals, metaGGA and hybrid functionals
  - From Quasipartical Spectra calculation types applying low scaling and standard GW, as well as optionally the Bethe-Salpeter approach to excitonic effects

- Low scaling technique supports finite temperature mode for metals

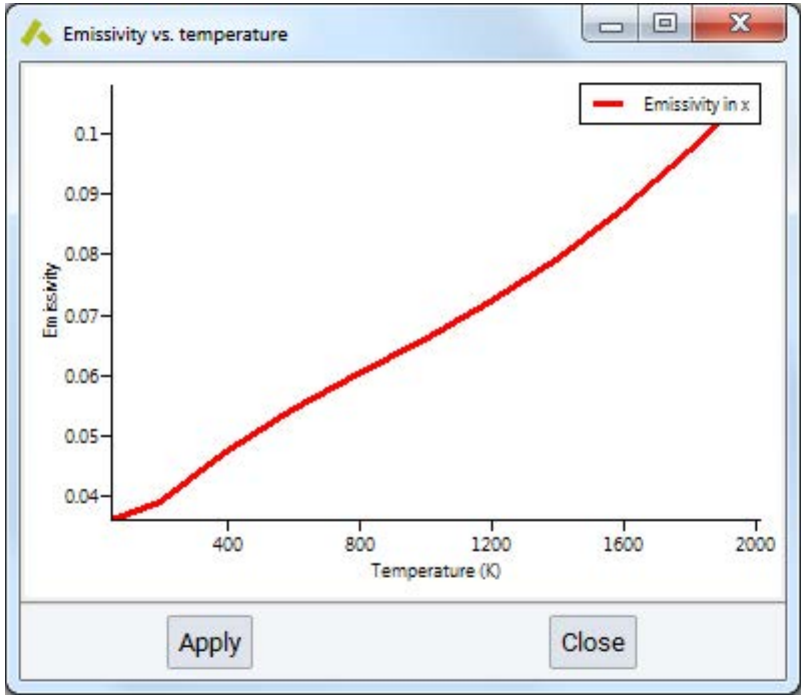
Optical Spectra and Color Analysis in *MedeA 3.1*

- New in *MedeA 3.1*: Spectral emissivity and black body radiation; Emissivity as a function of temperature; Color spaces: Spectral power distribution of fluorescent lamp FL2



Emissivity $\varepsilon(T) = \frac{\int \mathcal{E}(\omega) \int u_{BB}(\omega,T)\,d\omega}{\int u_{BB}(\omega,T)\,d\omega}$

Emissivity vs. Temperature of W

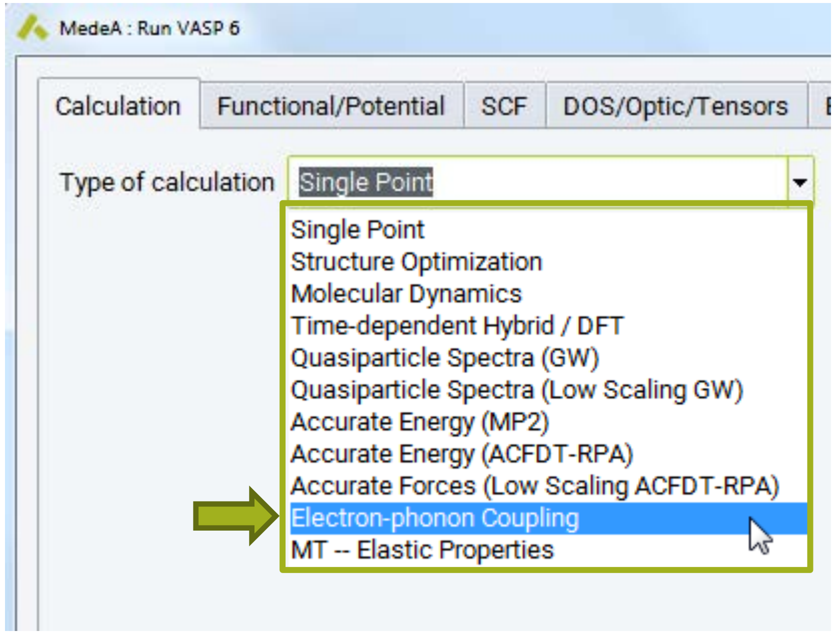


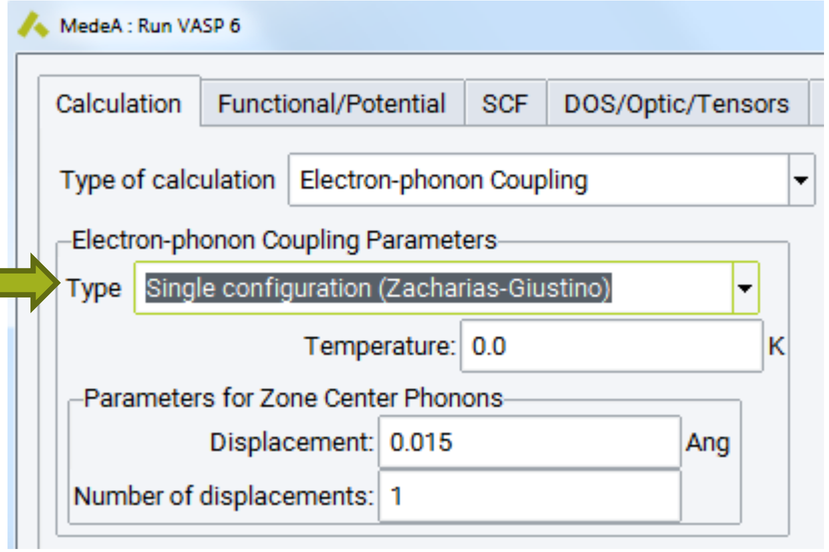
Electron Phonon Coupling from Stochastic Displacements

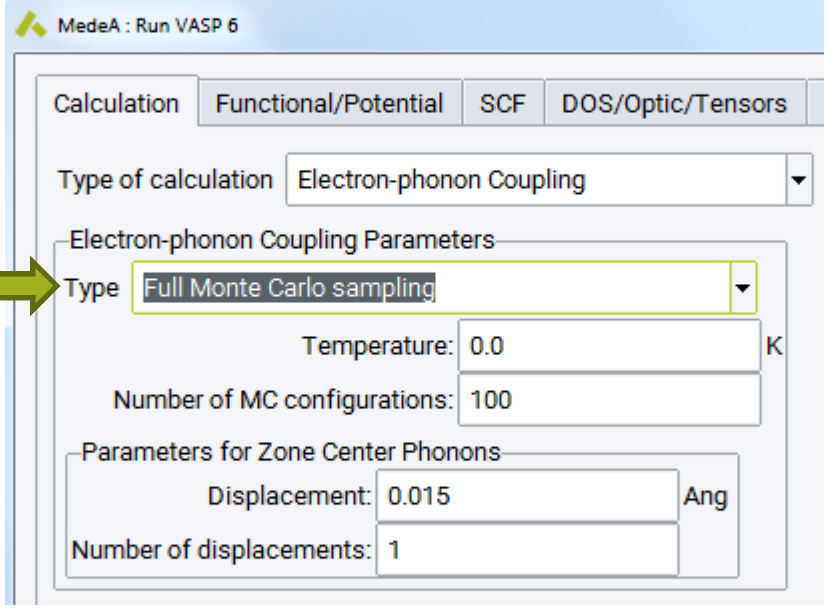
- Single displacement configuration

  M. Zacharias, F. Giustino, Phys. Rev. B 94, 075125 (2016)

- Full Monte Carlo sampling of displacement configurations

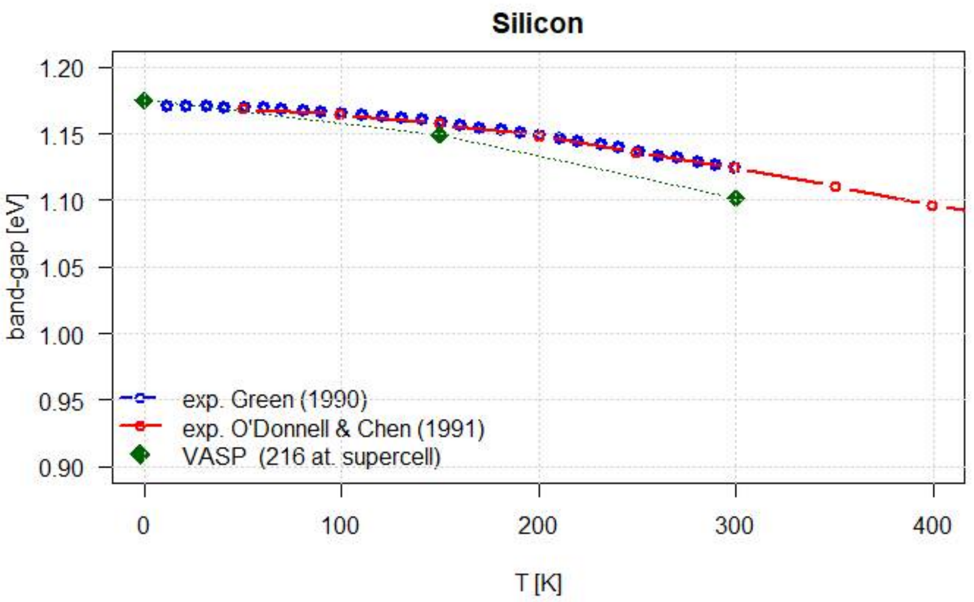


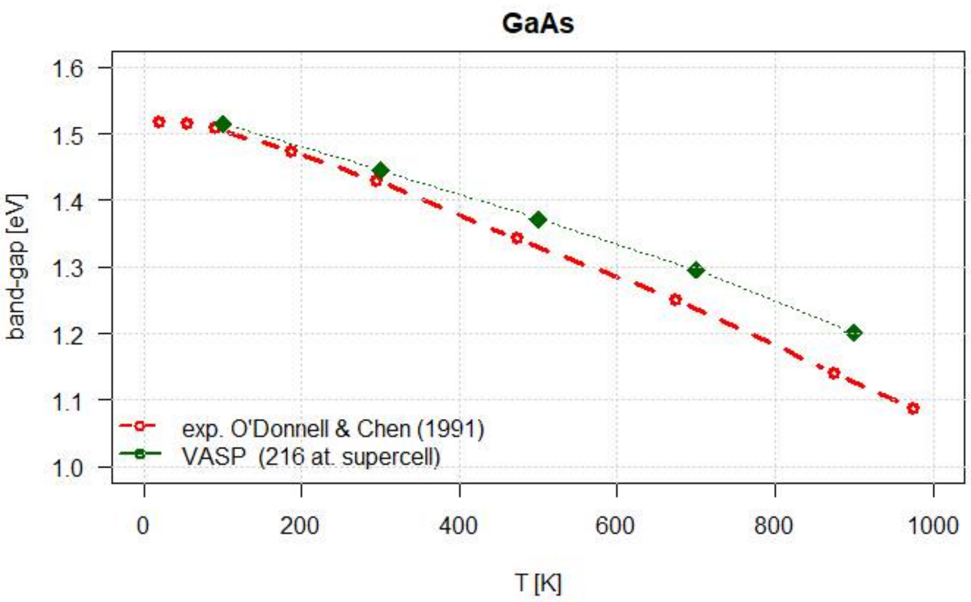


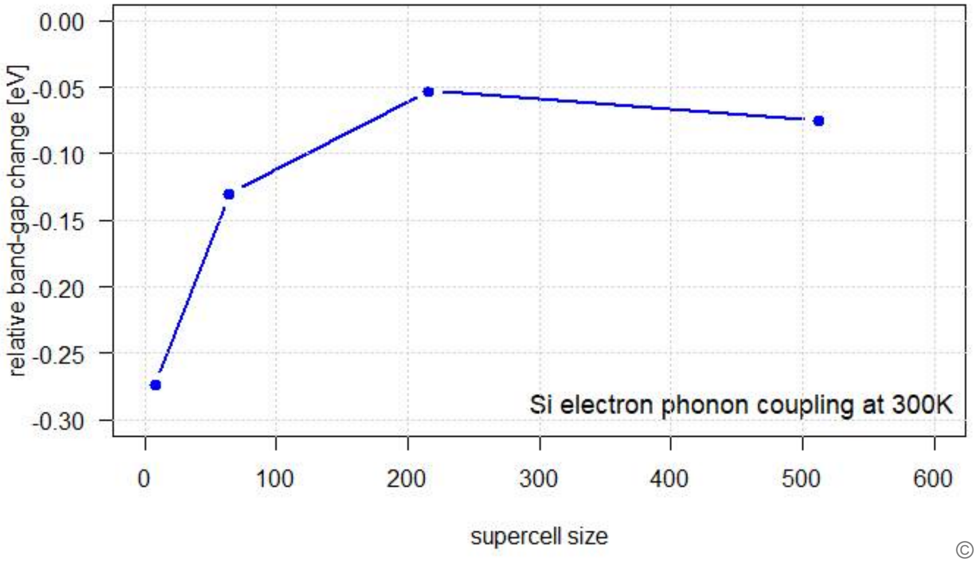


- For a given temperature any of the available properties can be computed

Temperature Dependence of Band Gaps





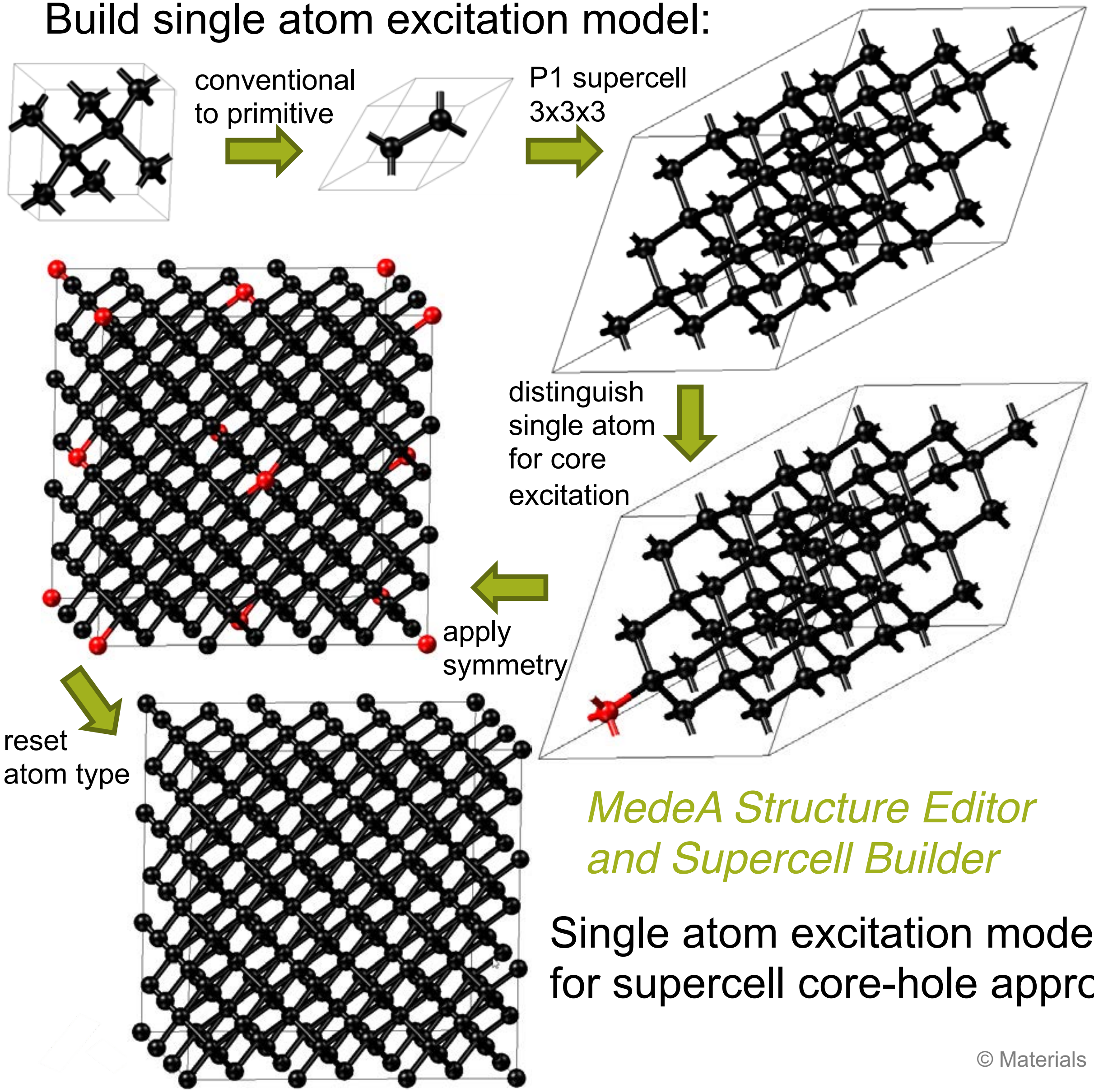


- Need of large supercells!
- Lattice optimization of Si/GaAs: PBE/PBEsol
- Band gaps: Modified Becke Johnson LDA
- Thermal expansion is not included

Exp.: M. A. Green, J. Appl. Phys. **67**, 2944 (1990)
K. P. O'Donnell, X. Chen, Appl. Phys. Lett. **58**, 24 (1991)

XAS, XANES, Core Excitation Spectroscopy

Build single atom excitation model:



MedeA Structure Editor and Supercell Builder

Single atom excitation model for supercell core-hole approach

MedeA VASP 6

Advanced Tab

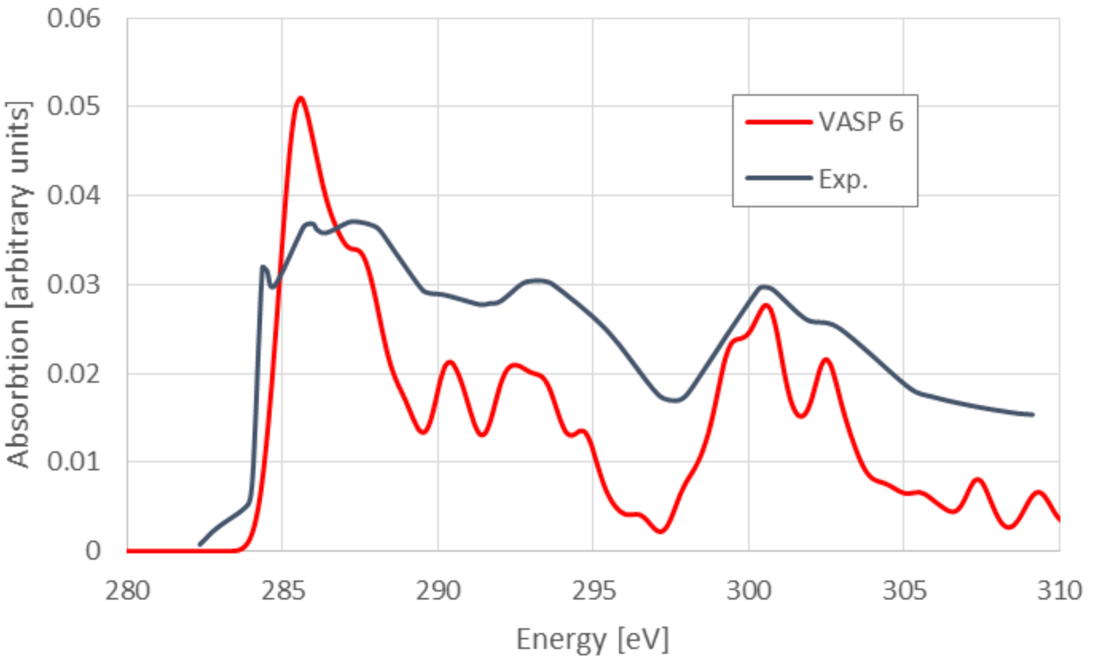
Enable choices specific for	sites

Number of bands (default):	136
Number of bands:	300

Add to Input Tab

```
ICORELEVEL = 2
CLNT = 1
CLN = 1
CLL = 0
CLZ = 1.0
CH_LSPEC = .TRUE.
CH_SIGMA = 0.5
```

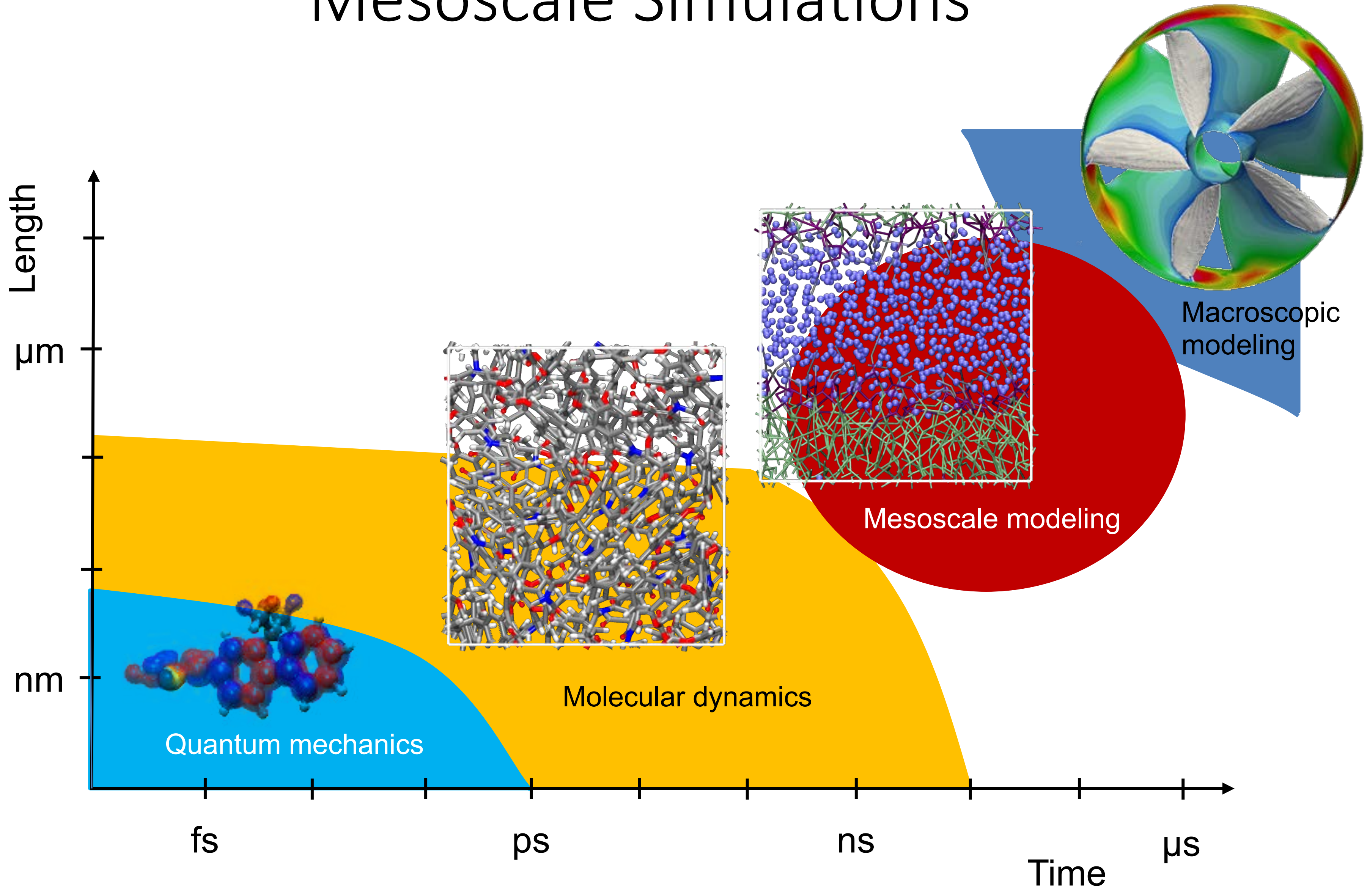
XANES K-edge spectrum of diamond



Exp.: Y. Ma *et al.*, Phys. Rev. Lett. **69**, 2598 (1992)

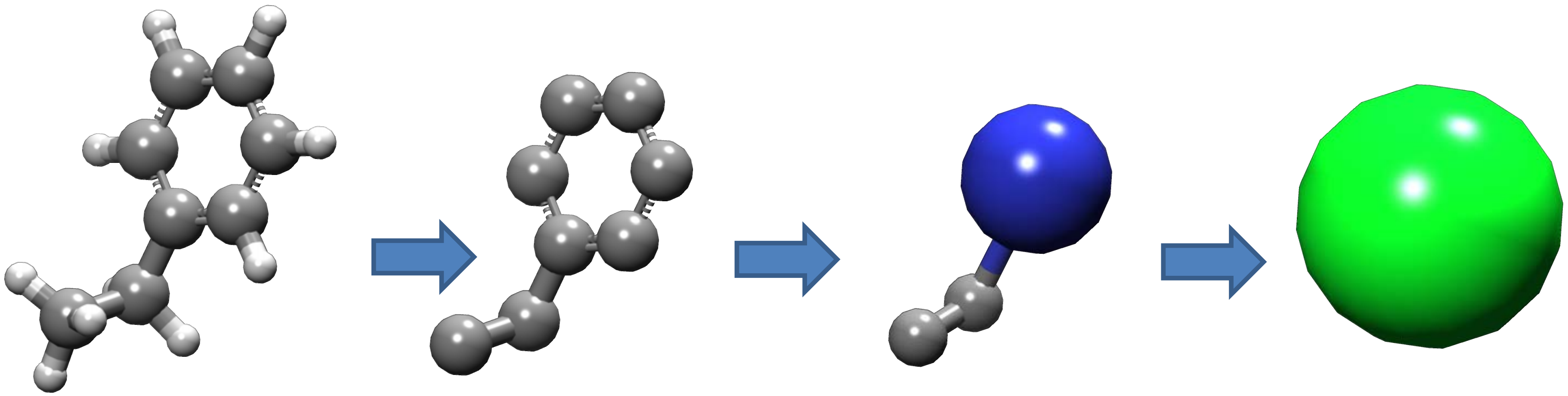
Mesoscale Simulations

Mesoscale Simulations



Mesoscale Simulations

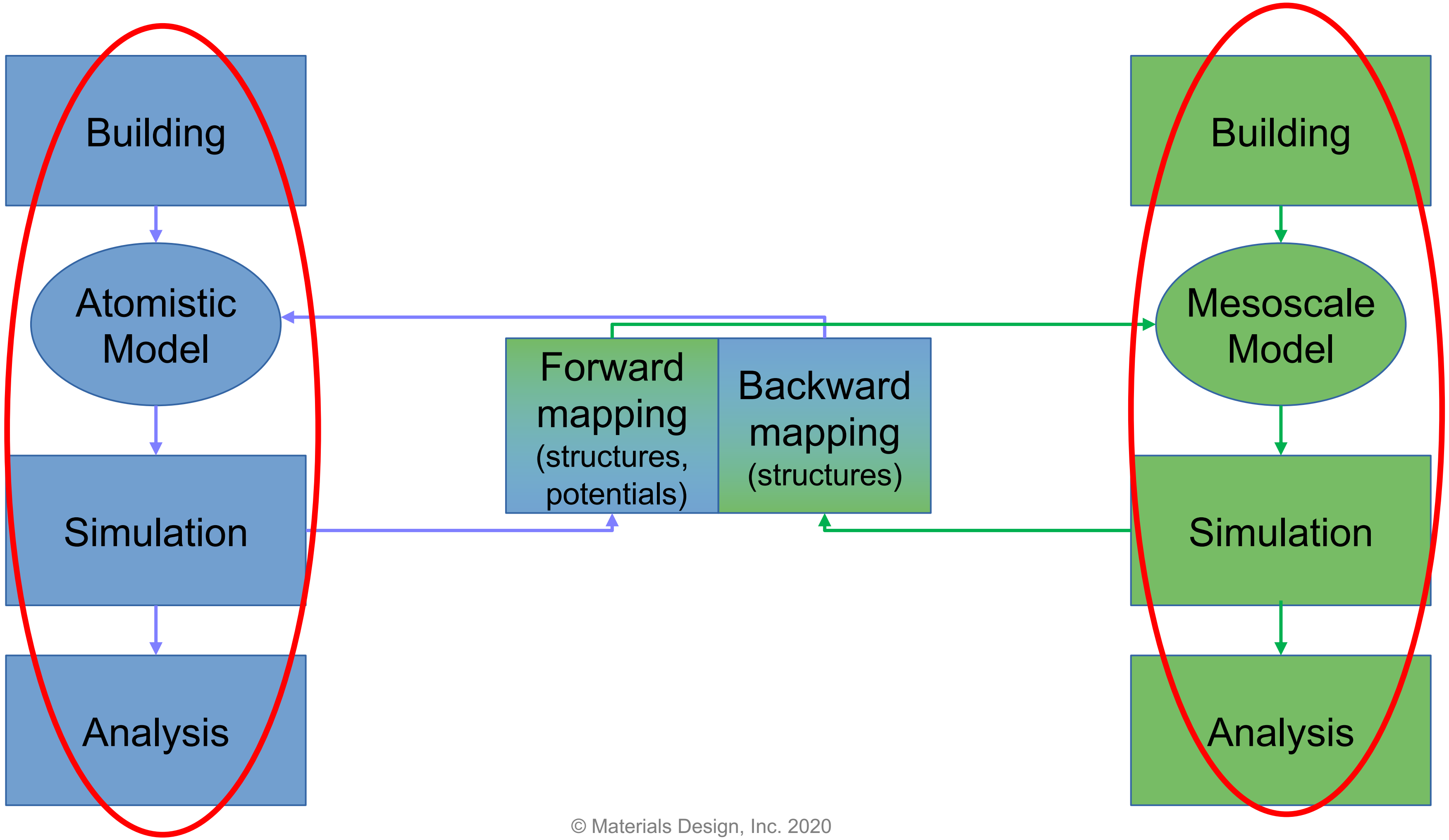
Coarse graining of a styrene monomer



atomistic | united atom | coarse grained 1 | coarse grained 2

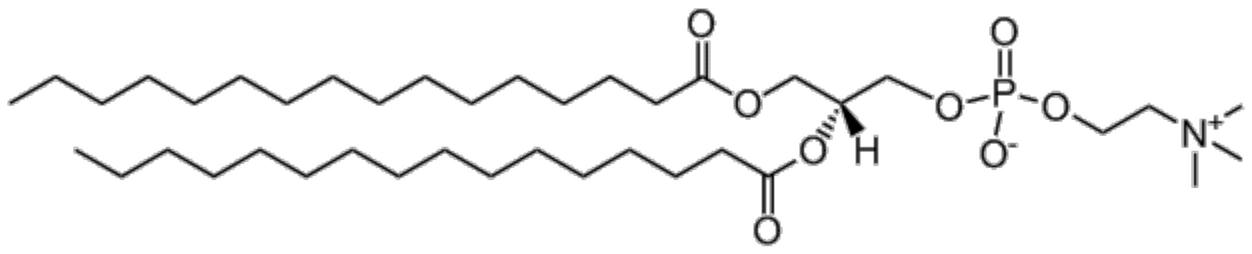
Mesoscale Simulations

- Users expect smooth switching between atomistic and mesoscale simulations



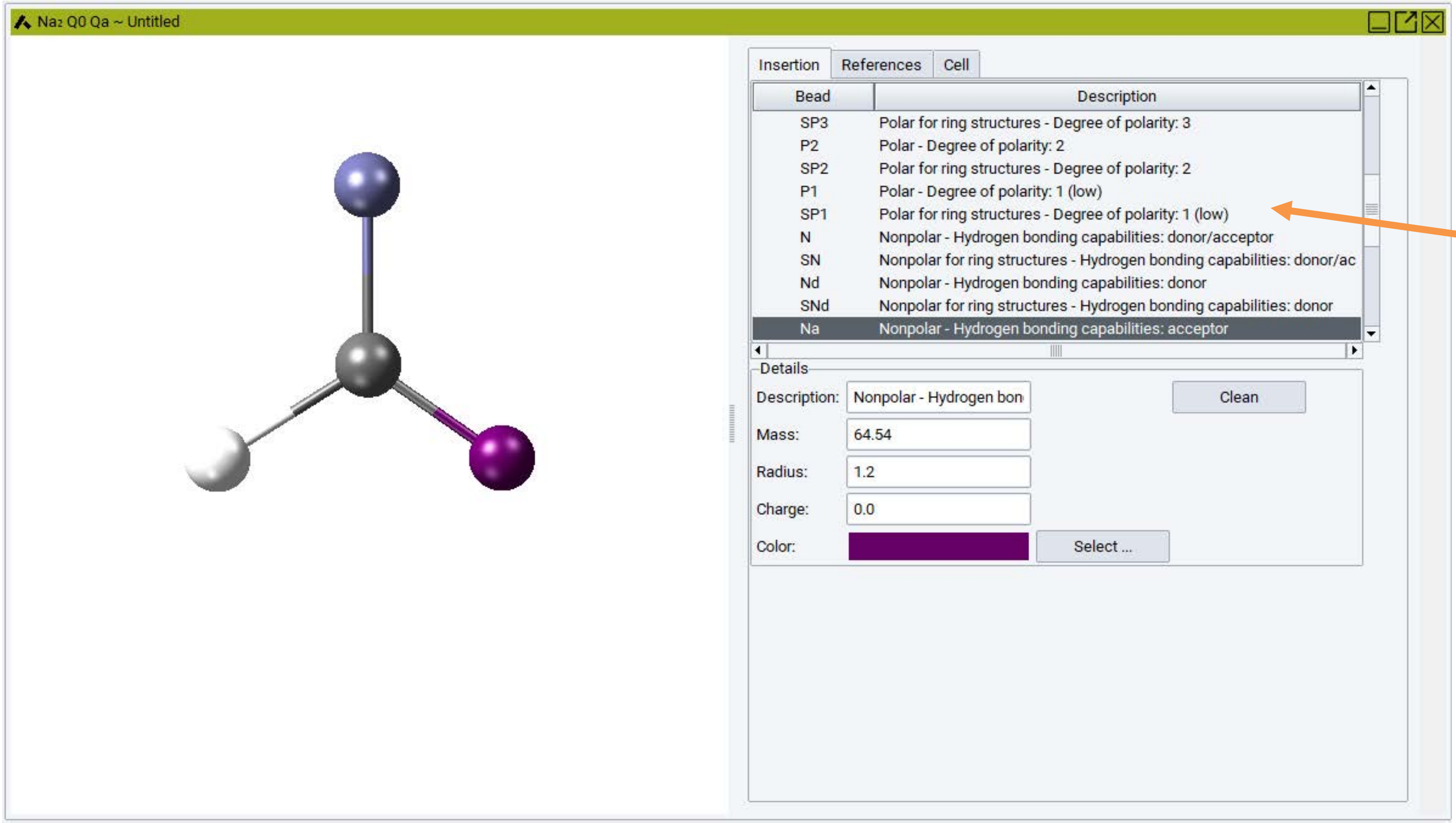
Self-assembly of Lipid Bilayer

- Self-assembly of a lipid bilayer (dipalmitoylphosphatidylcholine) in water with the Martini forcefield
- 128 DPPC lipid and 4800 coarse-grained water molecules randomly distributed, 250 ns simulation time
- Bilayer starts to form after around 7 ns



S. J. Marrink, A. H. de Vries, A. E. Mark, J. Phys. Chem. B (2004), 108, 750-760; S. J. Marrink, H. J. Risselada, S. Yefimov, D. P. Tieleman, A. H. de Vries, J. Phys. Chem. B (2007), 111, 7812-7824

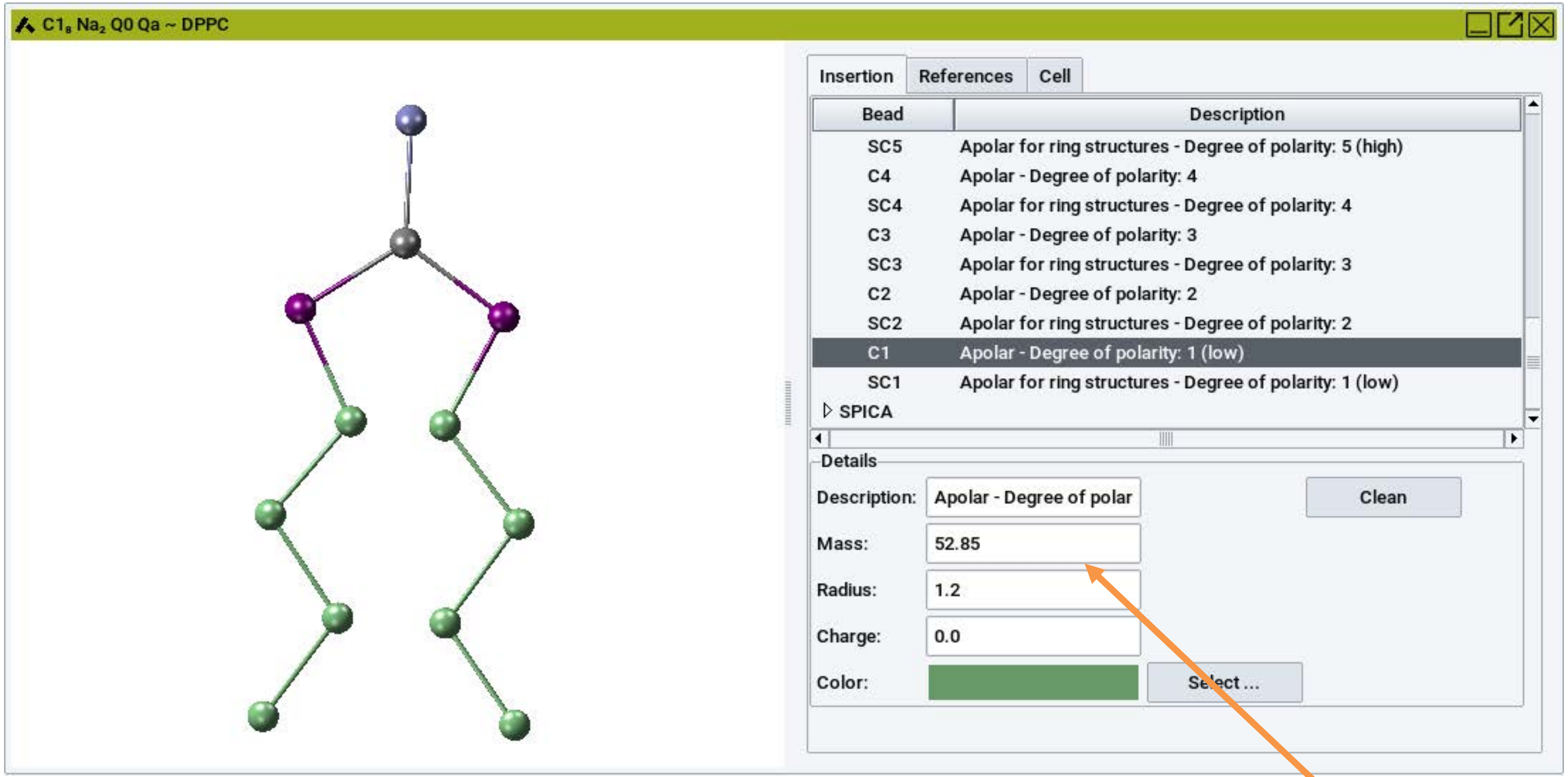
Mesoscale Simulations with *MedeA 3.1*



Martini and SPICA forcefields are available

Sketching mesoscale structures

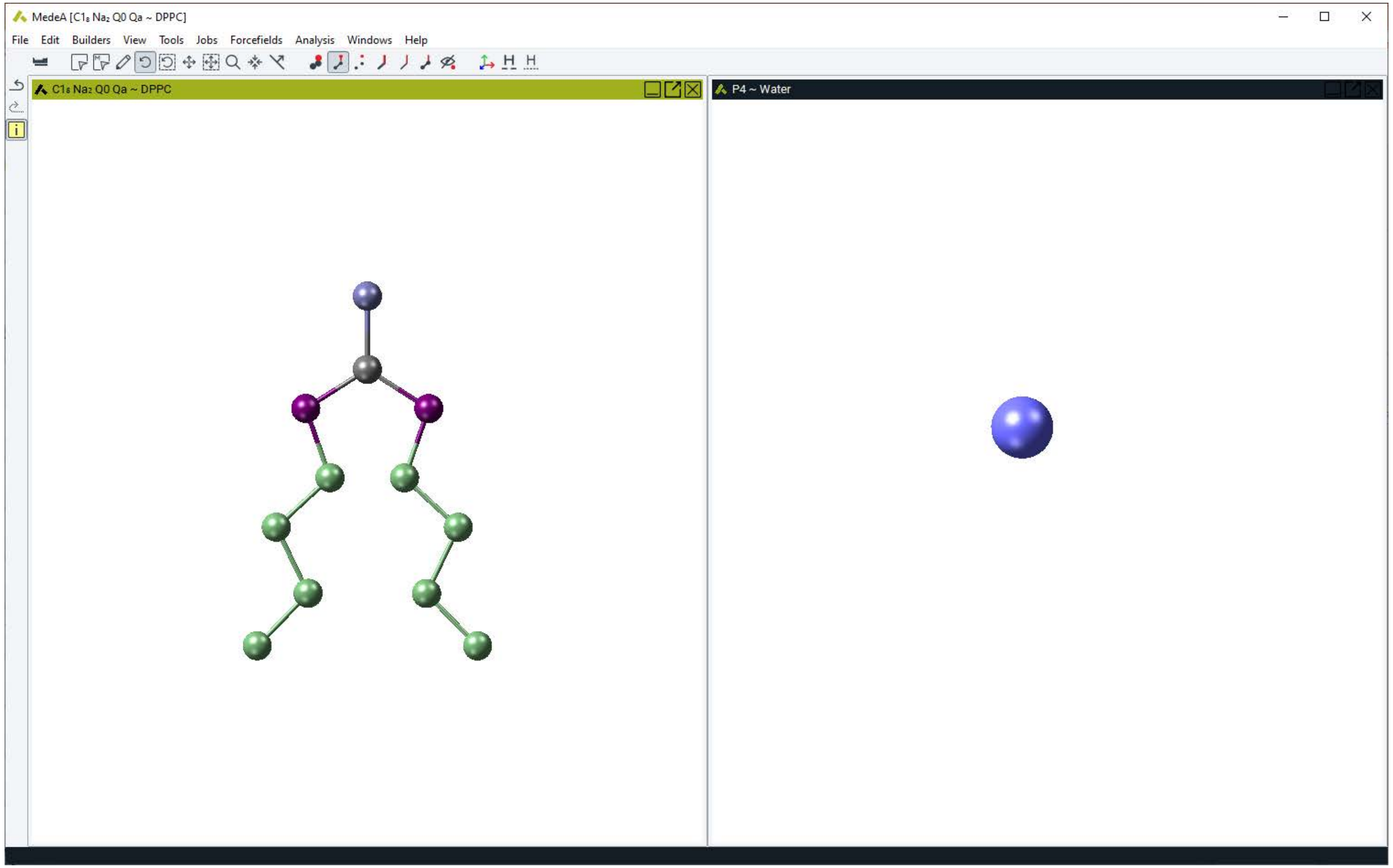
Mesoscale Simulations with *MedeA* 3.1



Coarse-grained DPPC molecule

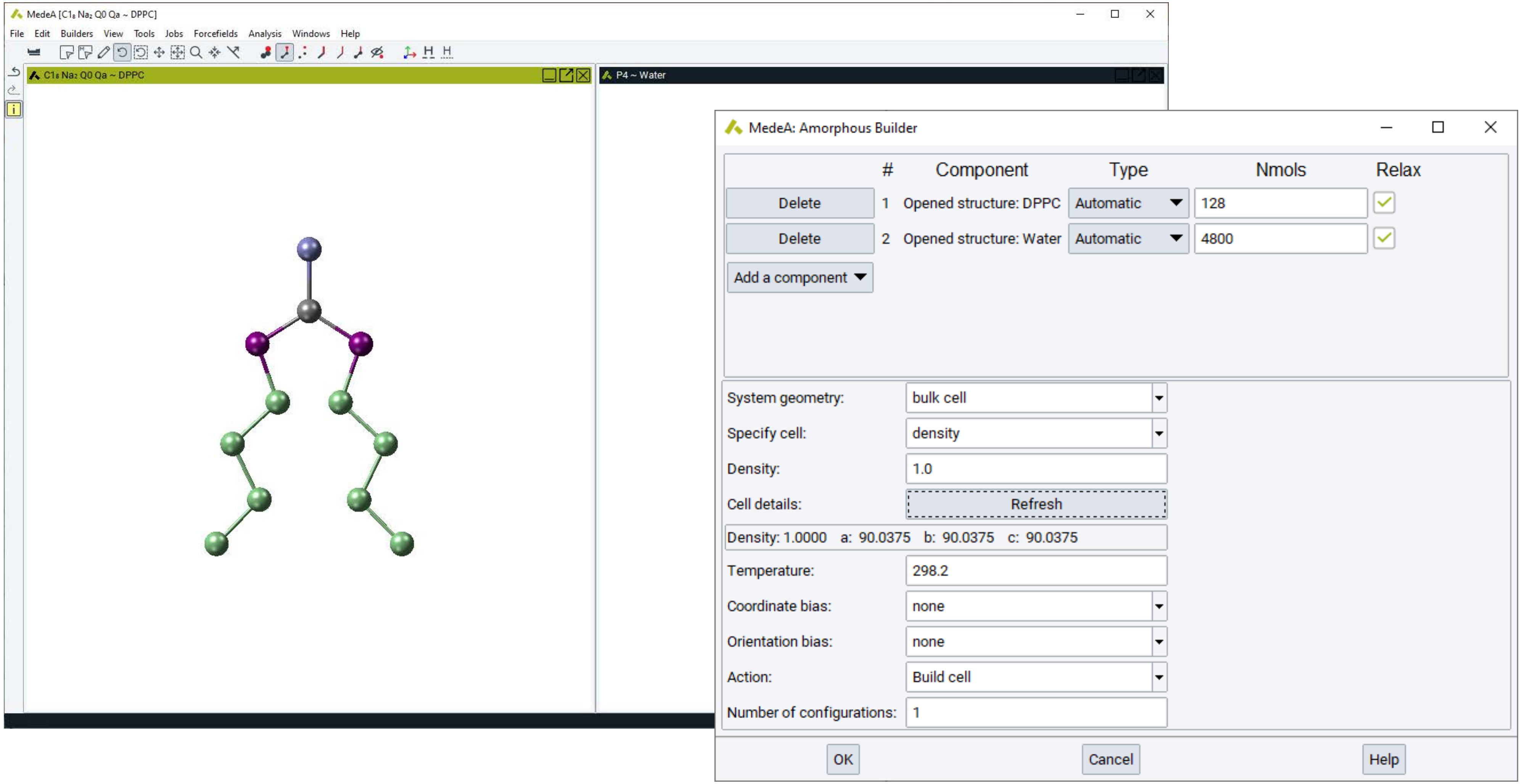
Parameters can be overwritten

Mesoscale Simulations with *MedeA 3.1*



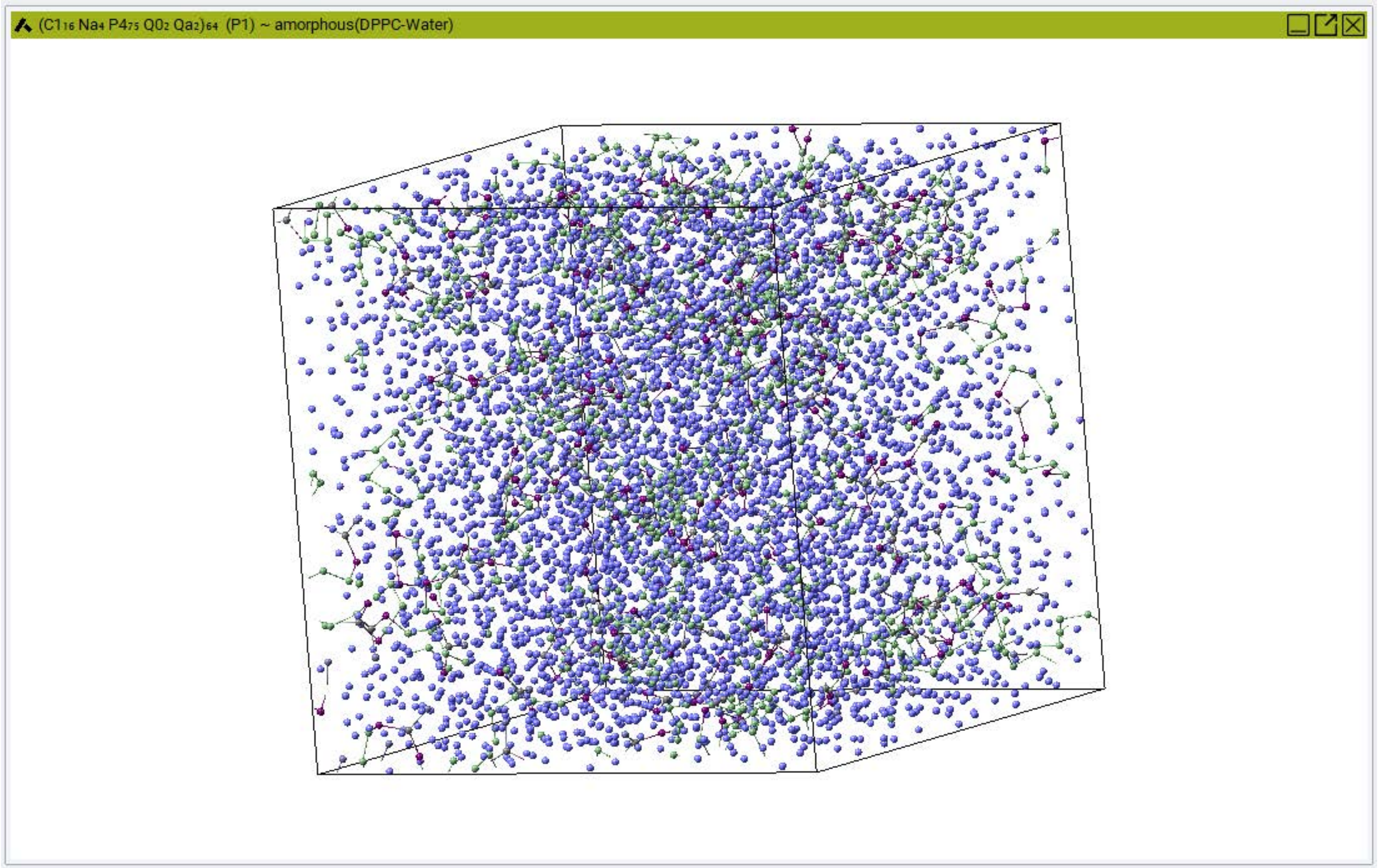
Coarse-grained DPPC and water molecules

Mesoscale Simulations with *MedeA 3.1*



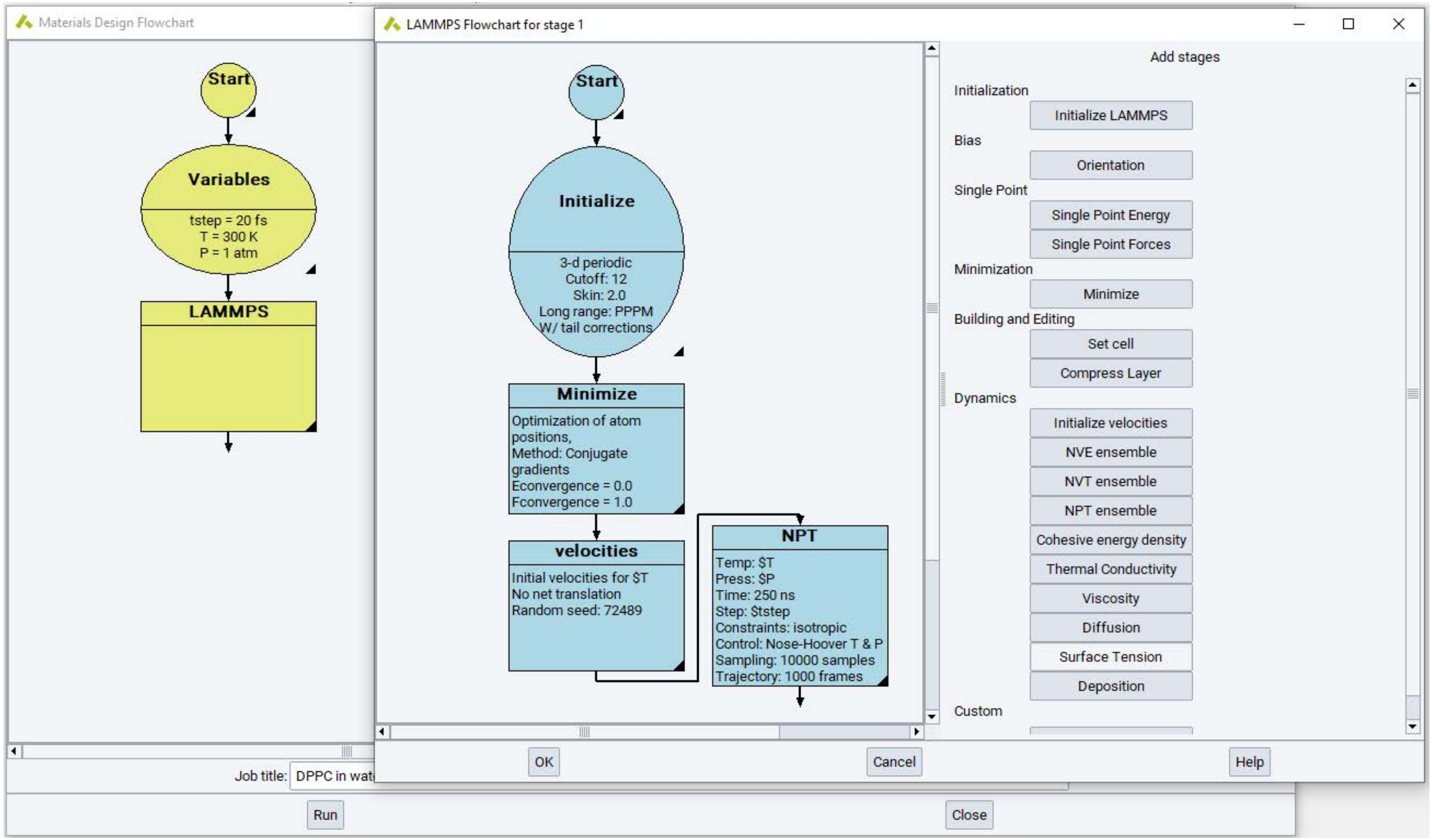
Amorphous builder can handle mesoscale systems

Mesoscale Simulations with *MedeA 3.1*

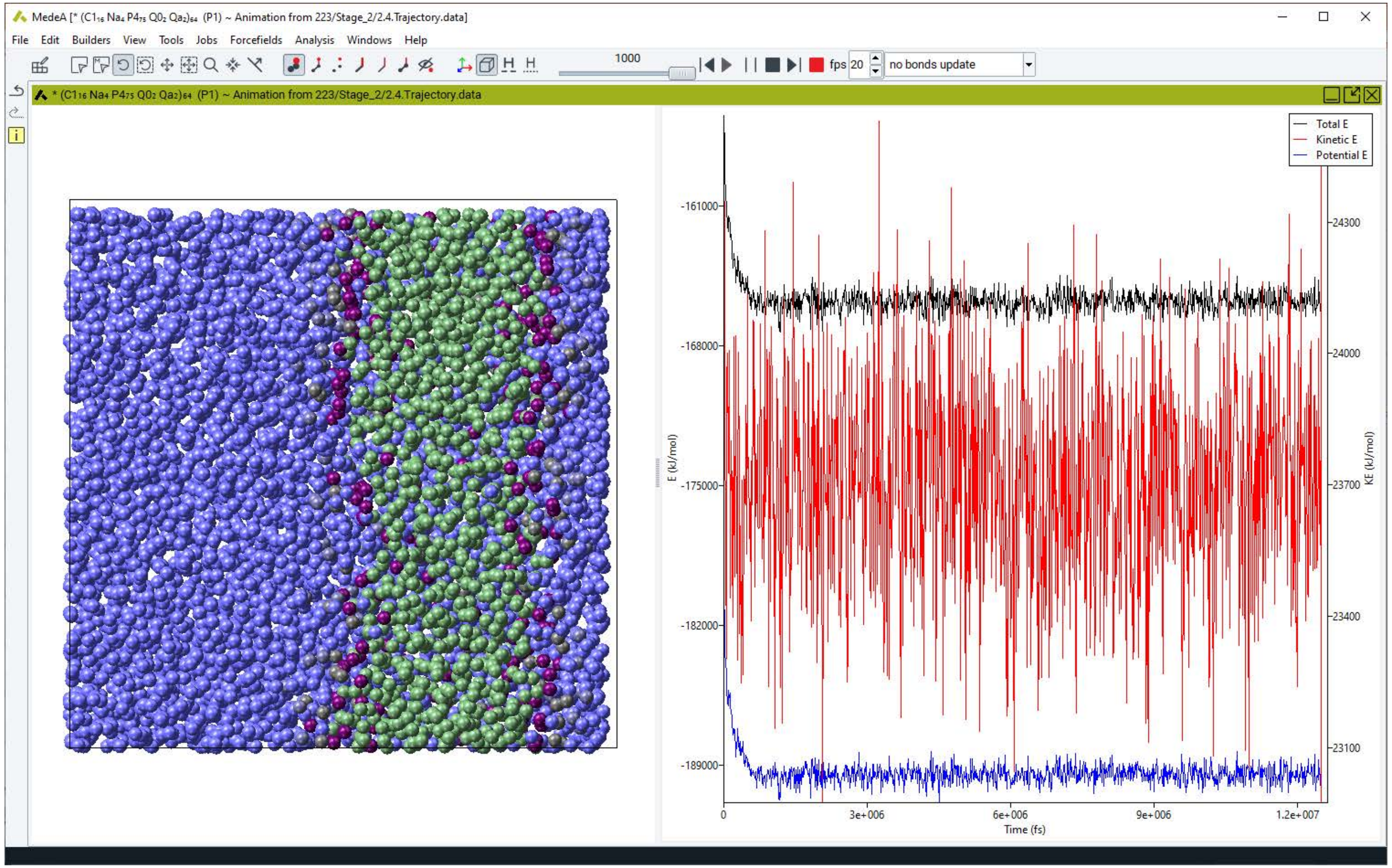


An amorphous mesoscale system

Mesoscale Simulations with *MedeA 3.1*



Mesoscale Simulations with *MedeA 3.1*



Mesoscale system after 250 ns, bilayer has formed

[Watch video]

Mesoscale Simulations with *MedeA 3.1*

Forcefields are standard frc files

```
#scaling           Martini

!Ver  Ref     I     J     K     L     Coulomb      VdW
!---- ---    ----  ----  ----  ----   -------    -------
1.0   1      *     *                   0.0         0.0
1.0   1      *     *     *             1.0         1.0
1.0   1      *     *     *     *       1.0         1.0

#quadratic_bond Martini

> E = K2 * (R - R0)^2

!Ver Ref    I     J       R0         K2
!--- ---  ----- -----  -------    --------
1.0  1     *       *   4.7000      1.4931

#quadratic_cosine_angle Martini

> E = K2 * (cos(th) - cos(th0))^2

!Ver Ref    I     J     K       th0          K2
!--- ---  ----- ----- -----   -------    --------
1.0  1   *      *      *     179.9000      2.9863

#nonbond(12-6) Martini

@type r-eps
@combination explicit

> E = 4*eps*[(sigma/r)^12-(sigma/r)^6]

!Ver  Ref     I     J          r             eps
!---- ---    ---- -----   -----------   -----------
 1.0   1    SQa    P5        5.2756      1.3380
 1.0   1    SQa    P4        5.2756      1.3380
 1.0   1    SQ     N         5.2756      1.1950
...
```

Online Training and Demo

MedeA 3.1

Next Tuesday, September 8, 2020

USA/EUROPE:

9:30 am EST/3:30 pm CEST

INDIA/CHINA/JAPAN:

7:00 pm IST/ 9:30 pm CST/ 10:30 pm JST

Emailed information coming soon!

All MedeA tutorials are available
at http://my.materialsdesign.com/tutorials

*Training and Demo available to customers
Who are currently on maintenance


Materials Design UGM
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October
www.materialsdesign.com/ugm-2020

MedeA 3.1 Webinars

- June 2020: Elasticity and Beyond – Predicting Mechanical Properties with *MedeA*, by Ray Shan
- June 2020: Diffusion by Erich Wimmer and Benoît Minisini
- July 2020: VASP 6 by Martijn Marsman
- July 2020: Mesoscale Modeling by Jörg-Rüdiger Hill
- August 2020: Exploring Battery Materials...by René Windiks
- September 2020: *MedeA* 3.1 by Marianna Yiannourakou, Walter Wolf and Jörg-Rüdiger Hill

Materials Design *MedeA 3.1* Webinar Links

- MedeA modules mentioned in today's webinar
  - https://www.materialsdesign.com/builders
  - https://www.materialsdesign.com/compute-engines
  - https://www.materialsdesign.com/property-modules

  - *MedeA* Mesoscale Builder
  - *MedeA* VASP
  - *MedeA Amorphous Materials Builder*
  - *MedeA* Thermoset Builder
  - *MedeA LAMMPS*
  - *MedeA Diffusion*
  - *MedeA GIBBS*
  - *MedeA Transition State Search*

- UGM
  - https://www.materialsdesign.com/ugm-2020

- Webinar: Live and Recorded
  - https://www.materialsdesign.com/webinars

- Publications
  - https://www.materialsdesign.com/Publications

- Application Notes
  - https://www.materialsdesign.com/application-notes

- For questions or comments contact
  - Katherine Hollingsworth
    - khollingsworth@materialsdesign.com

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Innovation by Simulation