



materials design®

WEBINAR

MedeA 3.1

Marianna Yiannourakou, Walter Wolf, Jörg-Rüdiger Hill

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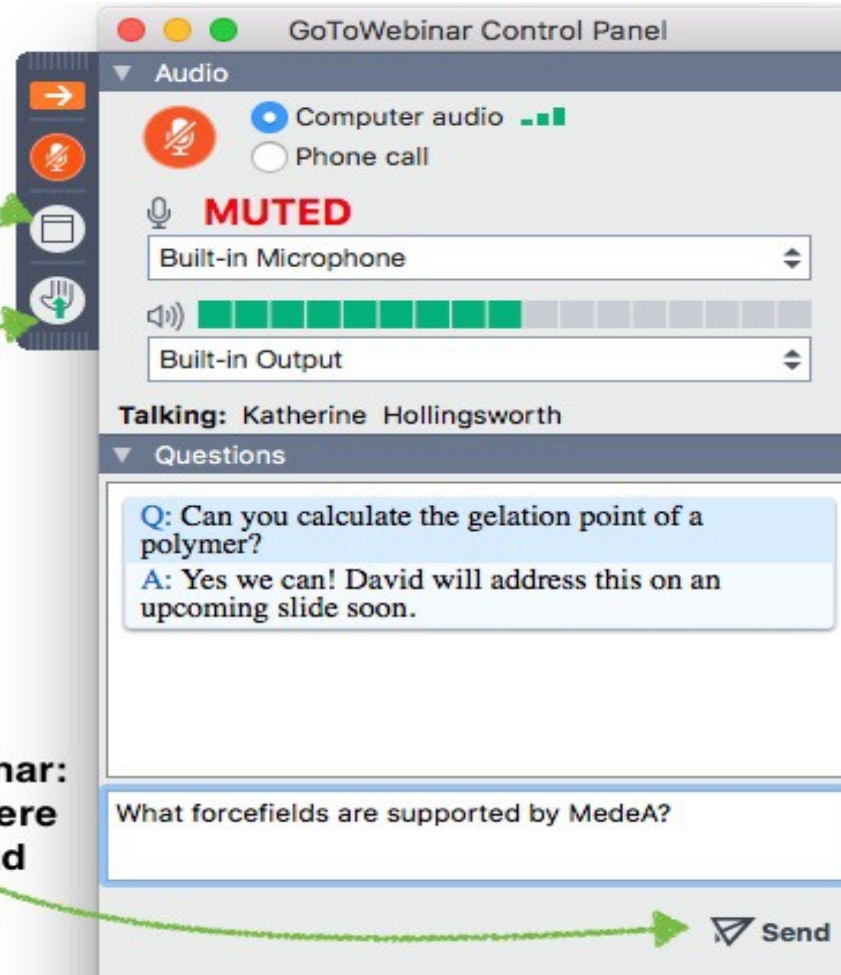
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type your question here
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Webinar Speakers

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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

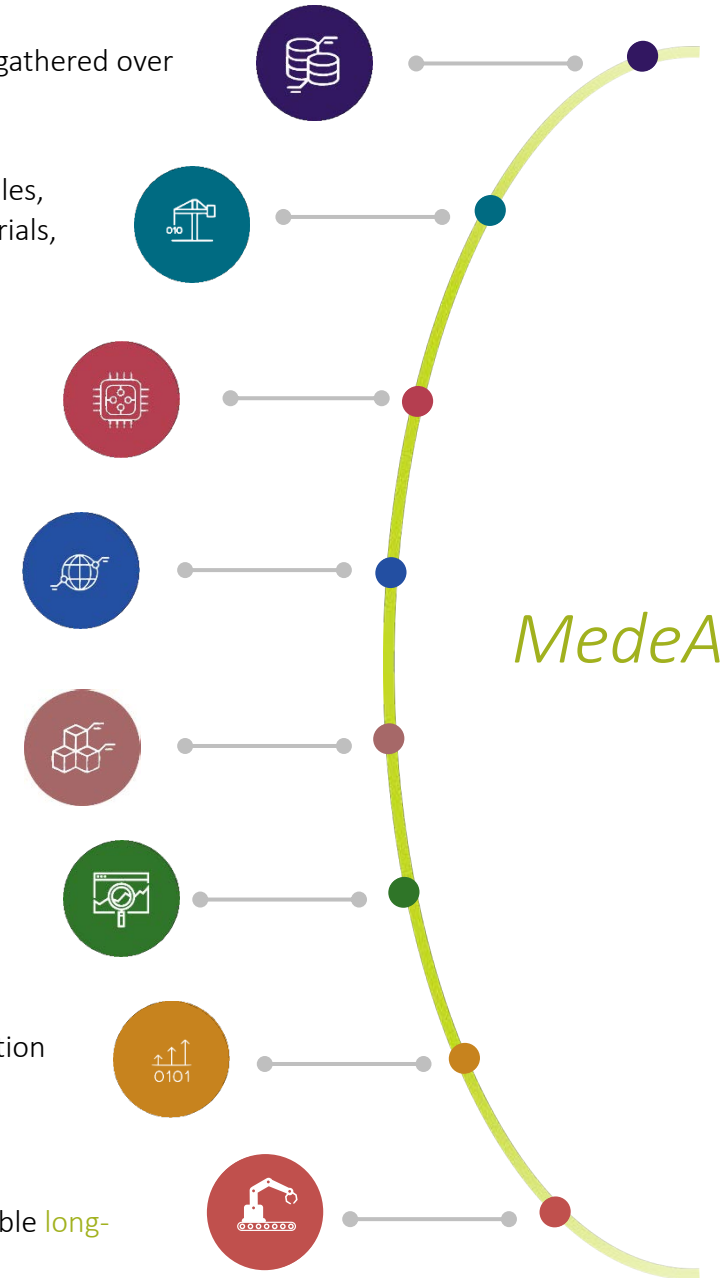
Generation of **large and consistent sets of computed data & descriptors**

Analysis Tools

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

JobServer & TaskServer

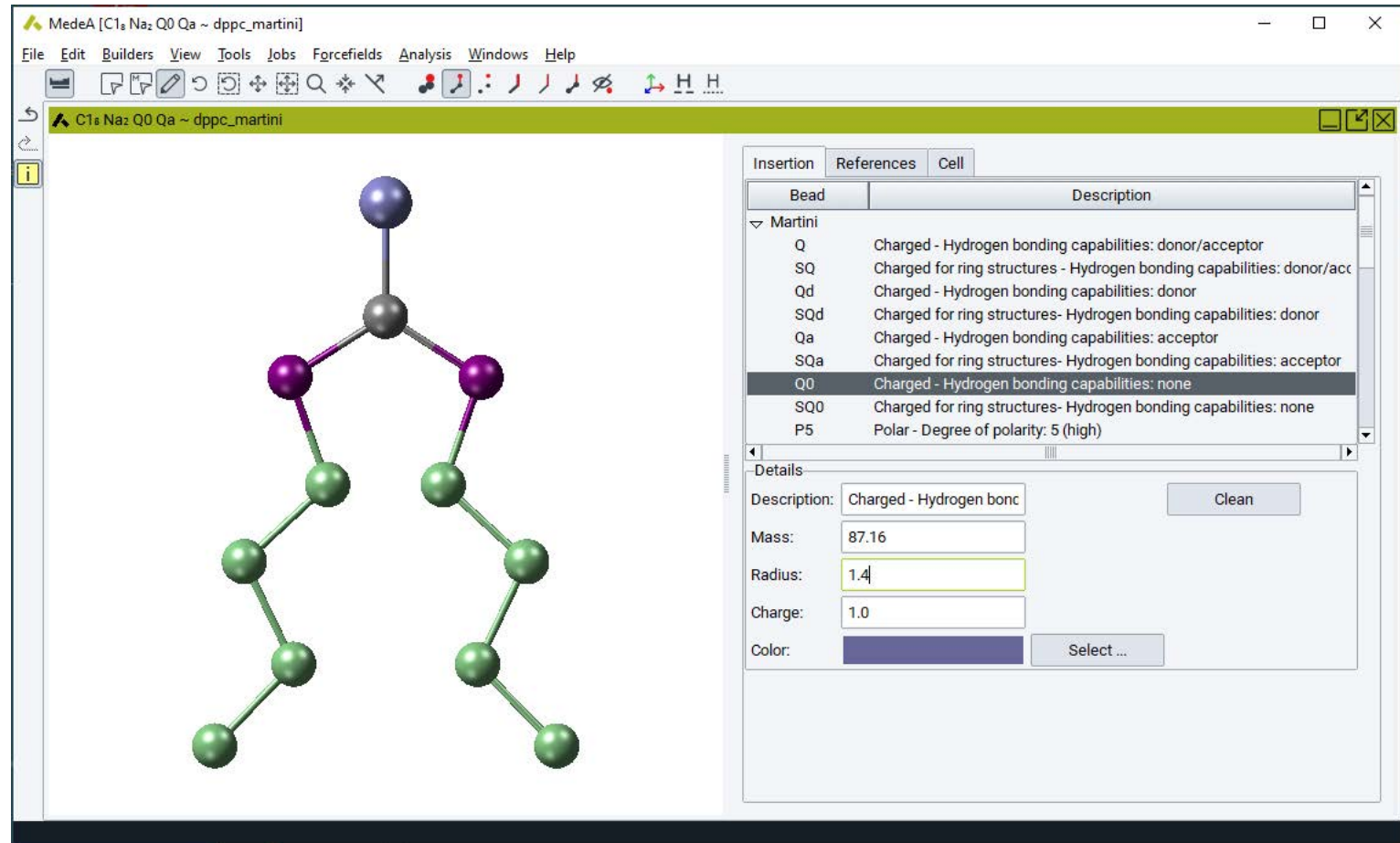
Automated processing of **compute protocols & workflows**; Reliable **long-term archiving & accounting** of computed data





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**

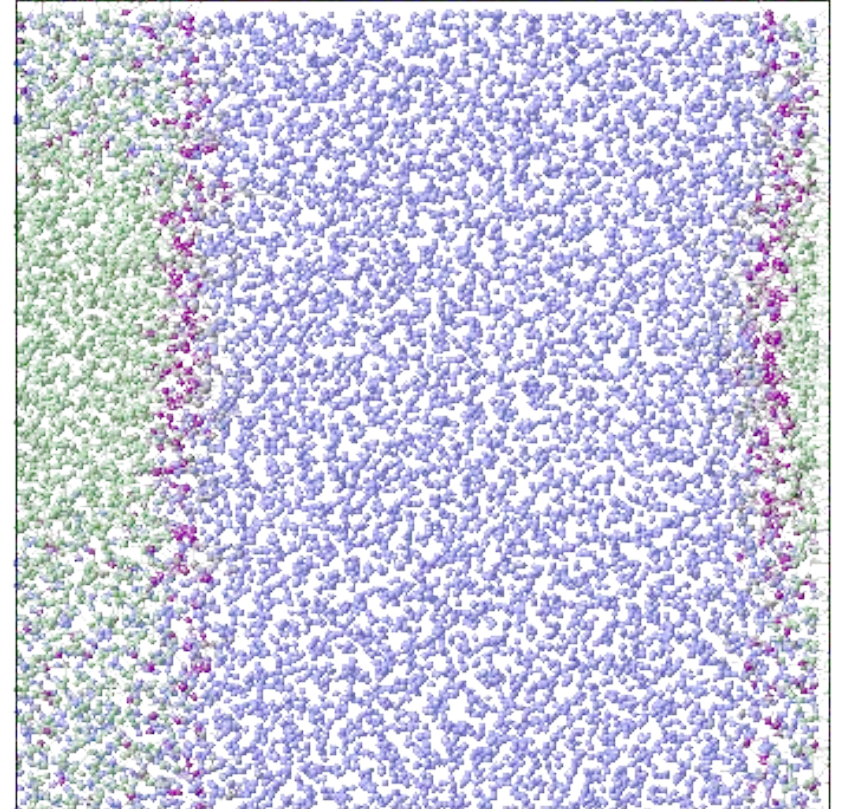




Mesoscale Simulations With *MedeA* 3.1

► *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





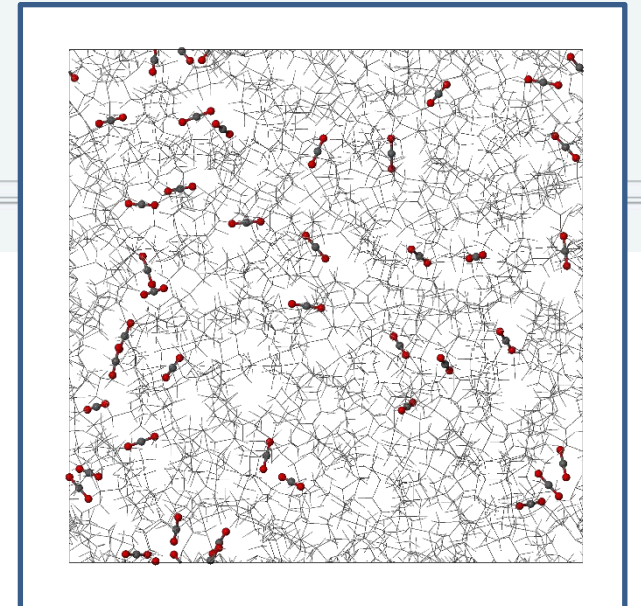
What's new in *MedeA GIBBS*

- ▶ 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

The screenshot displays the 'Advanced settings' dialog box in MedeA GIBBS. The 'Start this calculation' dropdown is set to 'from a built system'. The 'Use the:' dropdown is set to 'Osmotic', and the 'ensemble' label is visible. The 'Temperature:' field is set to '\$T' and the 'Pressure:' field is set to '\$P'. The 'Calculate the radial distribution function' checkbox is checked. Below this is a table of components:

Formula	Name	Type	Insertion Type	Charges	Use	Fugacity/ChemPot	# of Molecules	Volatile	Delete	Replace...	View
C44H90	C44	flexible	CH3-TraPPE-UA	<input checked="" type="checkbox"/>	Fugacity	1 bar	40	<input type="checkbox"/>			
CO2	CO2	rigid	C-CO2	<input type="checkbox"/>	Fugacity	1 bar	1	<input checked="" type="checkbox"/>			

Buttons for 'Add system from MedeA' and 'Add system from a file' are located below the table. The 'System' section includes a 'Specify cell:' dropdown set to 'a,b,c' and three input fields for 'Cell length x (Ang):', 'Cell length y (Ang):', and 'Cell length z (Ang):', all set to '38.015'. A 'Refresh' button is below these fields. At the bottom of the dialog are 'OK' and 'Cancel' buttons.





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

The screenshot displays the Materials Design Flowchart interface. On the left, a flowchart shows a 'Start' node leading to a 'New List' stage (name: Deformation, file: Deformation.sli), which then leads to a 'Deformation' stage (tension deformation, Max strain: 0.50 (relative) in Z, Strain increment: 0.0025, Save to list 'Deformation').

The main window is titled 'Materials Design Flowchart' and contains a 'Deformation stage' configuration dialog. The dialog has three tabs: 'Control', 'Relaxation Flowchart', and 'Stress Flowchart'. The 'Control' tab is active, showing the following settings:

- Deformation type: tension
- Direction: Z
- Keep volume constant
- Total strain (relative): 0.50
- Strain Increment (relative): 0.0025
- Append to structure list Registered lists: Deformation
- Run the different loop iterations simultaneously Maximum number of jobs to submit simultaneously: 20

Below the dialog, there are 'OK' and 'Cancel' buttons. At the bottom of the main window, there is a 'Job title:' field, a 'Run' button, and a 'Close' button. On the right side, there is a 'Reading and writing flowcharts' panel with buttons for 'Open Library...', 'Open User...', and 'Save...'. Below this, there is a 'From job:' field with the value '33108' and an 'Open' button. A list of 'Add stages' is visible, including 'Subchart', 'Set Variables', 'Print Variables', 'Custom Tcl Script', 'For Loop', 'Foreach Loop', 'While Loop', and 'Foreach Structure Loop'. At the bottom right, there is a list of VASP versions: 'VASP 5.4: High Throughput', 'VASP 5.2: Plane Wave DFT', and 'VASP 4.6: Plane Wave DFT'.



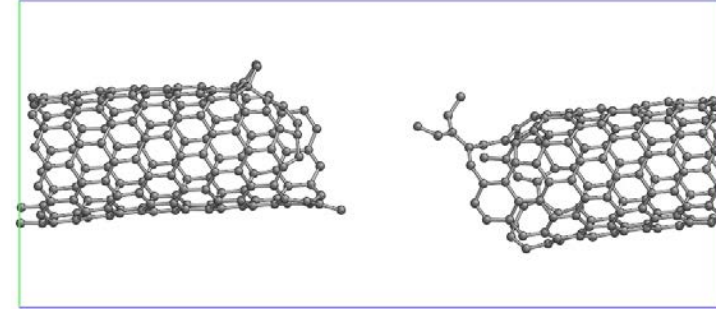
MedeA Deformation

The screenshot displays the 'Materials Design Flowchart' interface. A central window titled 'Deformation stage' is open, showing a flowchart with a 'Start' node leading to a 'LAMMPS' stage. The 'LAMMPS' stage is currently selected, and its configuration options are visible in a panel on the right. This panel includes sections for 'Reading and writing flowcharts', 'Add stages', 'Initialization & Control', 'Tables and Graphs', 'General Properties', and 'Methods'. The 'Initialization & Control' section lists options like Subchart, Set Variables, Print Variables, Custom Tcl Script, For Loop, Foreach Loop, While Loop, Foreach Structure Loop, Catch, and If. The 'Tables and Graphs' section includes Table, Add Row, and Print. The 'General Properties' section includes Hill-Walpole Bounds, Mechanical Properties, Deformation, and Effective Mass. The 'Methods' section includes Gibbs: Monte Carlo and Gibbs: Adsorption Isotherm. The main flowchart on the left shows a 'New List' stage (name: Deformation, file: Deformation.sli) leading to a 'Deformation' stage (tension deformation, Max strain: 0.50 (relative) in Z, Strain increment: 0.0025, Save to list 'Deformation'). At the bottom of the interface, there is a 'Job title:' field and 'Run' and 'Close' buttons.

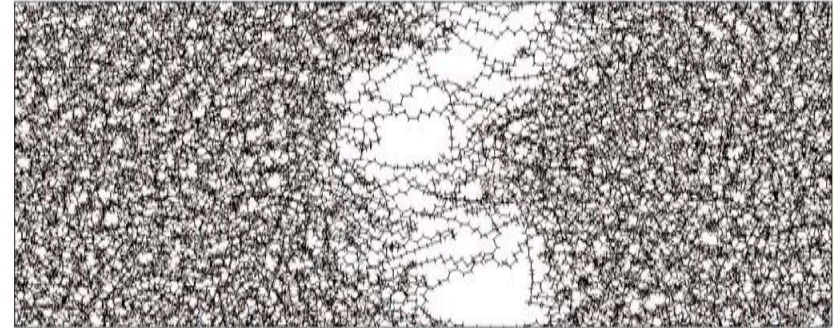


Deformation Simulations

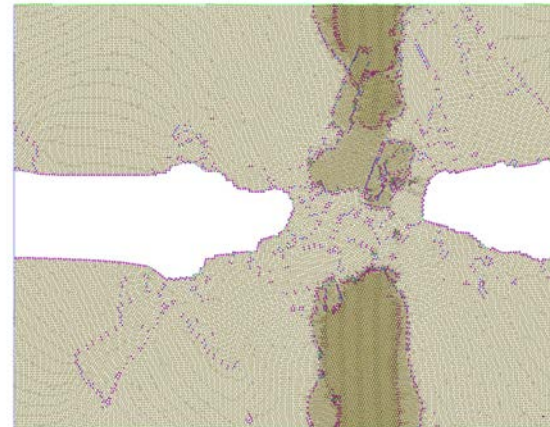
- ▶ Tensile deformation of CNT with Tersoff



- ▶ 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 (**UNIQUAC** Functional-group **Activity** Coefficients) 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

The screenshot displays the MedeA software interface for the UNIFAC model. The main window shows two molecular models: water (OH₂ ~ water) and ethanol (C₂OH₆ ~ ethanol). The UNIFAC dialog box is open, showing the following data:

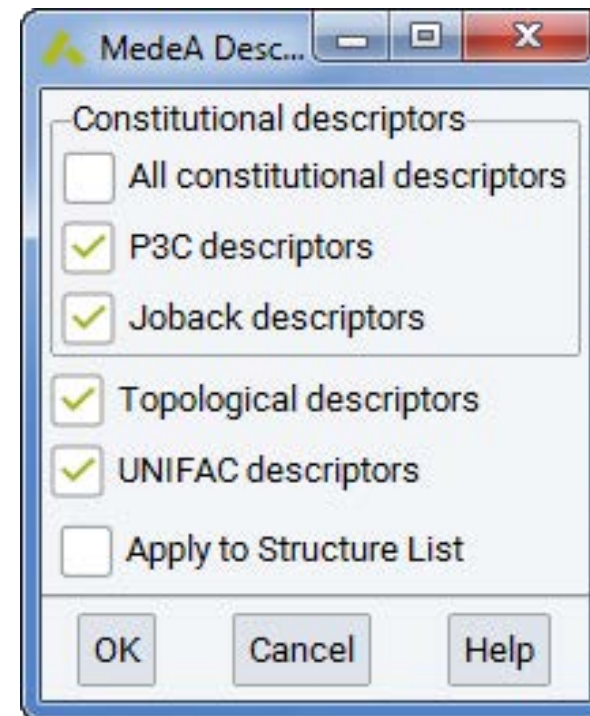
T(K)	x1	x2	Act. Coeff 1	Act. Coeff 2
298	0.05	0.95	5.93	1.00
298	0.10	0.90	4.76	1.02
298	0.15	0.85	3.94	1.03
298	0.20	0.80	3.35	1.05
298	0.25	0.75	2.92	1.07
298	0.30	0.70	2.53	1.11
298	0.35	0.65	2.27	1.13
298	0.40	0.60	2.03	1.16
298	0.45	0.55	1.84	1.20
298	0.50	0.50	1.67	1.25
298	0.55	0.45	1.54	1.28
298	0.60	0.40	1.42	1.34
298	0.65	0.35	1.32	1.40
298	0.70	0.30	1.25	1.46
298	0.75	0.25	1.17	1.54

The UNIFAC graph window shows the activity coefficient (ln gamma) versus the molecular fraction for ethanol (black line) and water (red line). The ethanol activity coefficient decreases from approximately 5.93 at x1=0.05 to 1.17 at x1=0.75, while the water activity coefficient increases from 1.00 at x1=0.05 to 1.54 at x1=0.75.



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

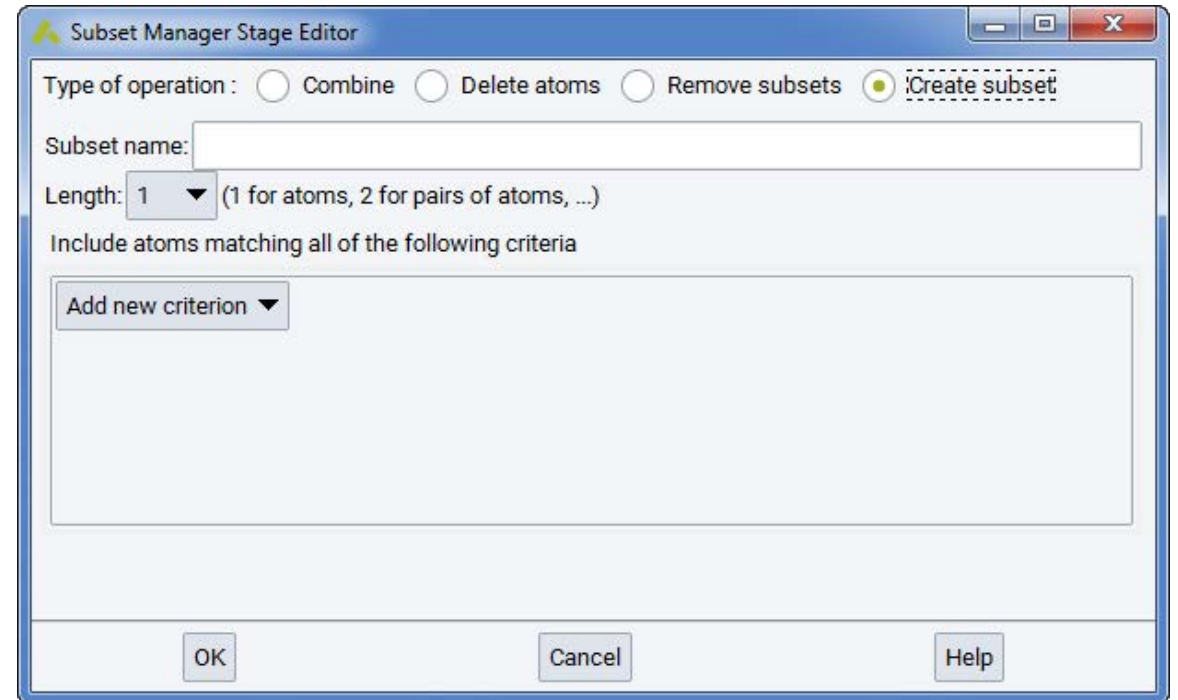
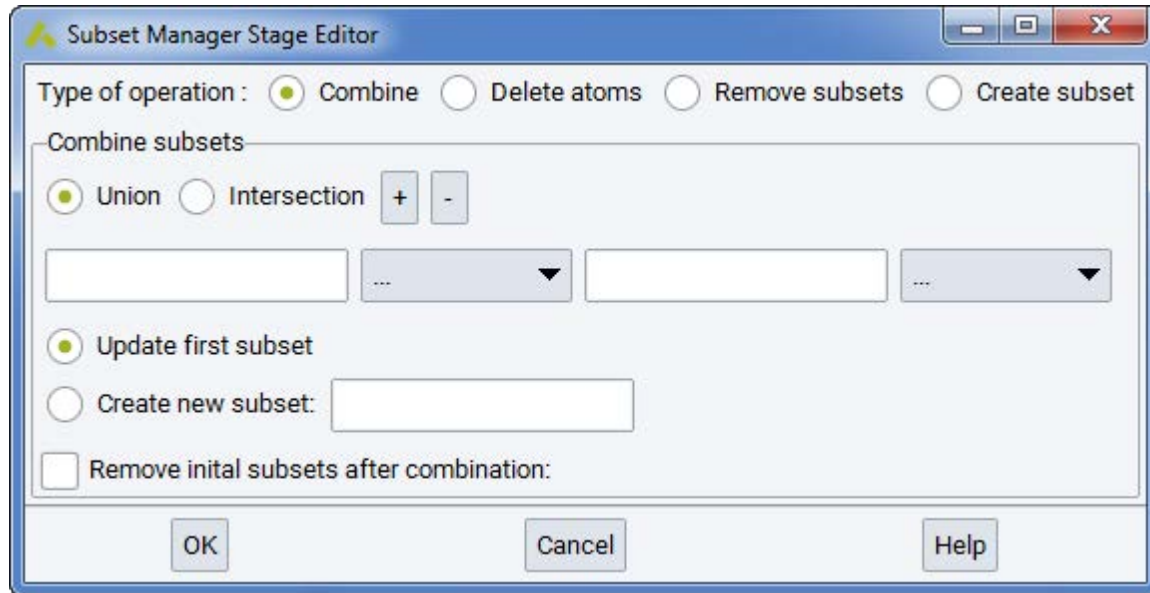
- Combination of morse FF with Streitzi-Mintmire charge equilibration
- ## ▶ Added explicit pair interactions handling in *MedeA LAMMPS*





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

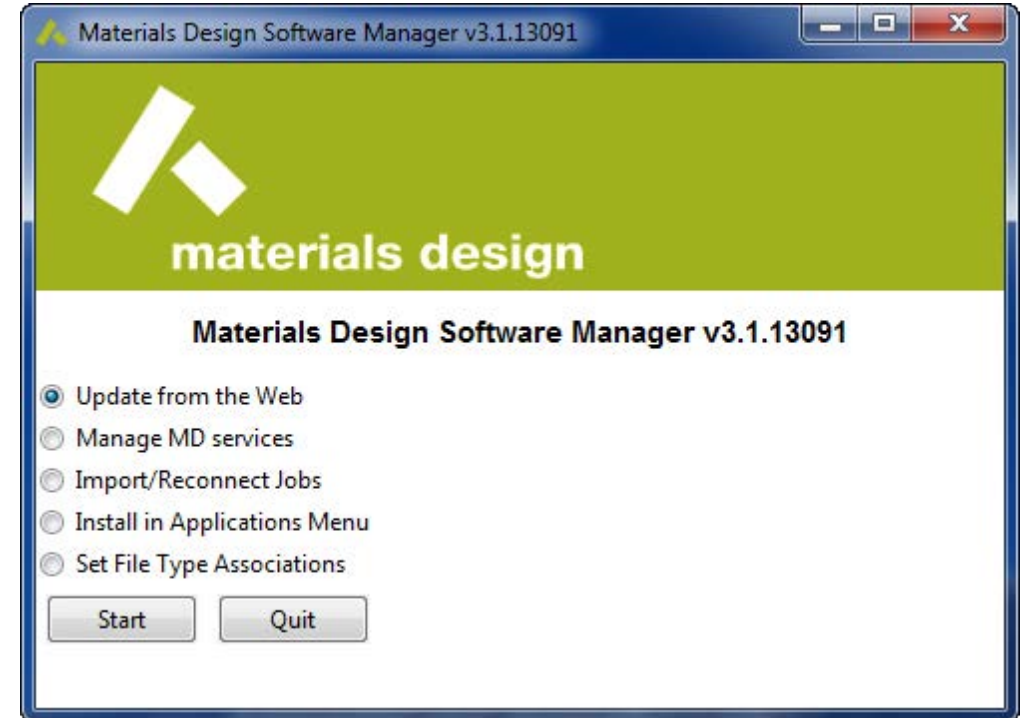
▶ Other





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

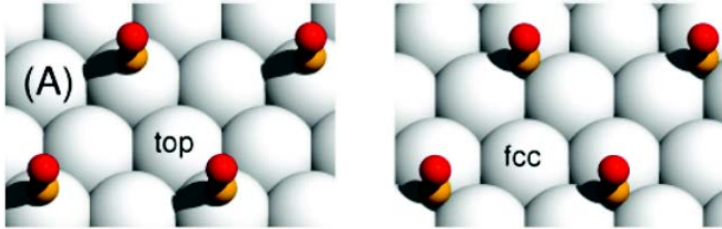
► *Solution Provided by VASP 6*

- 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



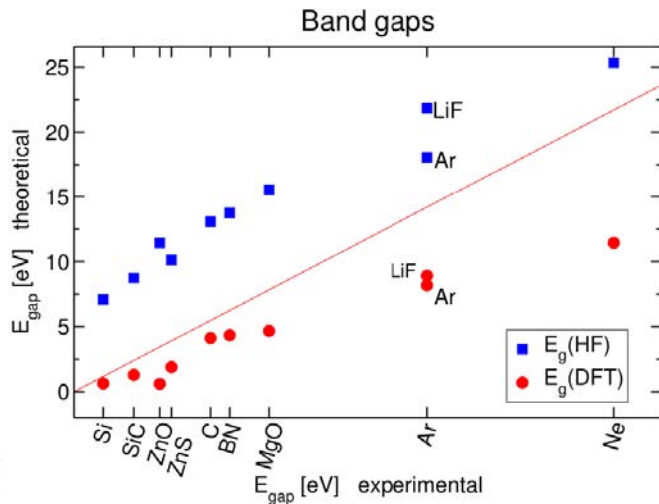
Need for Accurate Methods Beyond DFT and Hybrid

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

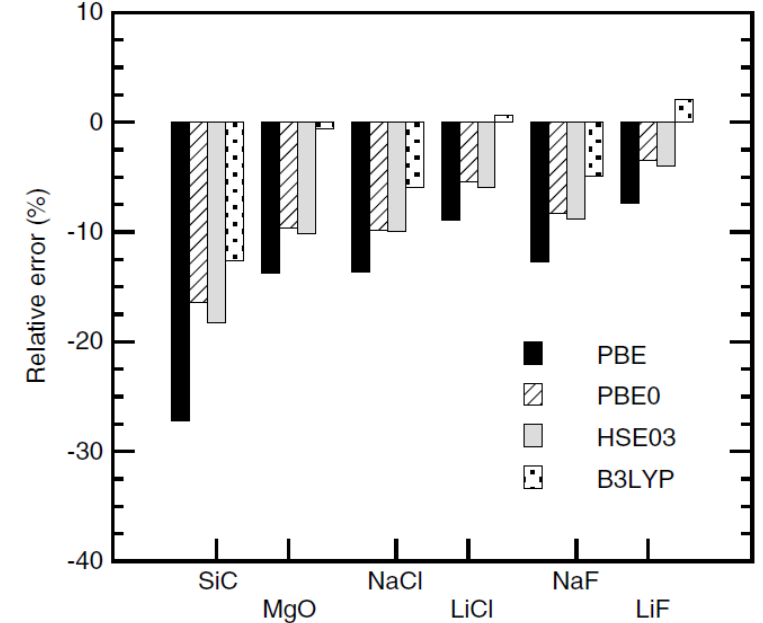


	Lattice constant	
	MRE	MARE
PBE	0.8	1.0
PBE0	0.1	0.5
HSE	0.2	0.5
B3LYP	1.0	1.2

	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

Heats of formation



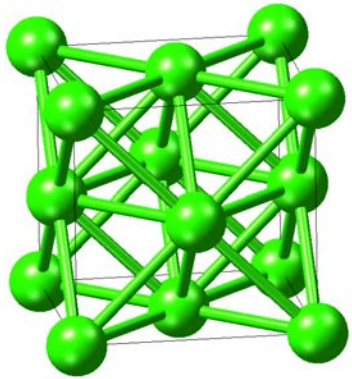
ΔH (kJ/mol)	PBE	EXP
$\text{Al} + \text{N}_2 \rightarrow \text{AlN}$	262	350
$\text{Mg} + \text{H}_2 \rightarrow \text{MgH}_2$	52	78
$\text{Si} + \text{C} \rightarrow \text{SiC}$	51	69
$\text{CO} \rightarrow \text{CO@Rh}$	183	144

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



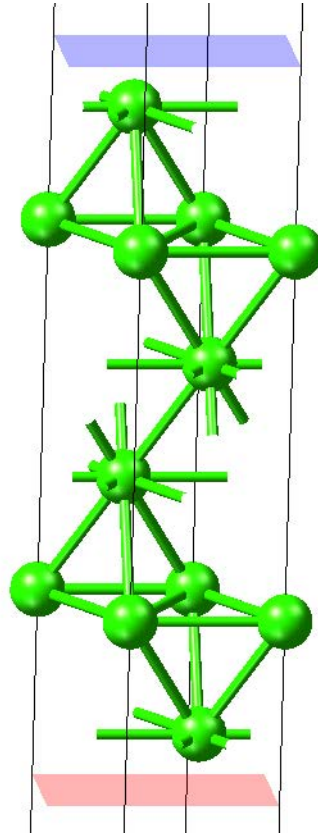
Build Model for CO Adsorbed on Pt(111) in *MedeA*

Retrieve fcc Pt from structural databases
MedeA InfoMaticA

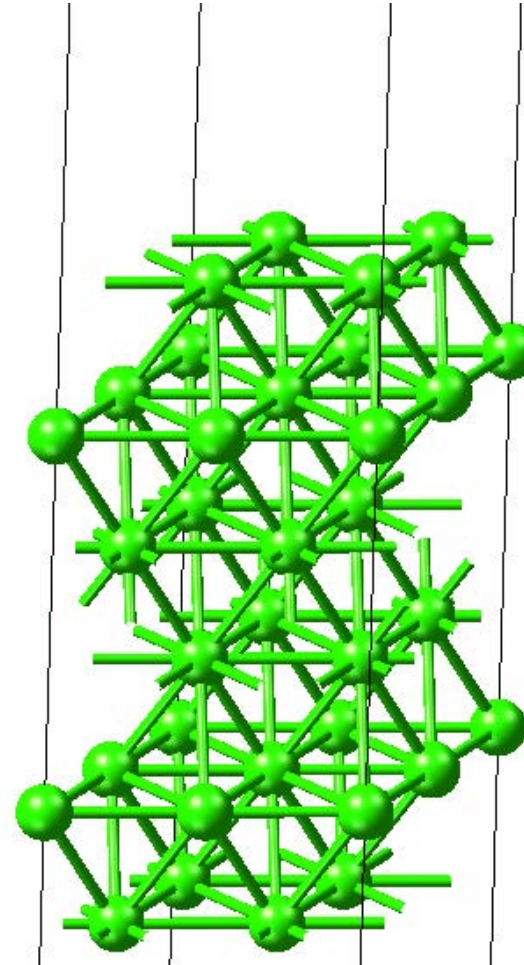


Optimize the lattice
MedeA VASP 6

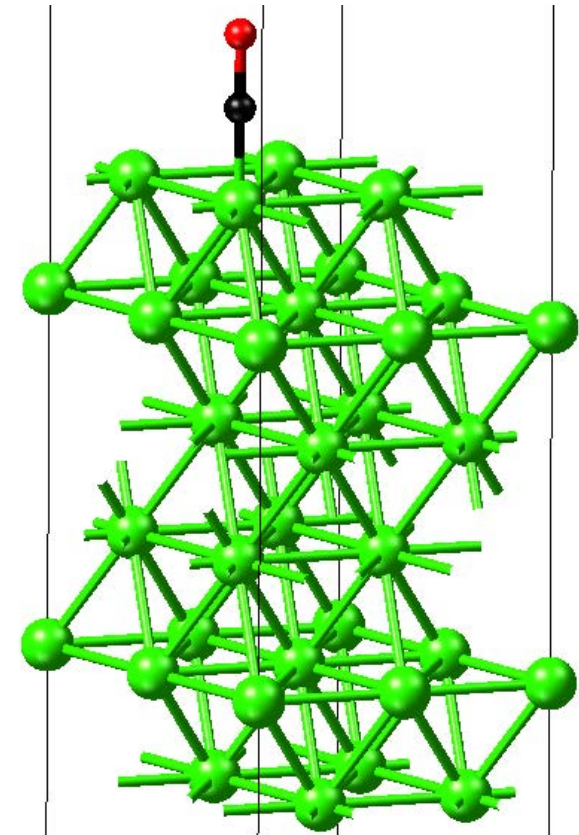
Build Pt(111) surface
MedeA Surface Builder



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*

The screenshot displays the MedeA VASP 6 software interface. On the left, a 3D ball-and-stick model of a Pt₂₄CO molecule is shown, with Pt atoms in green, C in black, and O in red. The main window is titled "MedeA : Run VASP 6" and contains several tabs: Calculation, Functional/Potential, SCF, DOS/Optic/Tensors, Band Structure, Advanced/Restart, Add to Input, and Preview Input. The "Calculation" tab is active, showing a dropdown menu for "Type of calculation" with "Accurate Forces (Low Scaling ACFDT-RPA)" selected. The "Properties" section includes checkboxes for various calculations like "Total local potential", "Wave functions", and "Electric field gradients". The "Interaction" section shows "Functional" set to "Density functional" and "DFT exchange-correlation" set to "GGA-PBE". The "General Setup" section shows "Precision" set to "Normal" and "Planewave cutoff" set to "400.000 eV". At the bottom, there are buttons for "Run", "Close", "Write input files", "Restore defaults", and "Restore from job".

MedeA [* Pt₂₄CO (P1) ~ 62359 minimized: Pt_1 (1 1 1) surface (#1)_2x2x1_1 + CO optpos (VASP)]

File Edit Builders View Tools Jobs Forcefields VASP 6 Analysis Windows Help

* Pt₂₄CO (P1) ~ 62359 minimized: Pt_1 (1 1 1) surface (#1)_2x2x1_1 + CO optpos (VASP)

MedeA : Run VASP 6

Calculation Functional/Potential SCF DOS/Optic/Tensors Band Structure Advanced/Restart Add to Input Preview Input

Type of calculation: Single Point

- Single Point
- Structure Optimization
- Molecular Dynamics
- Time-dependent Hybrid / DFT
- Quasiparticle Spectra (GW)
- Quasiparticle Spectra (Low Scaling GW)
- Accurate Energy (MP2)
- Accurate Energy (ACFDT-RPA)
- Accurate Forces (Low Scaling ACFDT-RPA)
- Electron-phonon Coupling
- MT -- Elastic Properties

Properties

- (Pseudo, difference, spin) charge density
- Total local potential
- Electron localization function
- Wave functions
- Electric field gradients
- Hyperfine parameters
- Work function (surfaces only)
- (Total, valence) charge density, Bader analysis
- Band structure
- Density of states
- Optical spectra
- Zone center phonons
- Response tensors
- NMR: chemical shifts

Solvation (for molecules or surfaces)

- Apply solvation model

External pressure: 0 GPa

Charge state: 0 e

External electrostatic field: none

Interaction

Functional: Density functional

DFT exchange-correlation: GGA-PBE

Van der Waals: None

Magnetism: Defined by model (to be non-magnetic)

General Setup

Precision: Normal

Increase planewave cutoff (cell optimizations)

Planewave cutoff (default): 400.000 eV

Planewave cutoff: eV

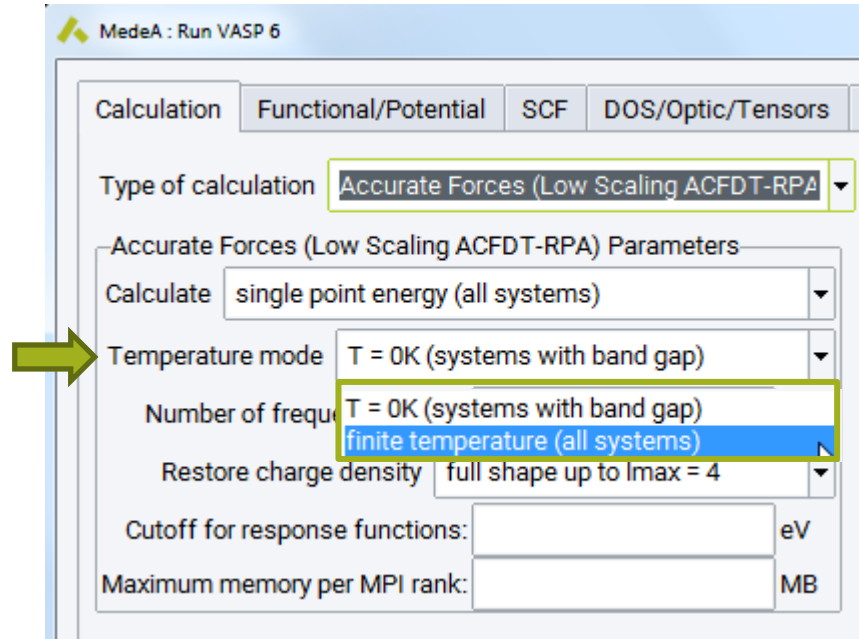
Projection: Real space

Title: Pt₂₄CO (P1) ~ 62359 minimized: Pt_1 (1 1 1) surface (#1)_2x2x1_1 + CO optpos (VASP)

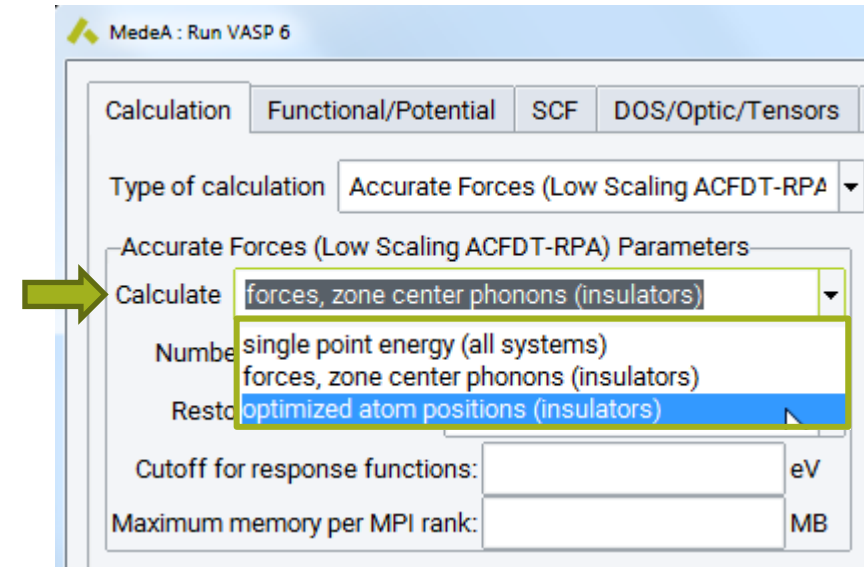
Run Close Write input files Restore defaults Restore from job



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
=====

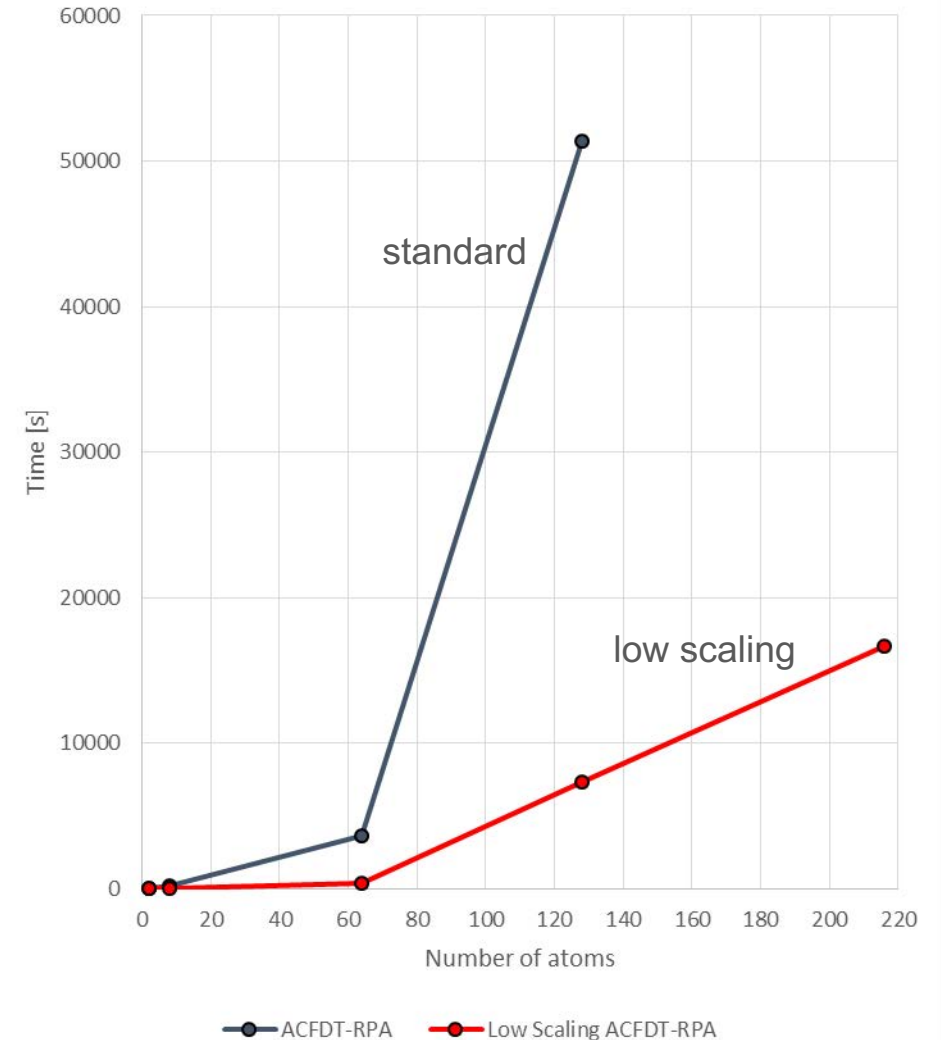
.....

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)
```

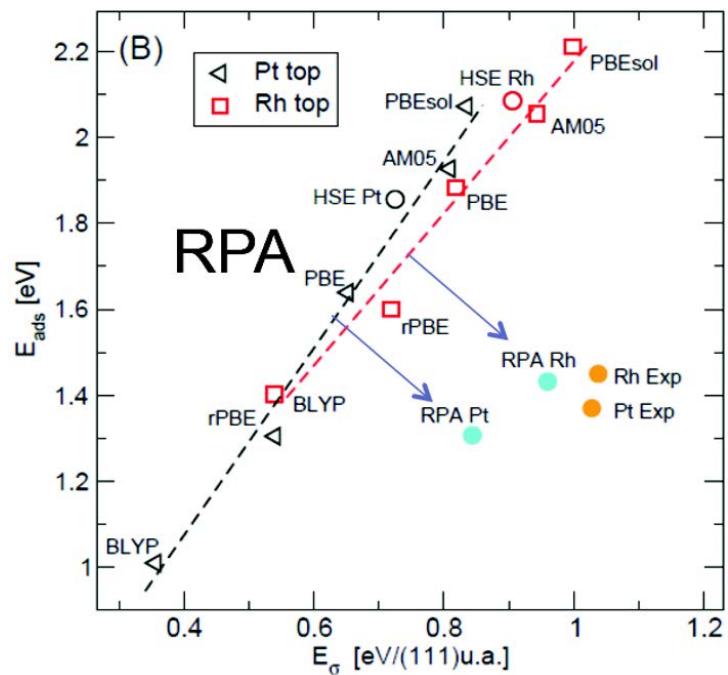


Compute time vs. supercell size for Si:

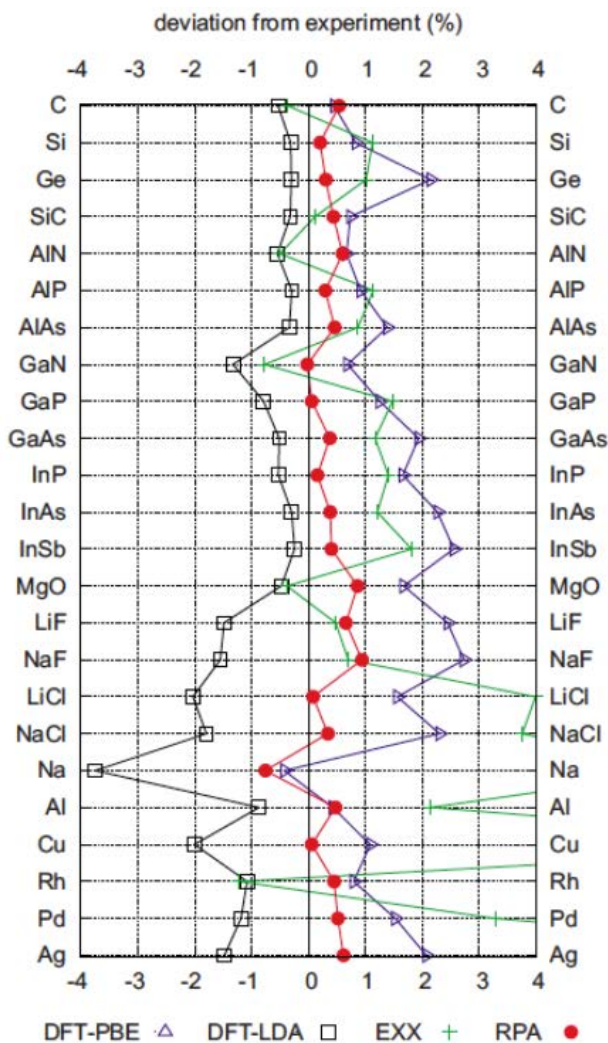


Benefit of Accurate Energies and Forces from ACFDT-RPA

Adsorption of CO on Rh, Pt (111)



Lattice parameters



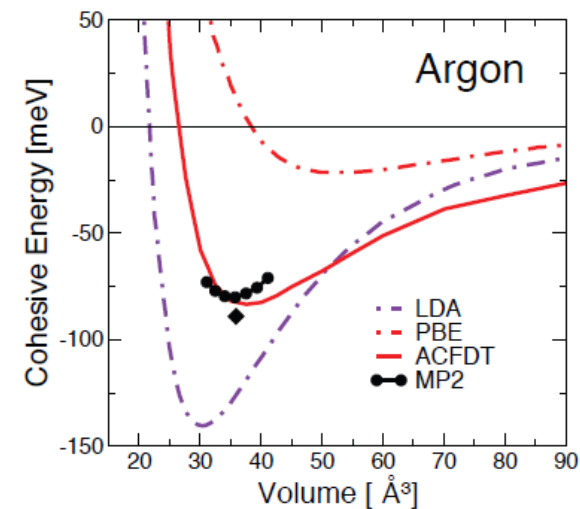
Heats of formation

	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

ACFDT-RPA delivers

- Correct site preference
- Good adsorption energies
- Excellent lattice constants
- Good surface energies

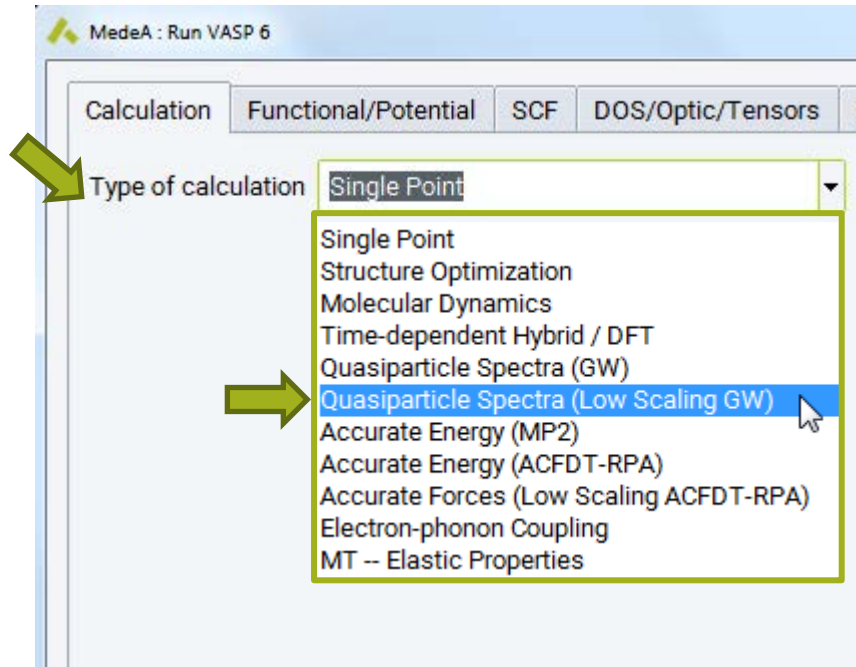
Van der Waals interactions



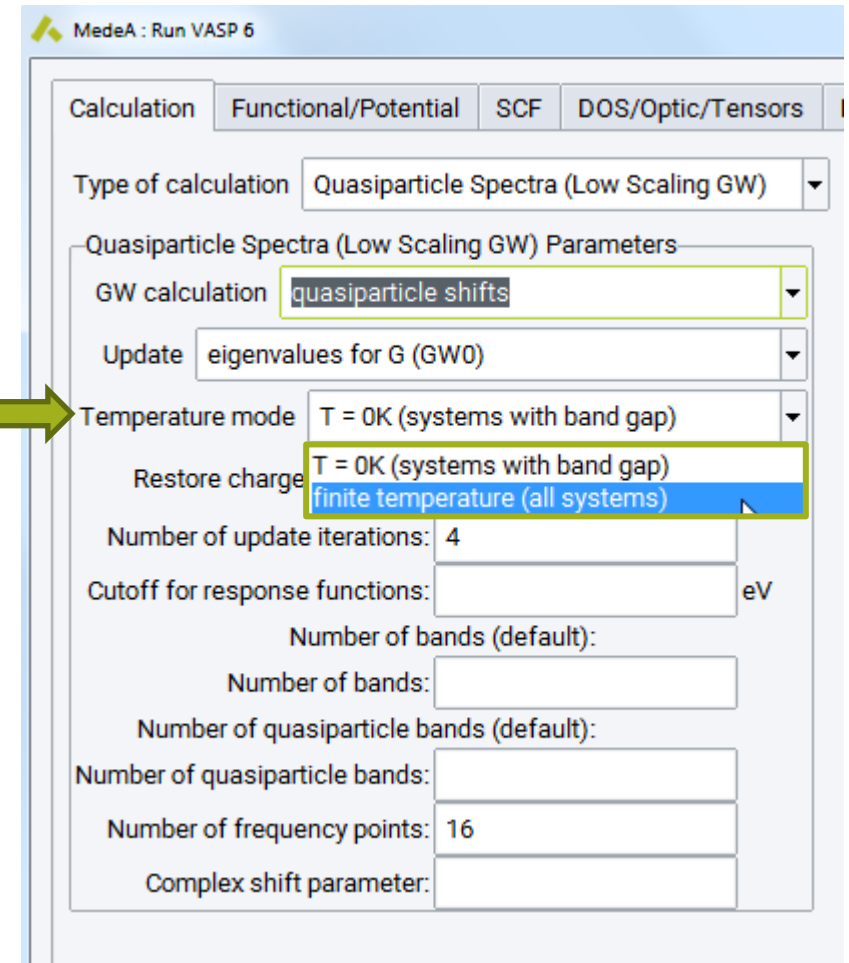
see Webinar “VASP 6: Total energies beyond DFT” by Martijn Marsman



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 **Quasiparticle Spectra** calculation types applying low scaling and standard GW, as well as optionally the Bethe-Salpeter approach to excitonic effects

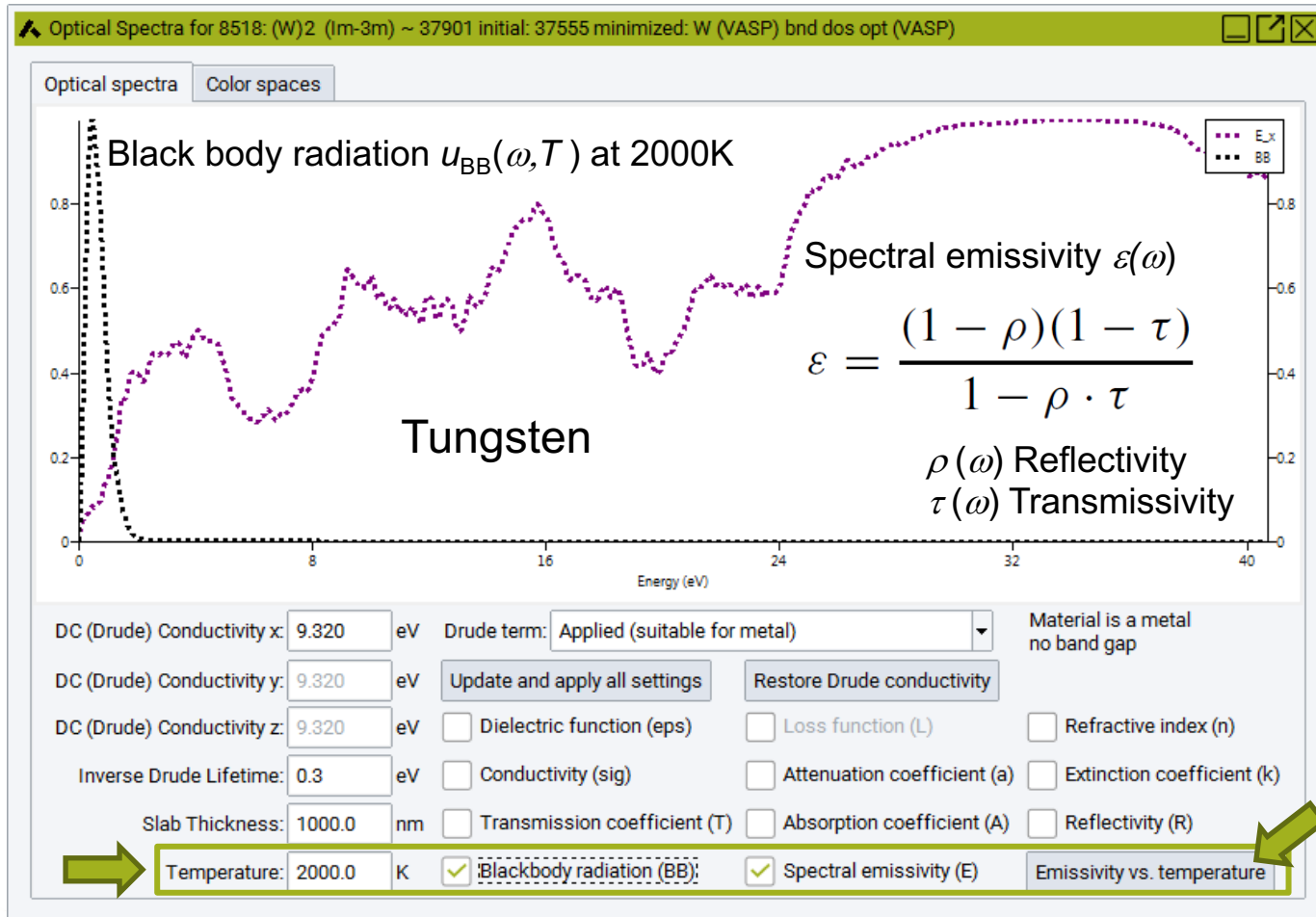


- ▶ Low scaling technique supports finite temperature mode for metals



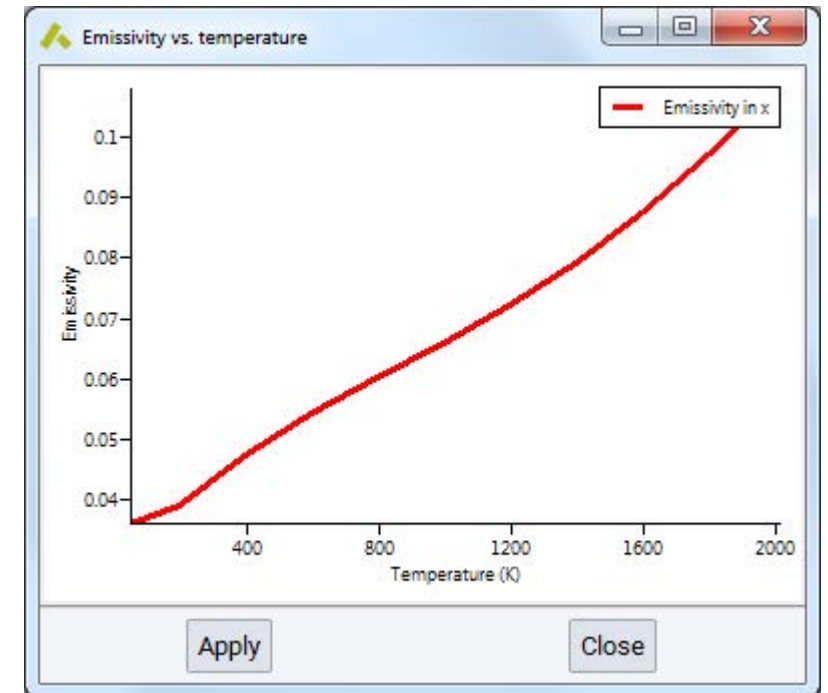
Optical Spectra and Color Analysis in *MedeA 3.1*

- ▶ 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



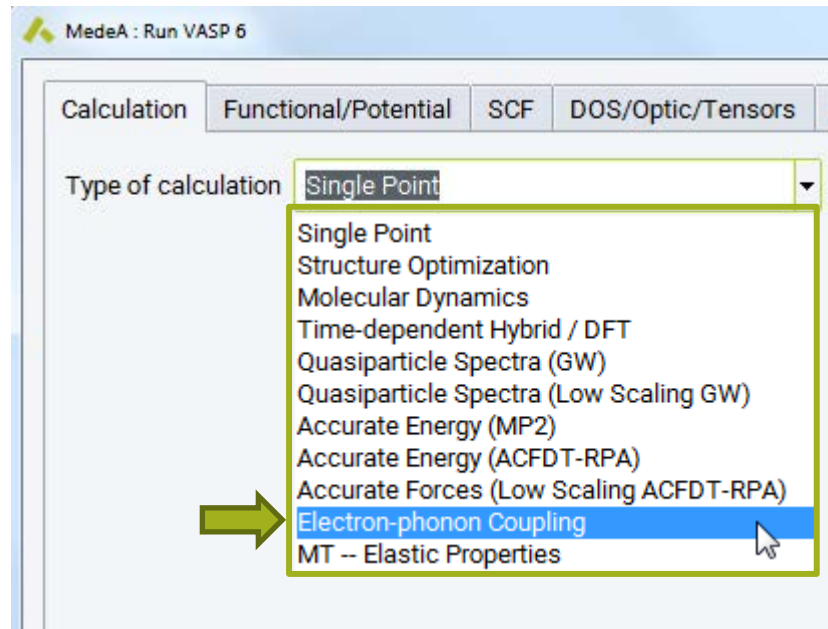
Emissivity $\epsilon(T) = \frac{\int \epsilon(\omega) \int u_{BB}(\omega, T) d\omega}{\int u_{BB}(\omega, T) d\omega}$

Emissivity vs. Temperature of W

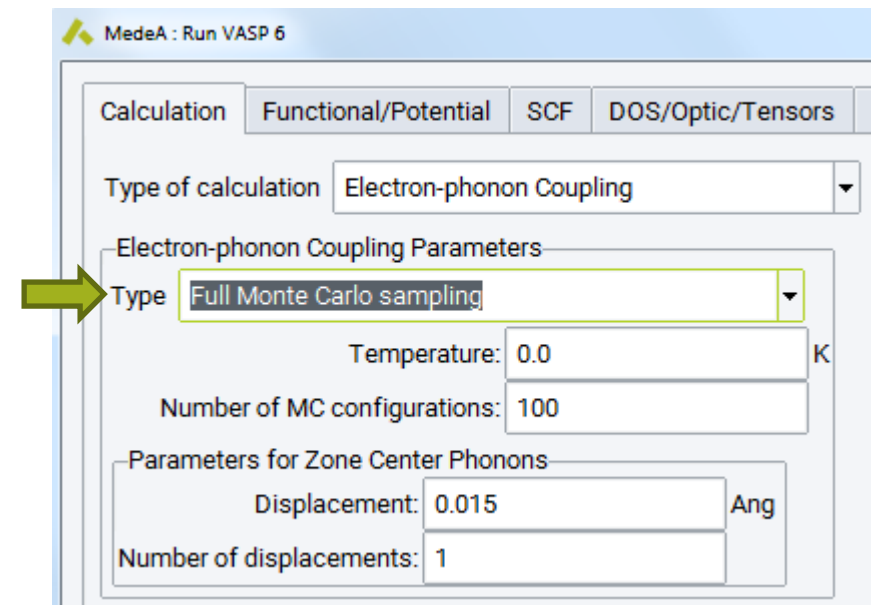
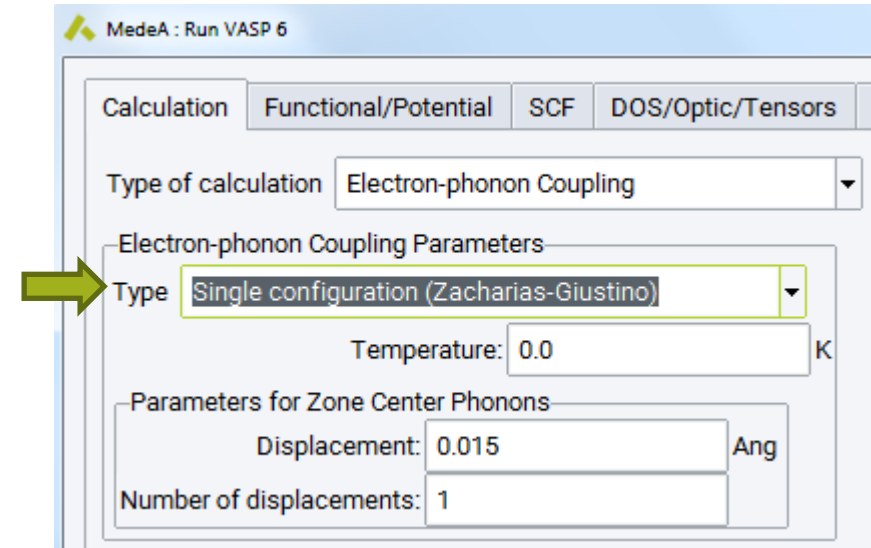


Electron Phonon Coupling from Stochastic Displacements

- ▶ Single displacement configuration
 - M. Zacharias, F. Giustino, Phys. Rev. B 94, 075125 (2016)
- ▶ Full Monte Carlo sampling of displacement configurations

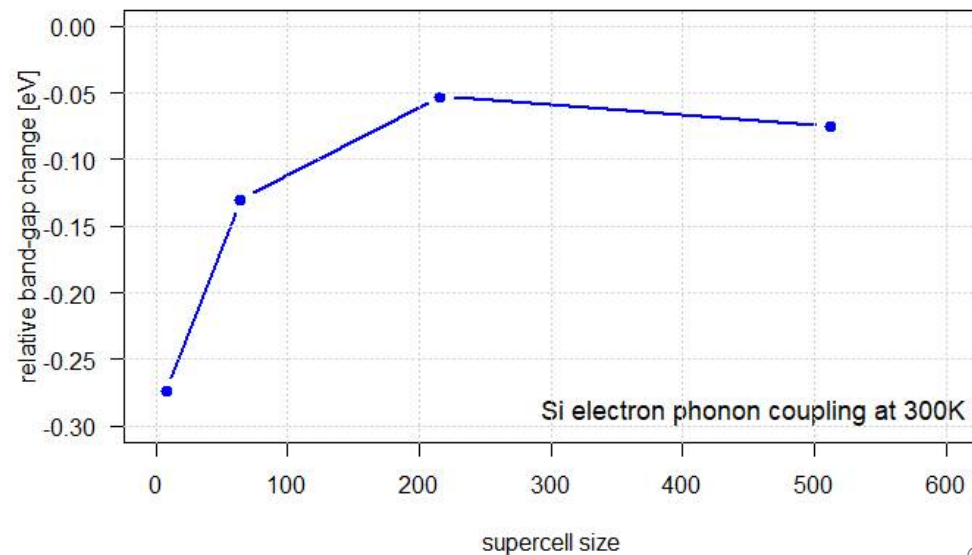
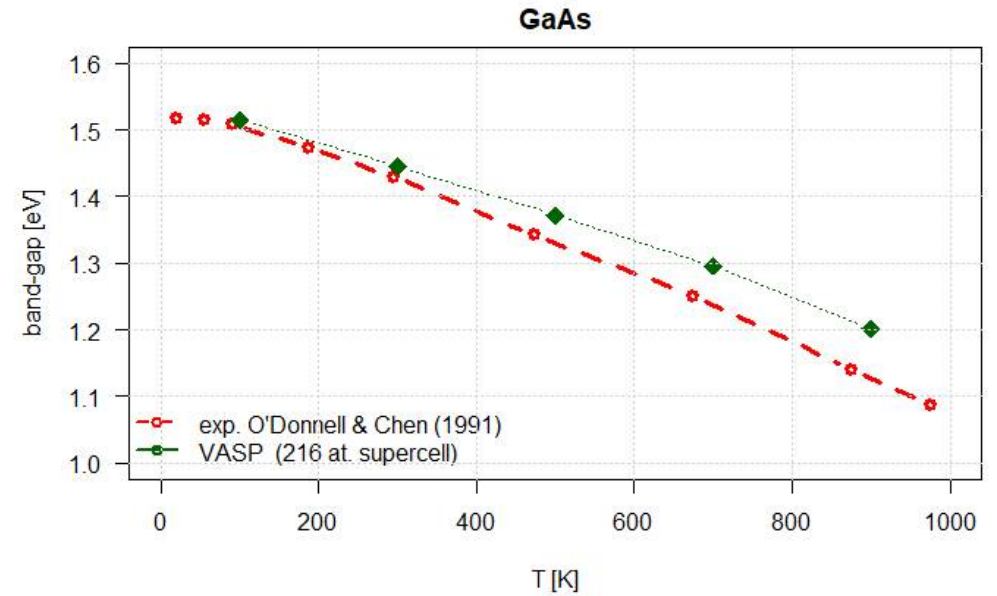
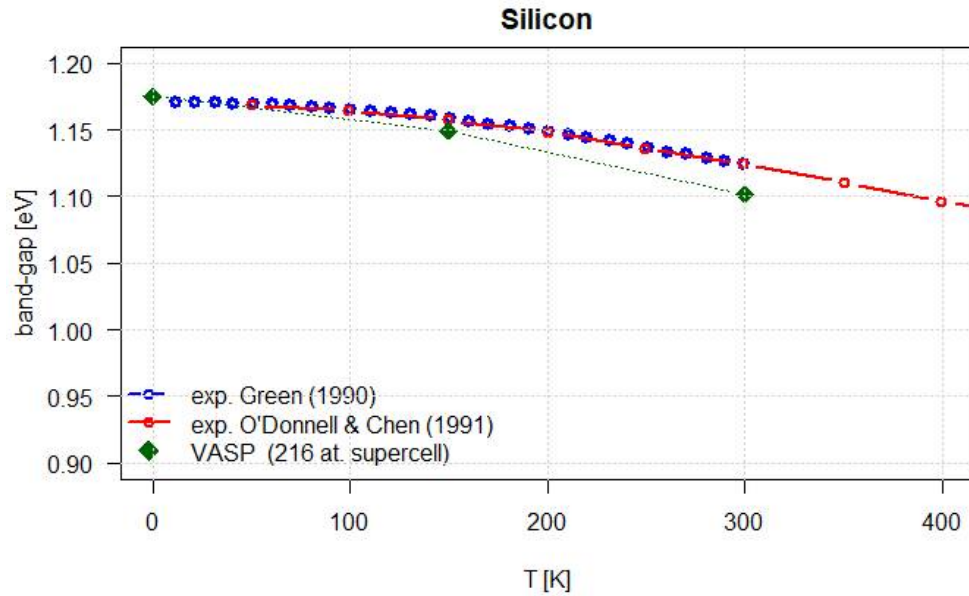


- ▶ For a given temperature any of the available properties can be computed





Temperature Dependence of Band Gaps



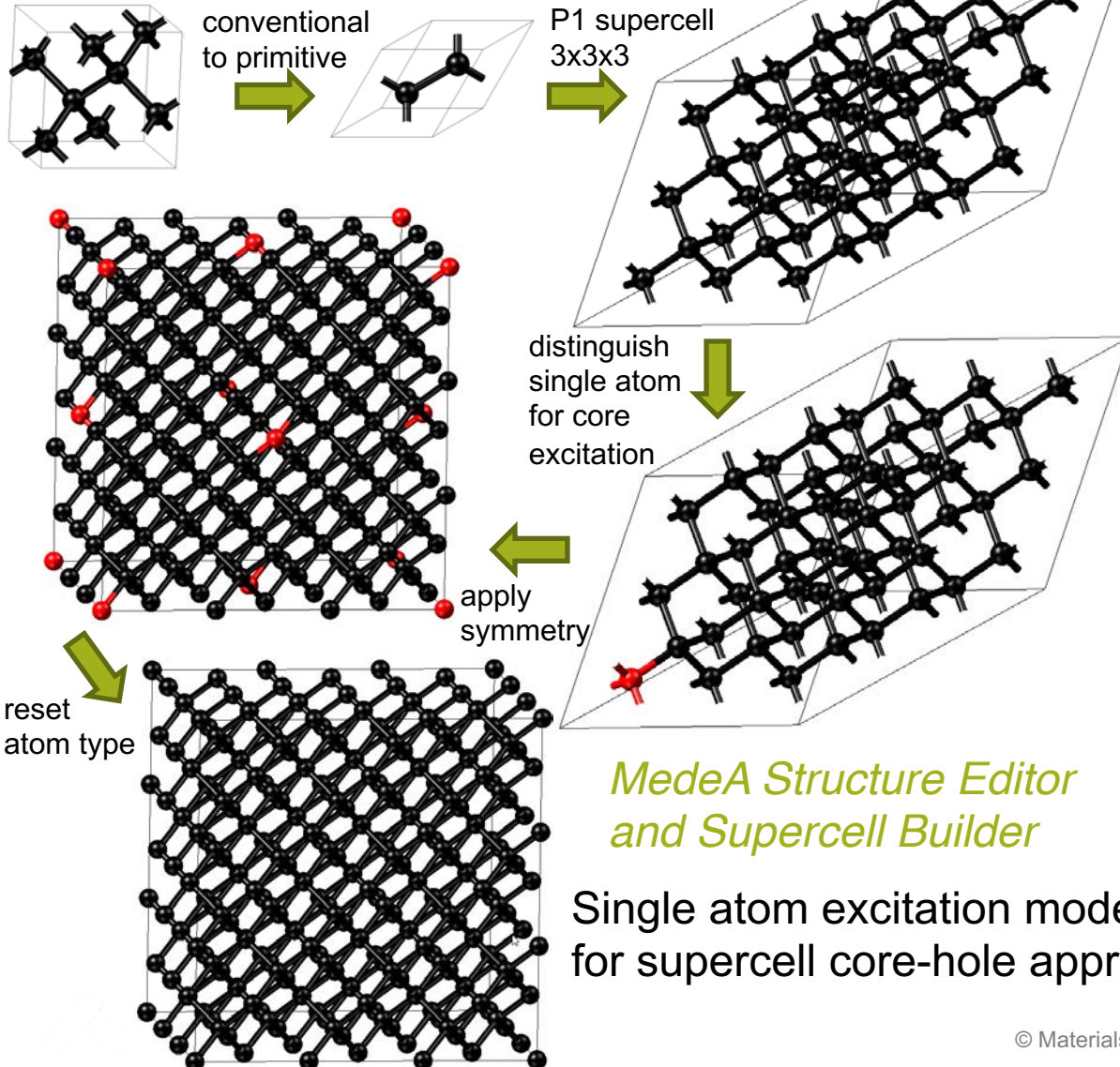
- ▶ Need of large supercells!
- ▶ Lattice optimization of Si/GaAs: PBE/PBEsol
- ▶ Band gaps: Modified Becke Johnson LDA
- ▶ Thermal expansion is not included

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 VASP 6

Advanced Tab

Enable choices specific for

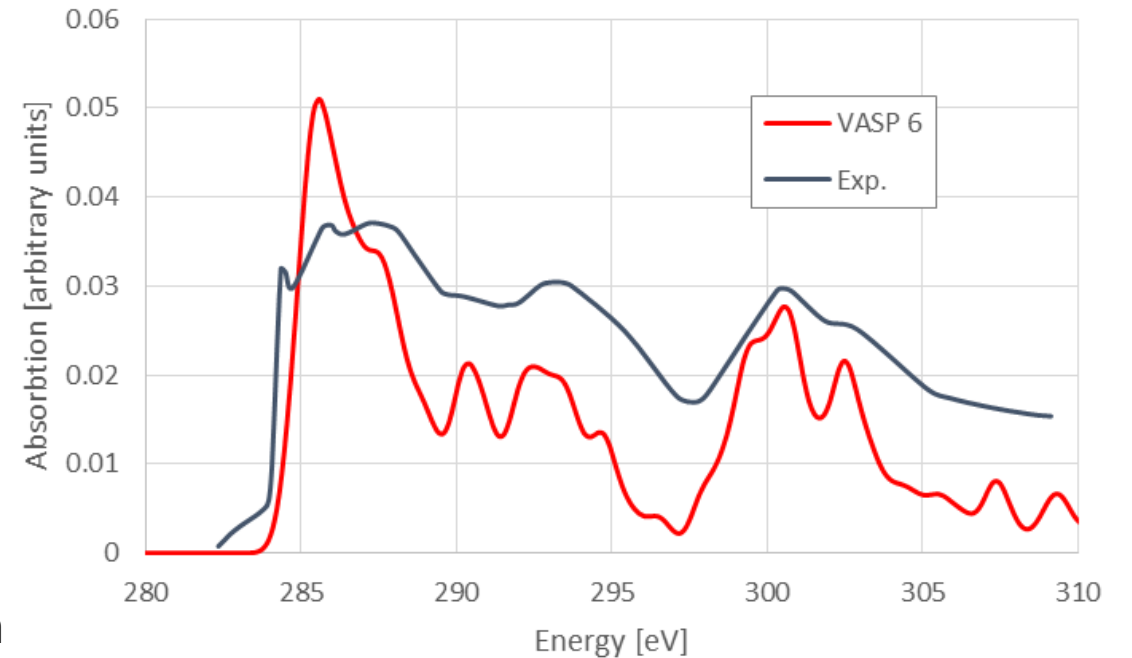
Number of bands (default): 136

Number of bands:

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

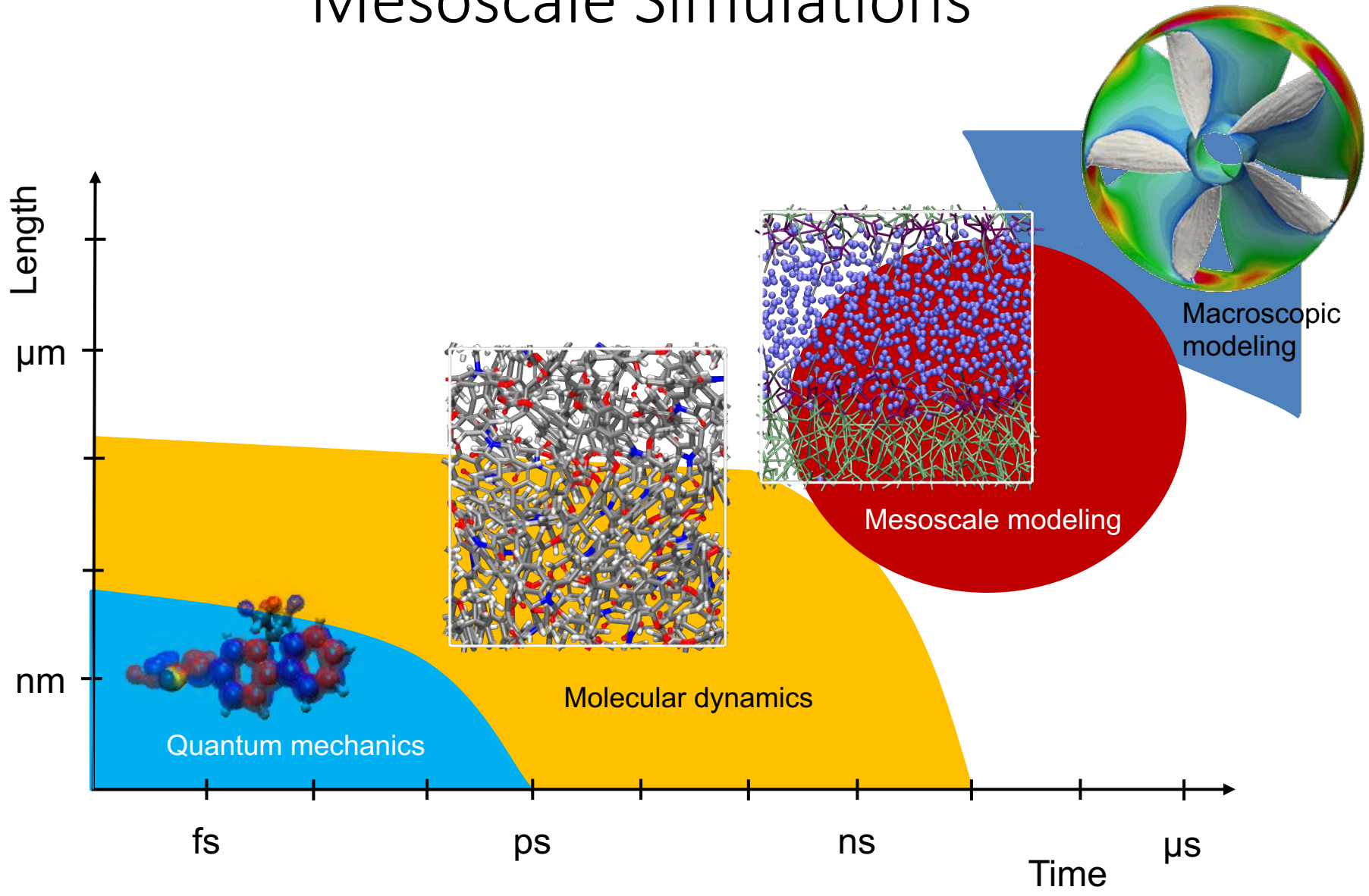




Mesoscale Simulations



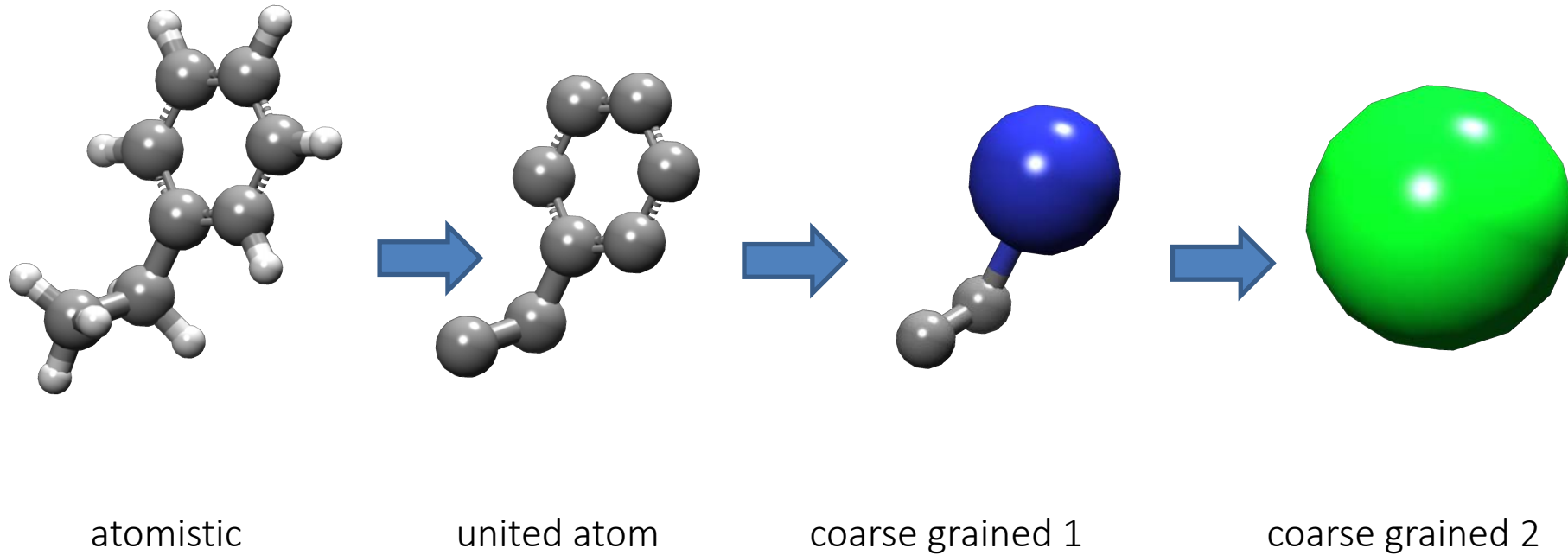
Mesoscale Simulations





Mesoscale Simulations

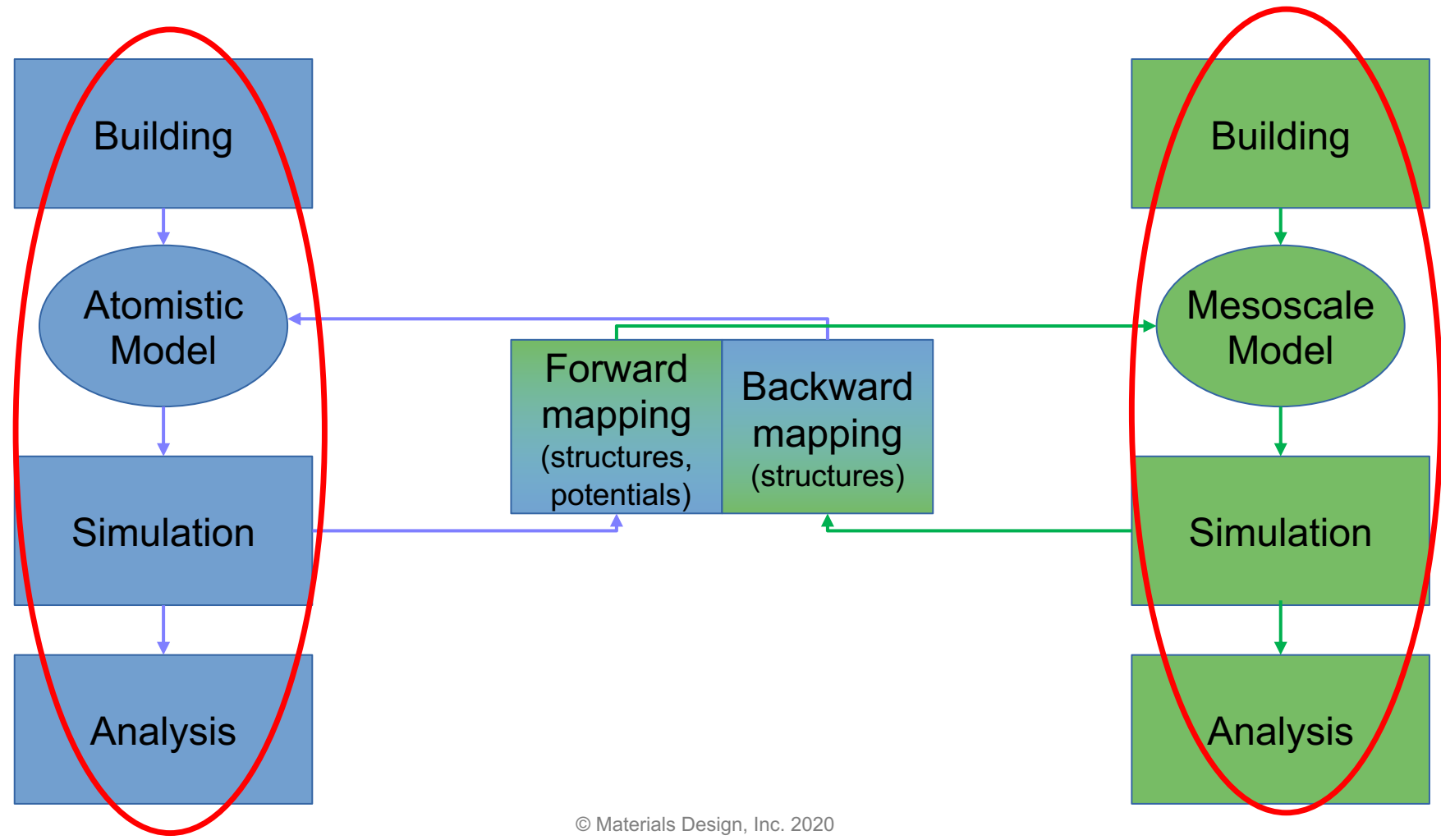
Coarse graining of a styrene monomer





Mesoscale Simulations

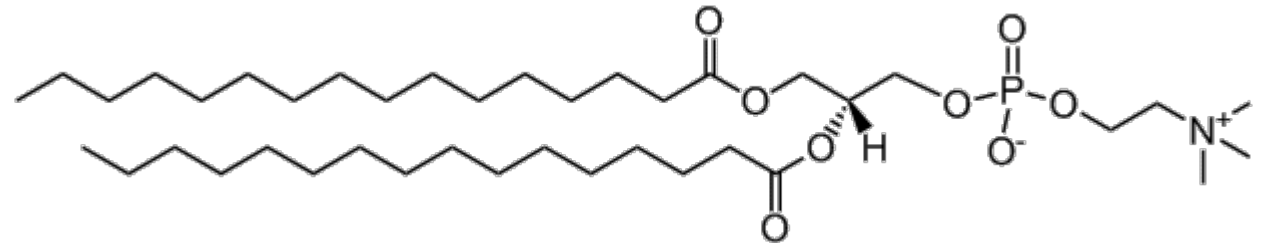
- Users expect smooth switching between atomistic and mesoscale simulations





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*

The screenshot shows the MedeA 3.1 software interface. On the left, a 3D ball-and-stick model of a molecule is displayed, featuring a central grey sphere bonded to a blue sphere above, a white sphere to the left, and a purple sphere to the right. On the right, a panel titled 'Insertion' contains a table of beads and their descriptions. An orange arrow points from the text 'Martini and SPICA forcefields are available' to the 'Na' bead entry in the table.

Bead	Description
SP3	Polar for ring structures - Degree of polarity: 3
P2	Polar - Degree of polarity: 2
SP2	Polar for ring structures - Degree of polarity: 2
P1	Polar - Degree of polarity: 1 (low)
SP1	Polar for ring structures - Degree of polarity: 1 (low)
N	Nonpolar - Hydrogen bonding capabilities: donor/acceptor
SN	Nonpolar for ring structures - Hydrogen bonding capabilities: donor/ac
Nd	Nonpolar - Hydrogen bonding capabilities: donor
SNd	Nonpolar for ring structures - Hydrogen bonding capabilities: donor
Na	Nonpolar - Hydrogen bonding capabilities: acceptor

Details for the selected bead (Na):

- Description: Nonpolar - Hydrogen bon
- Mass: 64.54
- Radius: 1.2
- Charge: 0.0
- Color: [Purple color swatch]

Martini and SPICA forcefields are available

Sketching mesoscale structures





Mesoscale Simulations with *MedeA* 3.1

The screenshot displays the MedeA 3.1 software interface. On the left, a coarse-grained DPPC molecule is shown with a head group (blue and grey spheres) and two tails (purple and green spheres). The right panel shows the 'Insertion' tab with a table of bead types and their descriptions. The 'C1' bead is selected, and its parameters are shown in the 'Details' section.

Bead	Description
SC5	Apolar for ring structures - Degree of polarity: 5 (high)
C4	Apolar - Degree of polarity: 4
SC4	Apolar for ring structures - Degree of polarity: 4
C3	Apolar - Degree of polarity: 3
SC3	Apolar for ring structures - Degree of polarity: 3
C2	Apolar - Degree of polarity: 2
SC2	Apolar for ring structures - Degree of polarity: 2
C1	Apolar - Degree of polarity: 1 (low)
SC1	Apolar for ring structures - Degree of polarity: 1 (low)

Details for selected bead C1:

- Description: Apolar - Degree of polar
- Mass: 52.85
- Radius: 1.2
- Charge: 0.0
- Color: [Green color swatch]

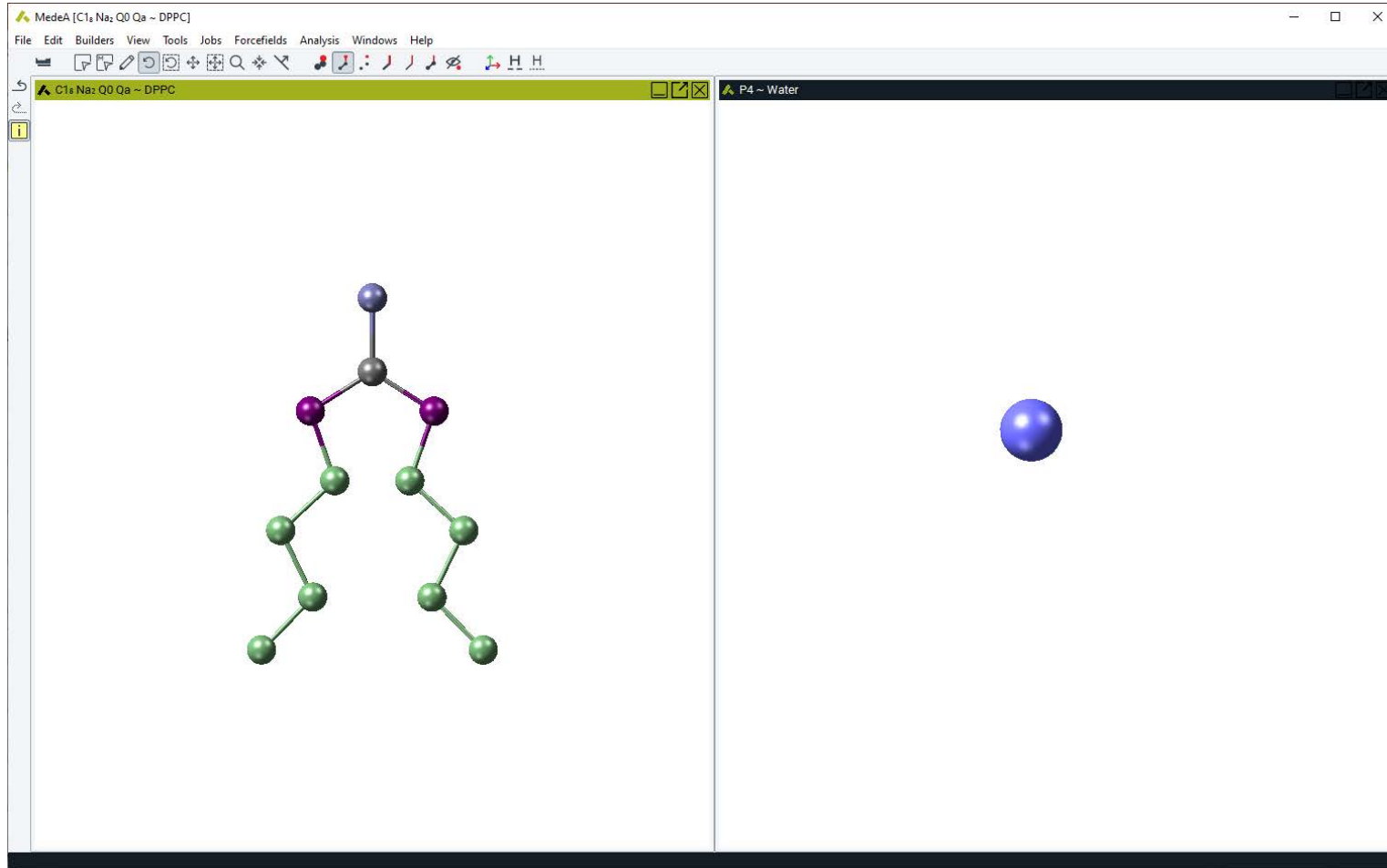
An orange arrow points from the text 'Parameters can be overwritten' to the 'Radius' field in the details panel.

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

The screenshot displays the MedeA software interface. The main window shows a ball-and-stick model of a DPPC molecule. Overlaid on the right is the 'MedeA: Amorphous Builder' dialog box. The dialog box contains a table with the following data:

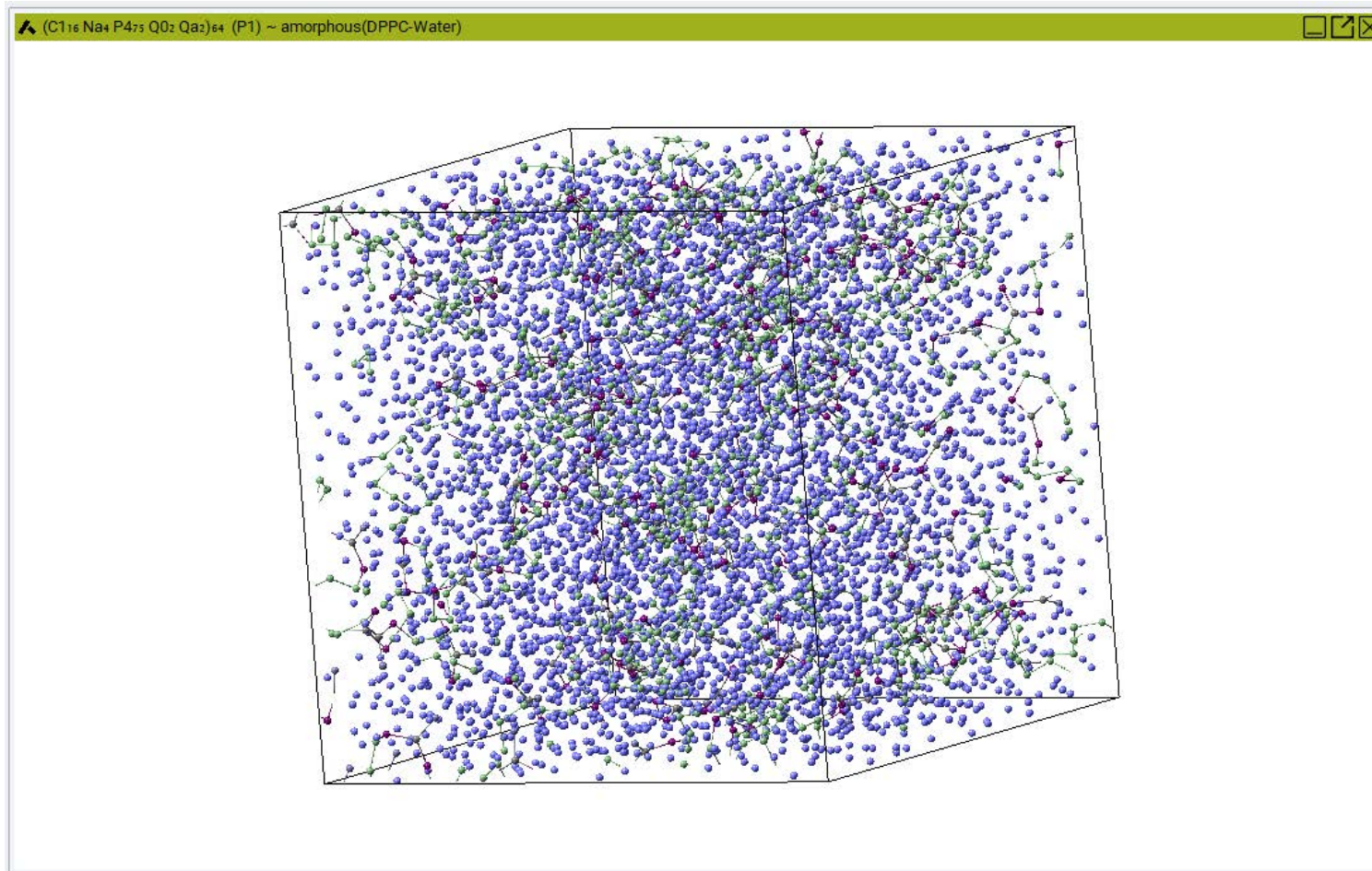
#	Component	Type	Nmols	Relax
1	Opened structure: DPPC	Automatic	128	<input checked="" type="checkbox"/>
2	Opened structure: Water	Automatic	4800	<input checked="" type="checkbox"/>

Below the table, there is an 'Add a component' button. The dialog also includes fields for 'System geometry' (set to 'bulk cell'), 'Specify cell' (set to 'density'), 'Density' (set to '1.0'), and 'Cell details' (with a 'Refresh' button). The 'Density' field shows calculated values: 'Density: 1.0000 a: 90.0375 b: 90.0375 c: 90.0375'. Other fields include 'Temperature' (298.2), 'Coordinate bias' (none), 'Orientation bias' (none), 'Action' (Build cell), and 'Number of configurations' (1). Buttons for 'OK', 'Cancel', and 'Help' are at the bottom.

Amorphous builder can handle mesoscale systems



Mesoscale Simulations with *MedeA 3.1*



An amorphous mesoscale system



Mesoscale Simulations with *MedeA* 3.1

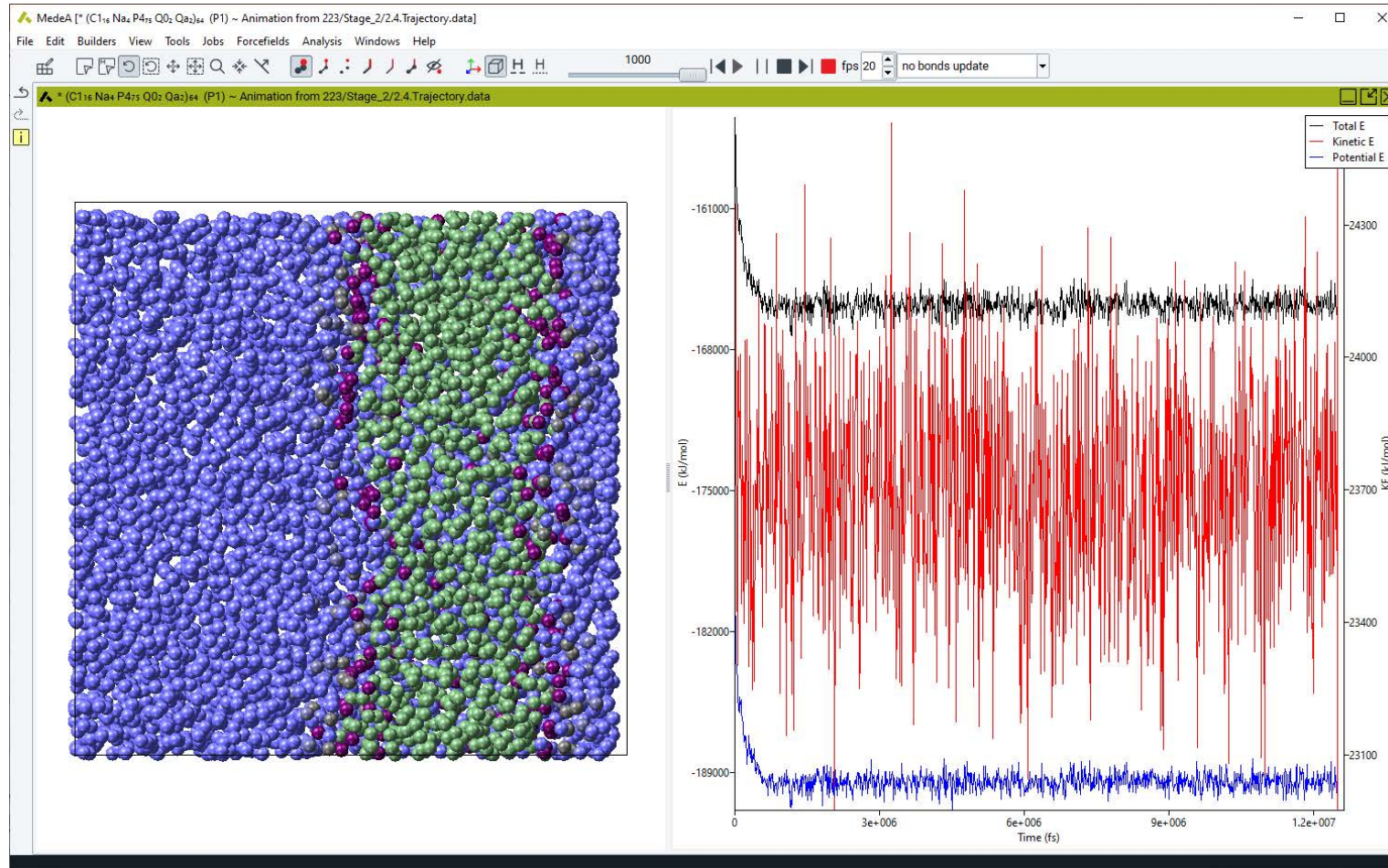
The screenshot displays the MedeA 3.1 interface, divided into three main sections:

- Materials Design Flowchart (Left):** A high-level flowchart starting with a 'Start' node, leading to a 'Variables' node (containing $tstep = 20$ fs, $T = 300$ K, $P = 1$ atm), and finally to a 'LAMMPS' node.
- LAMMPS Flowchart for stage 1 (Middle):** A detailed flowchart starting with 'Start', followed by 'Initialize' (3-d periodic, Cutoff: 12, Skin: 2.0, Long range: PPPM W/ tail corrections), 'Minimize' (Optimization of atom positions, Method: Conjugate gradients, Econvergence = 0.0, Fconvergence = 1.0), 'velocities' (Initial velocities for \$T\$, No net translation, Random seed: 72489), and 'NPT' (Temp: \$T\$, Press: \$P\$, Time: 250 ns, Step: \$tstep\$, Constraints: isotropic, Control: Nose-Hoover T & P, Sampling: 10000 samples, Trajectory: 1000 frames).
- Add stages (Right):** A panel with a scrollable list of simulation stages:
 - Initialization: Initialize LAMMPS
 - Bias: Orientation
 - Single Point: Single Point Energy, Single Point Forces
 - Minimization: Minimize
 - Building and Editing: Set cell, Compress Layer
 - Dynamics: Initialize velocities, NVE ensemble, NVT ensemble, NPT ensemble, Cohesive energy density, Thermal Conductivity, Viscosity, Diffusion, Surface Tension, Deposition
 - Custom: (empty)

At the bottom, there are buttons for 'OK', 'Cancel', and 'Help'. A status bar at the very bottom shows 'Job title: DPPC in wat' and a 'Run' button.



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




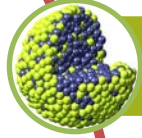

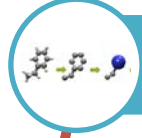
Online Training and
Demonstration:
MedeA 3.1

A world map with a dark blue background and glowing yellow city lights. The map is overlaid with a network of glowing blue lines connecting various global locations. The text is centered over the map.

**Materials Design UGM
GOING GLOBAL
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

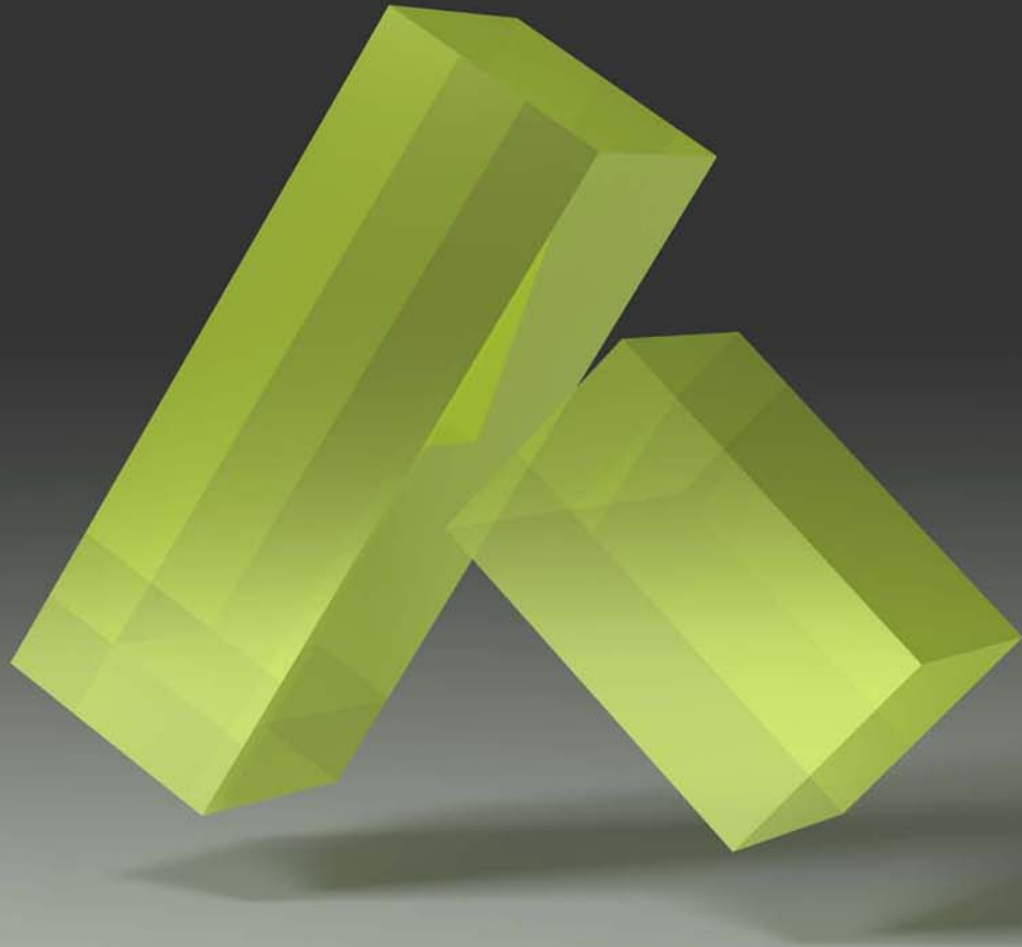
- <https://www.materialsdesign.com/Publications>

▶ Application Notes

- <https://www.materialsdesign.com/application-notes>

▶ For questions or comments contact

- Katherine Hollingsworth
 - khollingsworth@materialsdesign.com



Medea

Innovation by Simulation