materials design

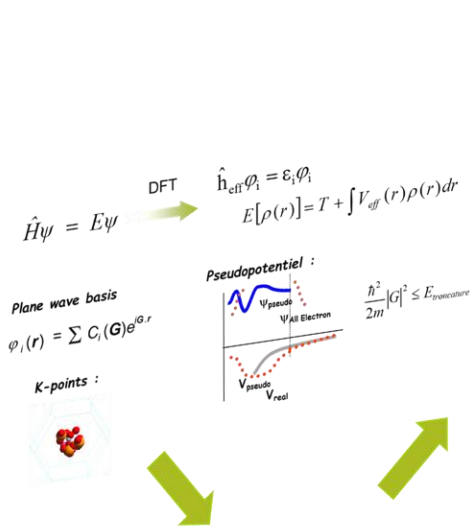
Monacoste 2022

Computational Materials Science in MedeA® environment

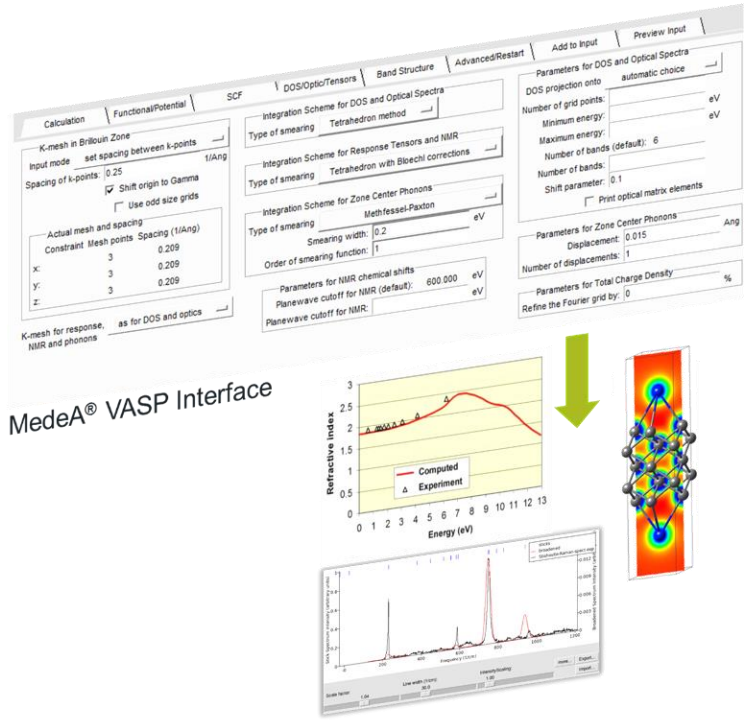
B. Minisini, J. Coll

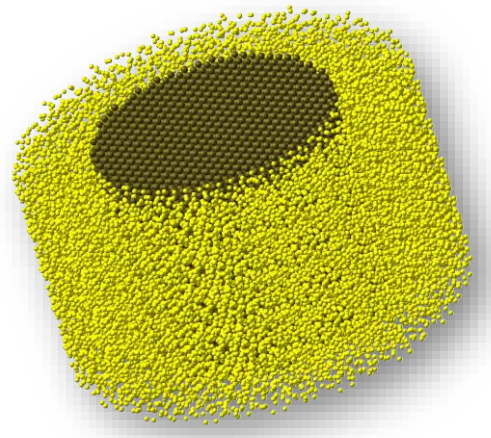
11th May 2022

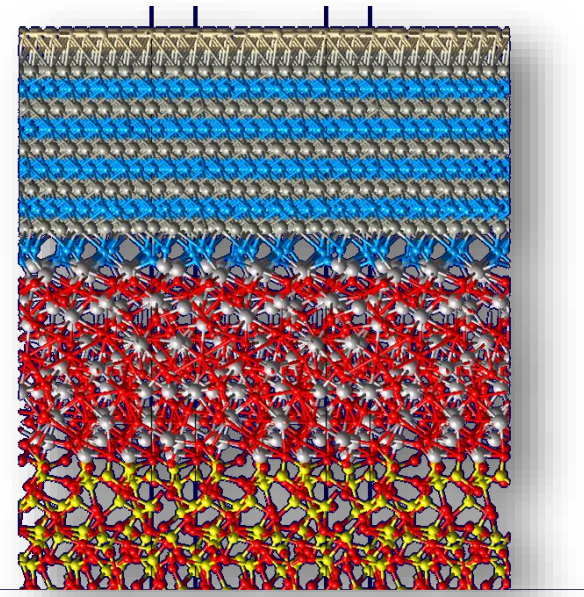
bminisini@materialsdesign.com



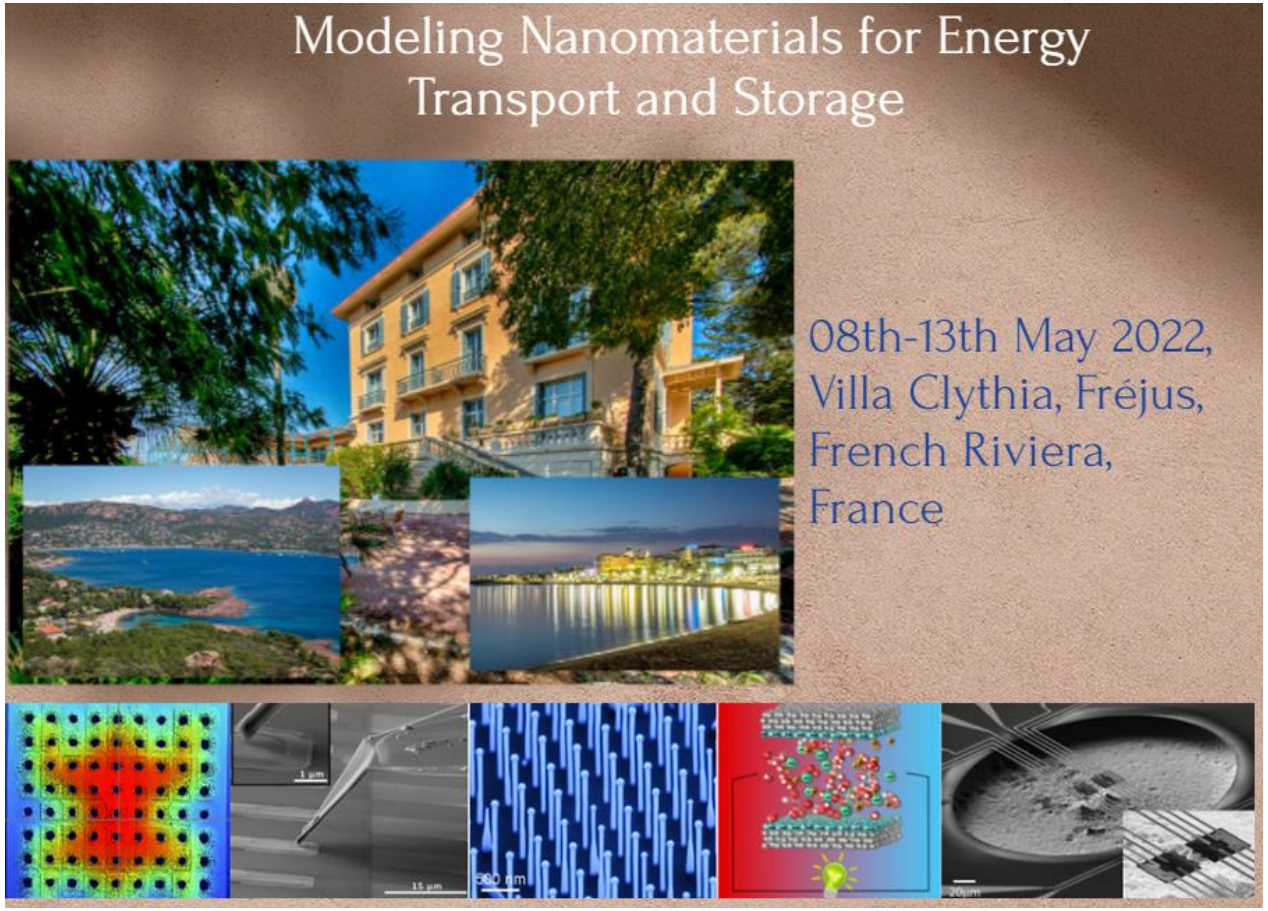
All the density functional theory calculations were performed using the Vienna Ab-initio Simulation Package (VASP) code.[43–45] Generalized gradient approximation in the parametrization of Perdew–Burke–Ernzerhof (PBE)[44] and the vdW correction proposed by Grimme are chosen.[46] The energy cutoff was set to be 550 eV. Geometry structures are fully relaxed until the convergence criteria of energy and force are less than 10^{-5} eV and 0.01 eV Å^{-1}, respectively. A Monkhorst–Pack mesh of $7 \times 7 \times 1$ *K*-points is used in the 2D Brillouin zone for geometry optimizations and electronic structure calculations. We also used a large vacuum space to

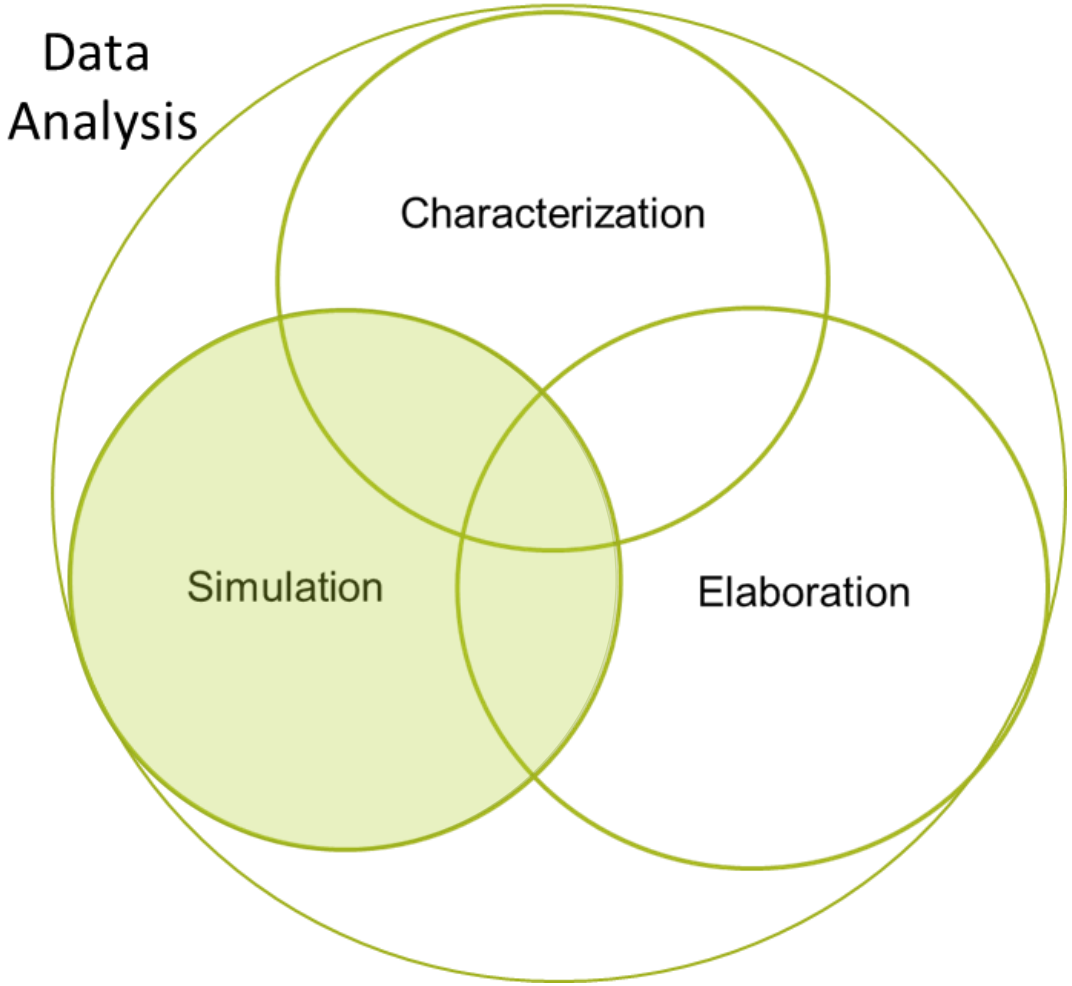






Introduction





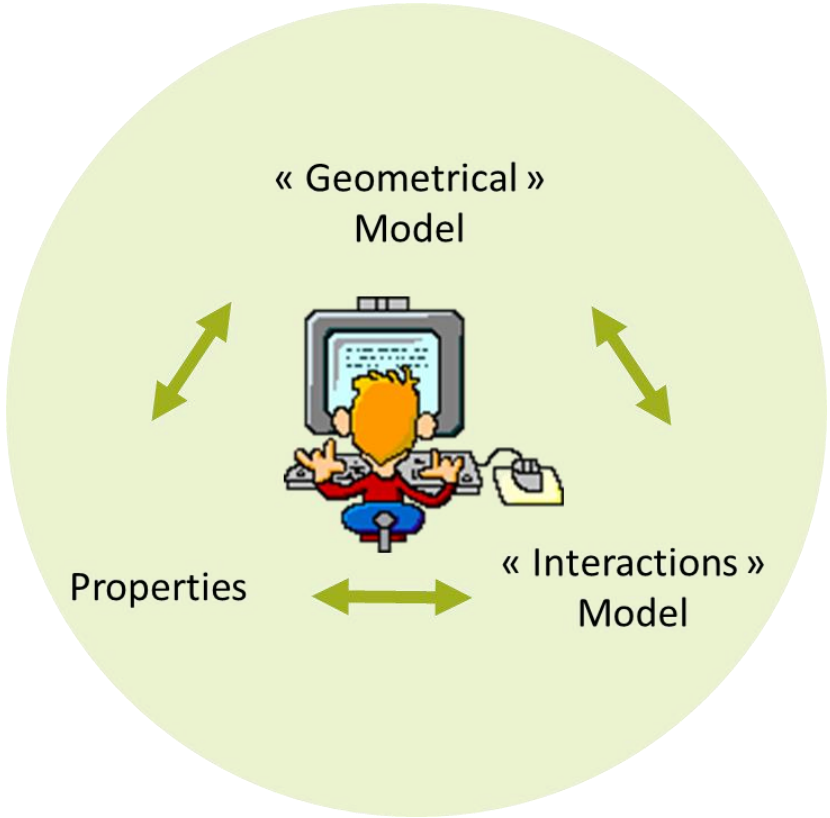
DATA :

1 number + 1 units + (1 uncertainty) obtained on 1 sample with 1 method under certain conditions

materials design

Introduction

COLOR CODE:		Physical Principles	Method	Workshop	Applications	
	Sunday 8th	Monday 9th	Tuesday 10th	Wednesday 11th	Thursday 12th	Friday 13th
8h00						
8h30		Materials : introduction				
9h00			Phonon transport (S. Merabia)	Near field radiation (R. Messina & S.A. Biehs) Photovoltaics (M. Amara)	Monte Carlo 1. phonon transport 2.electronic transport (D. Lacroix and J. St-Martin)	Ionic transport (A. Würger)
9h30		Ab initio modelling (N. Vast)				
10h00			pause			pause
10h30						
10h45		pause				
11h00			Electronic transport (F. Michelini)		pause	Thermoelectricity (P. Boulet)
11h15		Molecular dynamics (E. Martin)				
11h30				Thermo-photovoltaics (R. Vaillon)	Green's functions (M. Bescond)	
12h00						
12h30				Lunch		
13h00						
13h30		Materials 1 (A. Tanguy)	Materials 2 (E. Gaudry)			
14h00				free	Artificial Intelligence (T. Swinburne)	
14h30						
15h00					Empirical potentials	
15h20		Workshop ab-initio 1 (G. Fugallo & L. Paulatto)	Workshop ab-initio 2 (G. Fugallo & L. Paulatto)	free		
16h00					pause	
16h30					Finite element modelling (F. Xavier Alvarez)	
17h00		pause	pause			
17h20		Workshop molecular dynamics 1:activated processes (T. Albaret)	Workshop molecular dynamics 2: Transport (S. Merabia)			
18h00					pause	
18h30	Welcome and Aperitive	pause	pause		Round table	
19h00						
19h30		Dinner	Dinner	Free Dinner	Gala dinner	
20h00						
21h00		Poster session	Poster session			
22h00						



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Introduction

International Conference on Multiscale Approches for Process Innovation 2012

« One will have to train students and people to be expert at all scales ? »

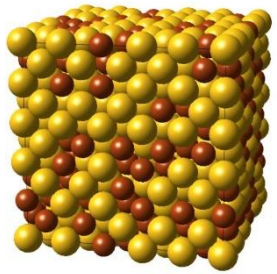
C. CHIZALLET (IFPEN), Oil & Gas Sci. Tech. 68, 110-1113, 2013

« If I need brain surgery I will not apply to a foot doctor »

R.J QUANN (Exxon Mobil),), Oil & Gas Sci. Tech. 68, 110-1113, 2013

« …promote a rather wide training and then on this broad training you need to build specialization »

P. SAUTET (ENS Lyon),), Oil & Gas Sci. Tech. 68, 110-1113, 2013



« …it is more important to teach the skills to use computational tools rather than the programming skills required to develop such tools. »

THORTON et al JOM, 61, 12-17, 2009

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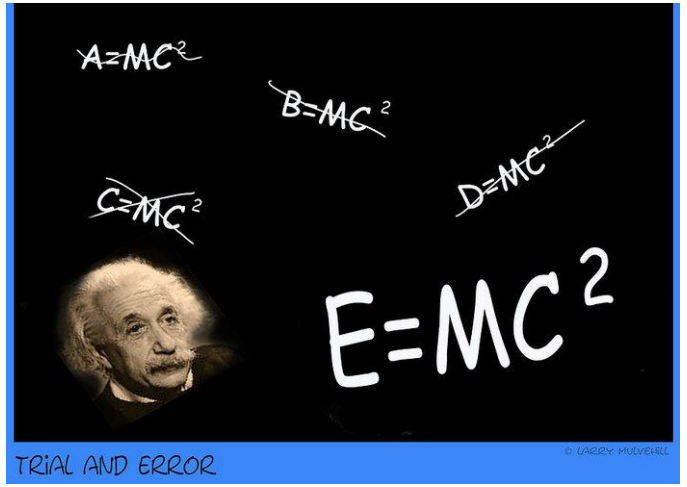
Introduction

- How reduce the learning curve ?
  - Lectures
  - Bibliography
    - Properties
    - Methods
    - Materials
  - Practice

reasoned



materials design

Introduction

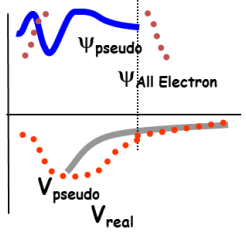
$$\hat{H}\psi = E\psi \xrightarrow{\text{DFT}} \hat{h}_{eff}\varphi_i = \varepsilon_i\varphi_i$$

$$E[\rho(r)] = T + \int V_{eff}(r)\rho(r)dr$$

Plane wave basis

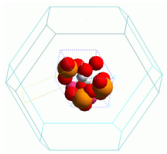
$$\varphi_i(\boldsymbol{r}) = \sum C_i(\boldsymbol{G})e^{i\boldsymbol{G}.\boldsymbol{r}}$$

Pseudopotentiel :



$$\frac{\hbar^2}{2m}|G|^2 \le E_{troncature}$$

K-points :



- NGX, NGY, NGZ and NGXF, NGYF, NGZF-tags
- KSPACING-tag and KGAMMA-tag
- NBANDS-tag
- NBLK-tag
- SYSTEM-tag
- NWRITE-tag
- ENCUT-tag
- ENAUG-tag
- PREC-tag
- ISPIN-tag
- MAGMOM-tag
- ISTART-tag
- ICHARG-tag
- INIWAV-tag
- NELM, NELMIN and NELMDL-tag
- EDIFF-tag
- EDIFFG-tag
- NSW-tag

- NBLOCK and KBLOCK-tag
- IBRION-tag, NFREE-tag
  - IBRION=-1
  - IBRION=0
  - IBRION=1
  - IBRION=2
  - IBRION=3
  - IBRION=5 and IBRION=6
  - IBRION=7 and IBRION=8
  - IBRION=44
  - IBRION some general comments (ISIF, POTIM)
- POTIM-tag
- ISIF-tag
- PSTRESS-tag
- IWAVPR-tag
- ISYM-tag and SYMPREC-tag
- LCORR-tag

```
# Time-averaged data for fix 2
# TimeStep v_time c_thermo_temp c_thermo_press v_sysvo
50000 25000.5 310.663 477.916 21226.2 1.301 1592.51 -1
100000 75000.5 312.475 662.159 21226.2 1.301 1626.3 -1
150000 125001 316.215 620.213 21226.2 1.301 1702.37 -6
200000 175001 318.552 186.784 21226.2 1.301 1729.92 -4
250000 225001 319.014 86.3631 21226.2 1.301 1739.07 -4
300000 275001 319.426 243.312 21226.2 1.301 1749.2 -35
350000 325001 319.482 217.45 21226.2 1.301 1779.71 -4.
```

```
Sub distance()

' copy data from sheet1 to sheet2 to evaluate the end_er

' position of the two atoms coordinates in the file

n = 16
m = 17

'loop to copy the atoms coordinates from sheet1 to sheet
    Worksheets("Sheet2").Activate
    Range("A2:H5002").Select
  Selection.ClearContents

    For i = 1 To 12000
        Worksheets("sheet2").Cells(i + 1, 1).Value =
        Worksheets("sheet2").Cells(i + 1, 5).Value =
        n = n + 11
        m = m + 11
    Next
```

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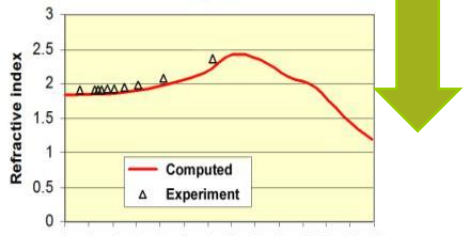

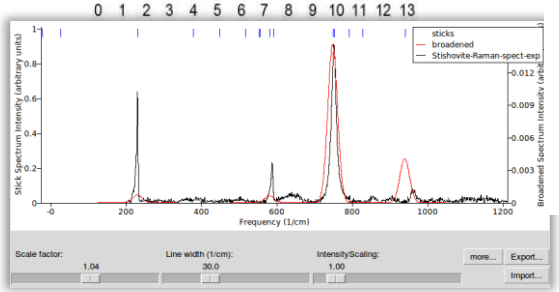

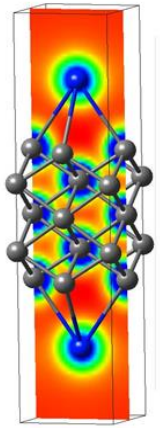

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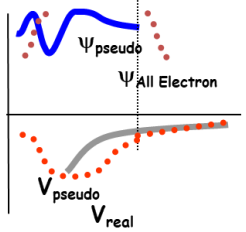

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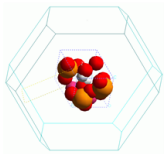

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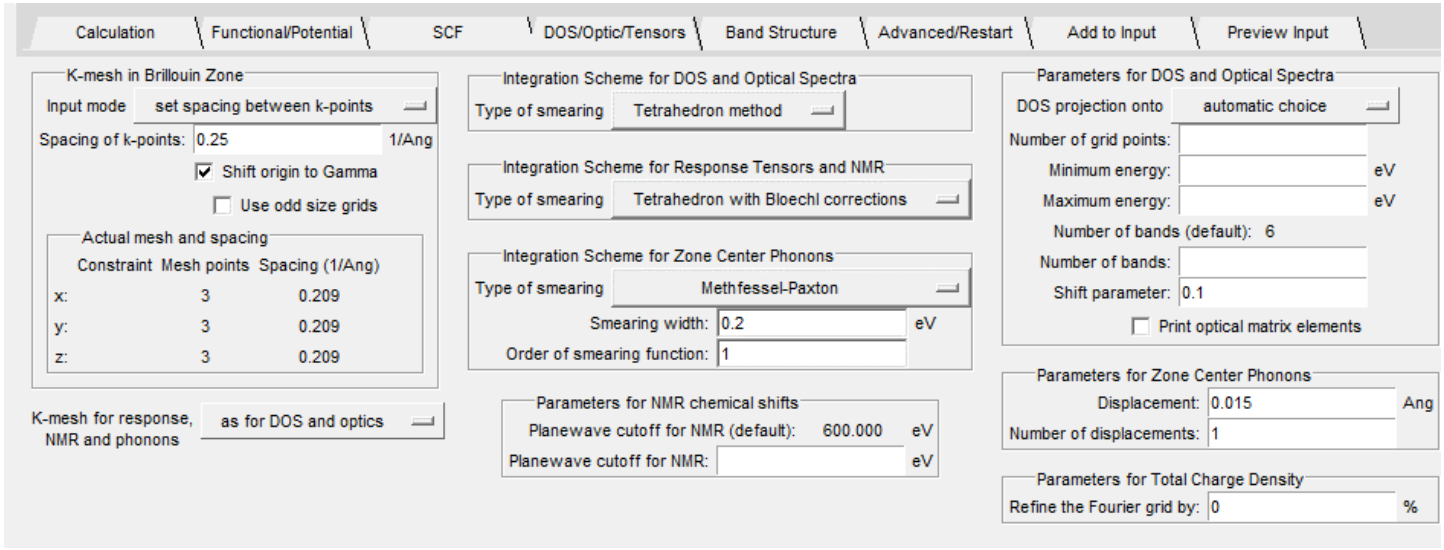
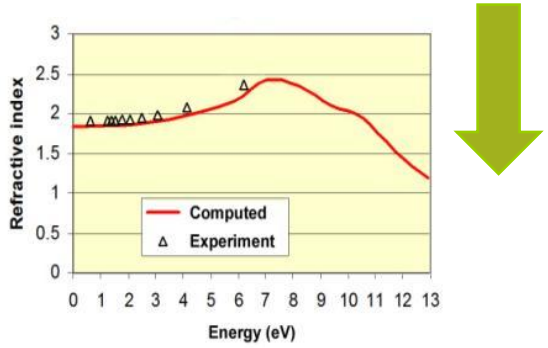
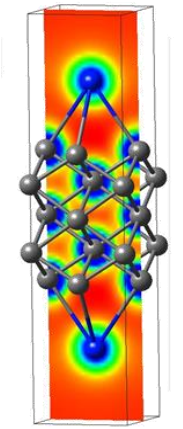
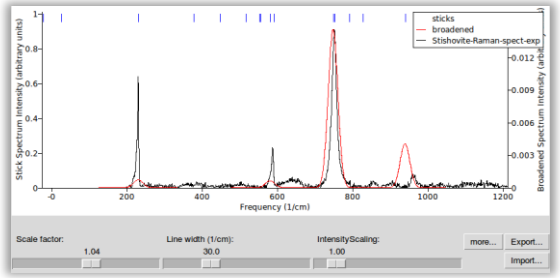


MedeA® VASP Interface







materials design

Introduction

“I like MedeA, it gives me more time to think.”

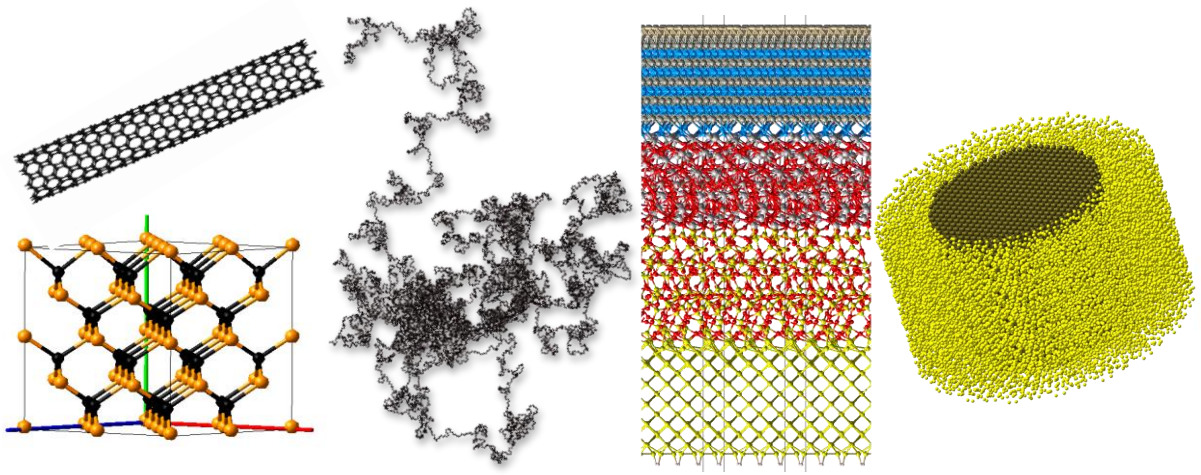
-Ryoji Asahi

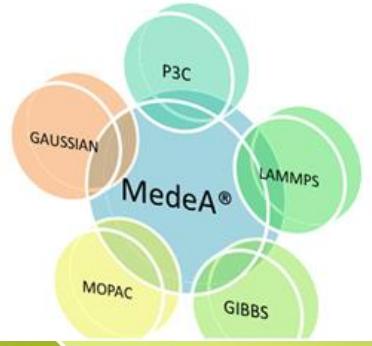
Toyota Central Research and Development Laboratories, Nagoya, Japan

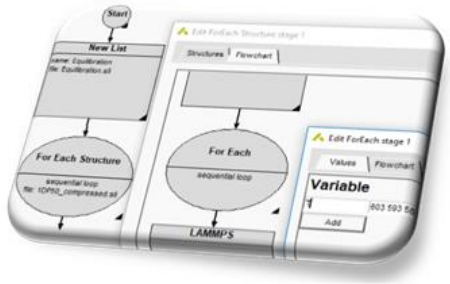
materials design

Introduction

Atomic-scale Simulations

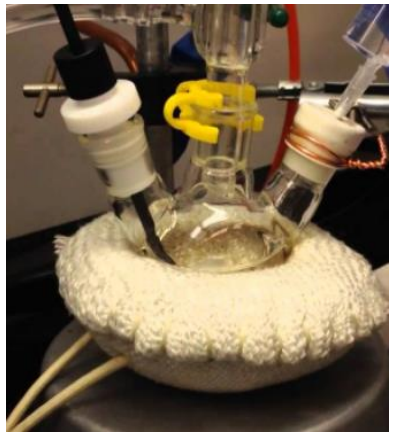


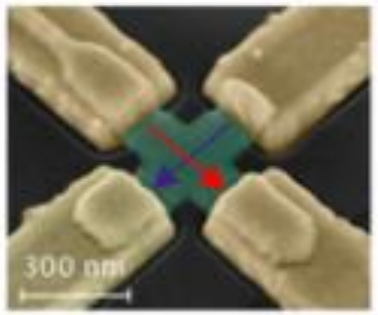


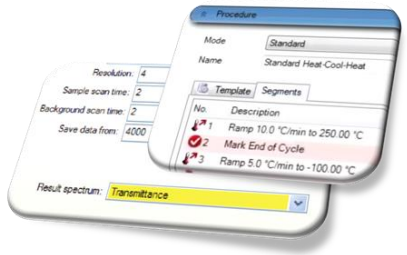


Formulation → Synthesis → Characterization

Laboratory Work







materials design

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

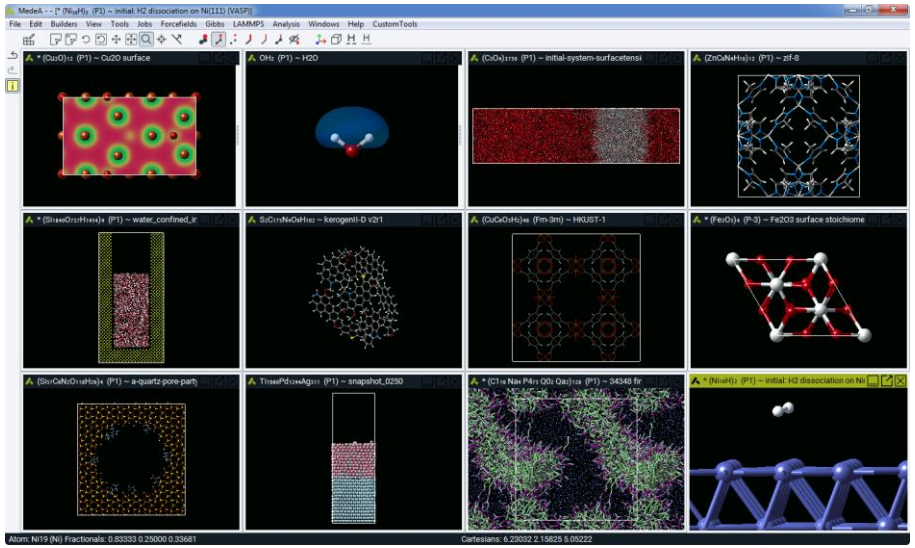
Analysis Tools

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

JobServer & TaskServer

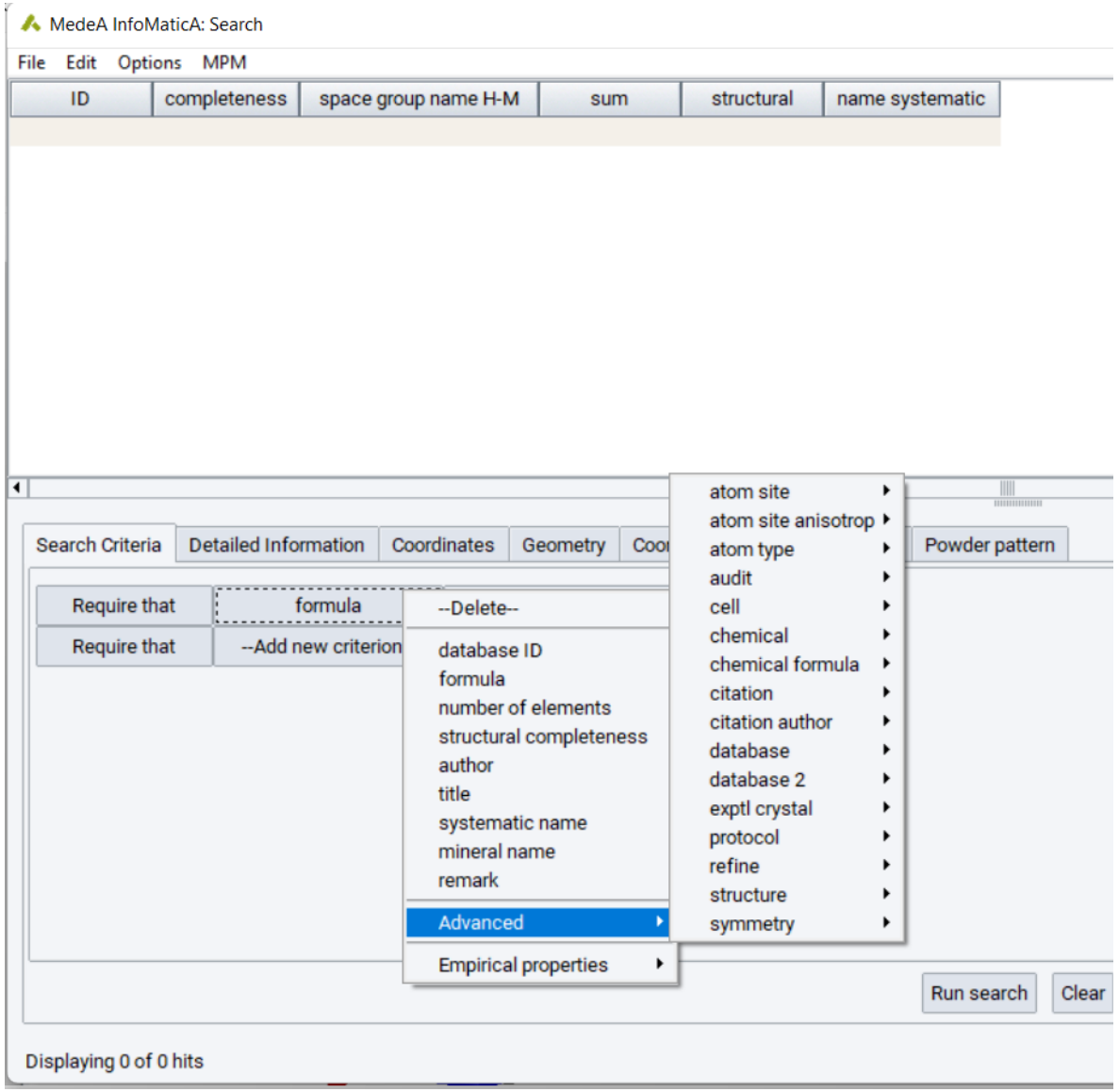
Automated processing of compute protocols & workflows; Reliable long-term archiving & accounting of computed data

MedeA environment



Databases

over 1.1 million entries



https://www.materialsdesign.com/databases

Databases

MedeA InfoMaticA: Search

File Edit Options MPM

ID	completeness	space group name H-M	sum	structural	name systematic
ICSD.2518	Complete	I4-2D	Cu1 Fe1 S2	Cu1 Fe1 S2	Copper iron sulfide
ICSD.67530	Complete	PCMN	Cu1 Fe2 S3	Cu1 Fe2 S3	Copper diiron sulfide
COD.152171[illegible]	Complete	F-43m	Cr2 Cu0.5 Fe0.5 S4	Cr2 Cu0.5 Fe0.5 S4	Fe0.5 Cu0.5 Cr2 S4
COD.900372[illegible]	Complete	F-43m	Cu2 Fe S2	Cu2 Fe S2	
COD.900372[illegible]	Complete	F-43m	Cu2 Fe S2	Cu2 Fe S2	
COD.901206[illegible]	Complete	I-42m	Cu2 Fe Ge S4	Cu2 Fe Ge S4	
COD.900372[illegible]	Complete	F-43m	Cu2 Fe S2	Cu2 Fe S2	
COD.900372[illegible]	Complete	F-43m	Cu2 Fe S2	Cu2 Fe S2	
COD.900006[illegible]	Complete	Pcmn	Cu Fe2 S3	Cu Fe2 S3	
COD.900820[illegible]	Complete	Pcmn	Cu Fe2 S3	Cu Fe2 S3	
COD.900410[illegible]	Complete	P-4m2	Cu6 Fe2 S8 Sn	Cu6 Fe2 S8 Sn	
COD.900820[illegible]	Complete	Pcmn	Cu Fe2 S3	Cu Fe2 S3	

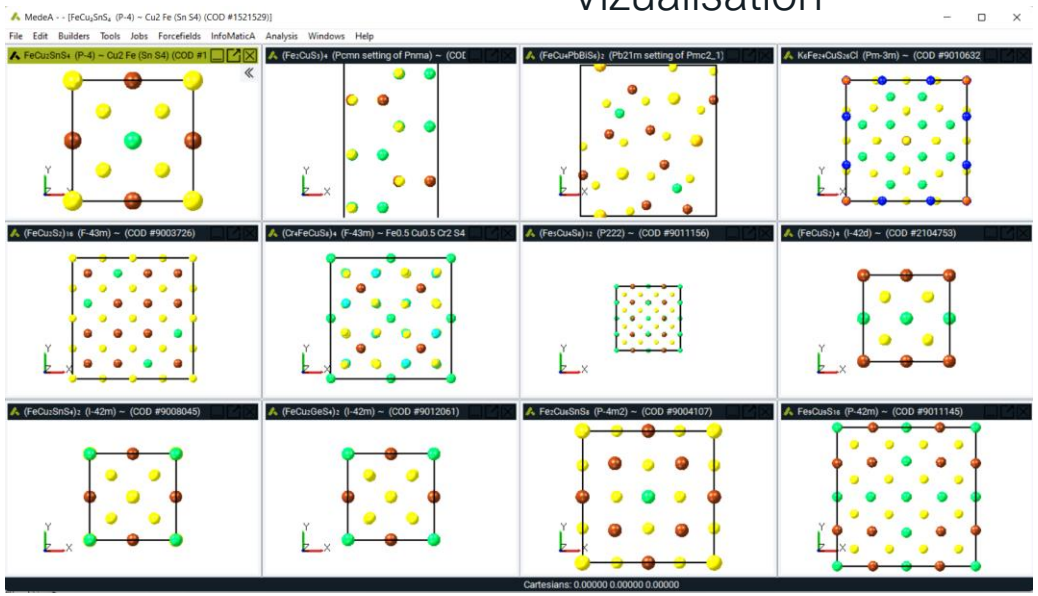
Search Criteria | Detailed Information | Coordinates | Geometry | Coordination | Pair Correlation | Powder pattern

Require that	formula	contains any number of	atoms of	Cu
Require that	formula	contains any number of	atoms of	Fe
Require that	formula	contains any number of	atoms of	S
Require that	formula	does not contain	atoms of	H
Require that	structural completeness	complete		
Require that	--Add new criterion--			

Run search | Clear

Displaying 29 of 29 hits

Vizualisation



Structure list

MedeA: structure list editor

File Add structure(s) Display Properties QT: QSAR Toolbox

SQLite structure list file (30720 bytes): C:/Users/BenoîtMinisini/OneDrive - Materials Design/Documents/etudes/molecules_of_interest/Compounds/chloro/structures/Cux
Containing 12 structure(s) and a total number of 12 configuration(s)

Display structures from: 1 to: 12 Apply

Structures | Properties

Order	Name	Structural Formula	# atoms	# configurations	Symmetry	Cell parameters
1	COD.9011145	Fe9Cu9S16	34	1	P-42m	10.585 10.585 5.383 90 90 90
2	COD.9004107	Fe2Cu6SnS8	17	1	P-4m2	7.603 7.603 5.358 90 90 90
3	COD.9012061	Fe2Cu4Ge2S8	16	1	I-42m	5.325 5.325 10.51 90 90 90
4	COD.9008045	Fe2Cu4Sn2S8	16	1	I-42m	5.46 5.46 10.725 90 90 90
5	COD.2104753	Fe4Cu4S8	16	1	I-42d	5.2888 5.2888 10.4221 90 90 90
6	COD.9011156	Fe60Cu48S96	204	1	P222	10.705 10.734 31.63 90 90 90
7	COD.1521718: Fe0.5 Cu0.5 Cr2 S4	Cr16Fe4Cu4S32	56	1	F-43m	9.90705 9.90705 9.90705 90 90 90
8	COD.9003726	Fe16Cu32S32	80	1	F-43m	10.71 10.71 10.71 90 90 90
9	COD.9010632	K6Fe24CuS26Cl	58	1	Pm-3m	10.385 10.385 10.385 90 90 90
10	COD.9011929	Fe2Cu8Pb2Bi2S12	26	1	Pb21m	10.88 12.003 3.874 90 90 90
11	COD.9001496	Fe8Cu4S12	24	1	Pcmn	6.455 11.102 6.226 90 90 90
12	COD.1521529: Cu2 Fe (Sn S4)	FeCu2SnS4	8	1	P-4	5.414 5.414 5.414 90 90 90

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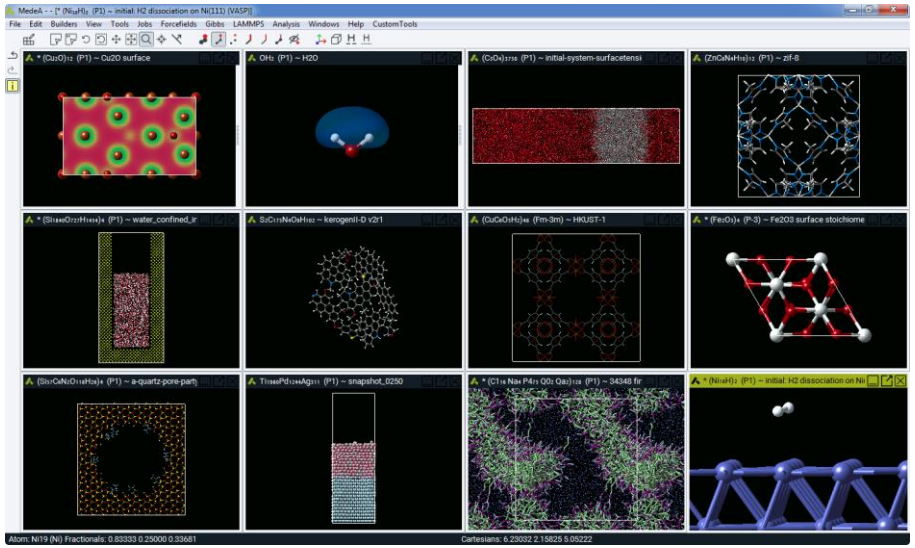
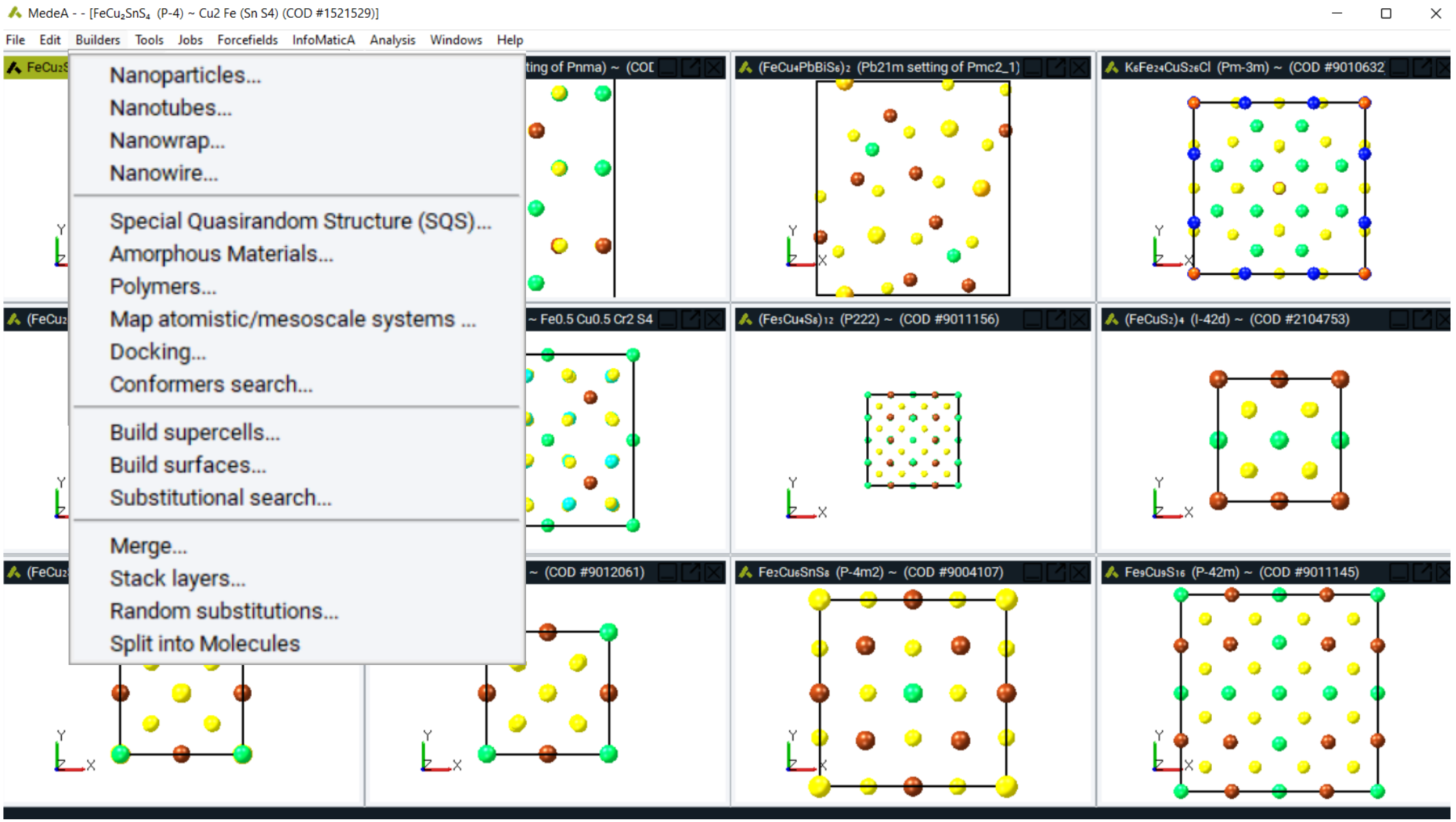
Automated processing of compute protocols & workflows; Reliable long-term archiving & accounting of computed data

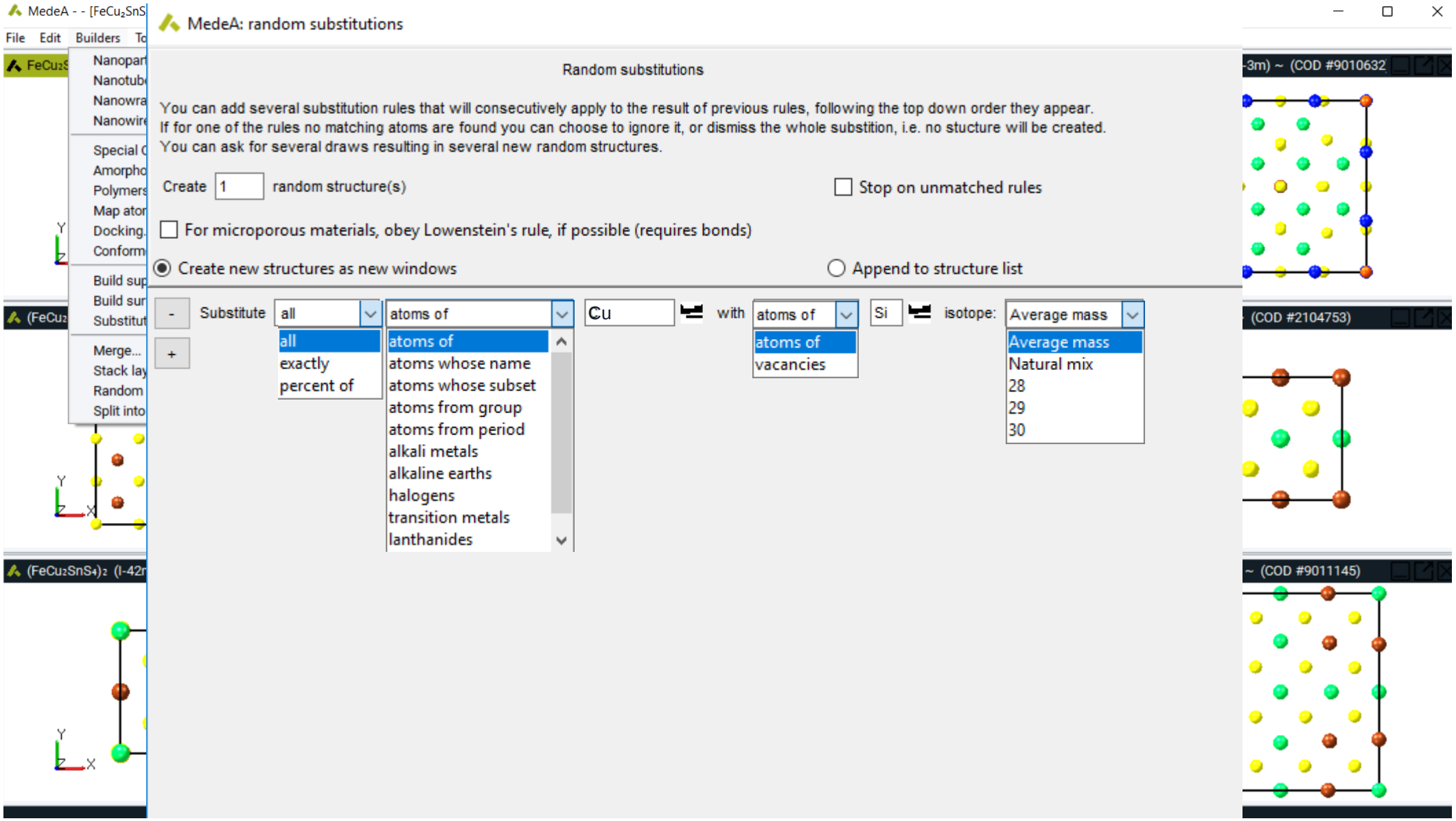
MedeA environment



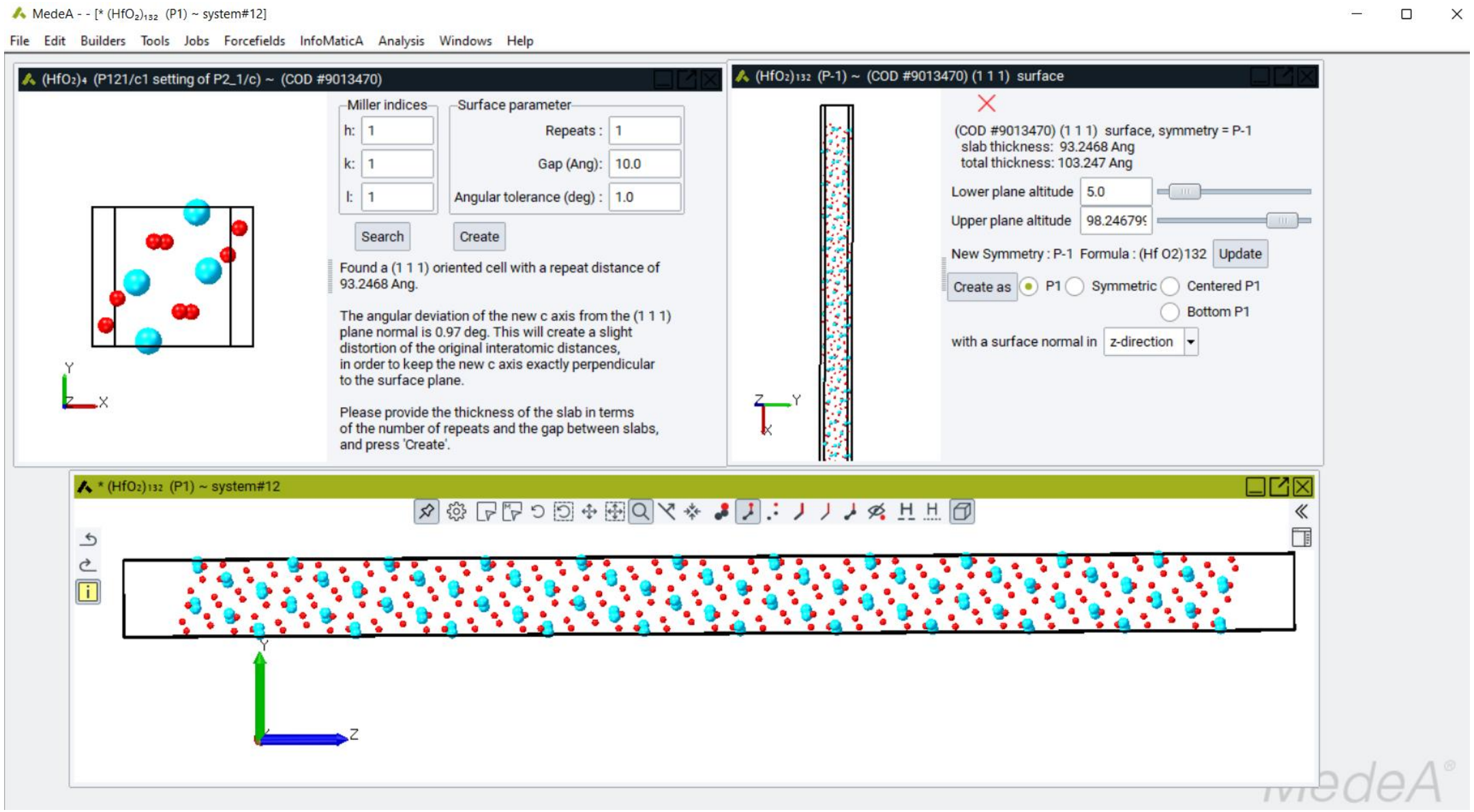
Builders


MedeA - - [FeCu2SnS4 (P-4) ~ Cu2 Fe (Sn S4) (COD #1521529)]
File
Edit
Builders
Tools
Jobs
Forcefields
InfoMaticA
Analysis
Windows
Help
Nanoparticles...
Nanotubes...
Nanowrap...
Nanowire...
Special Quasirandom Structure (SQS)...
Amorphous Materials...
Polymers...
Map atomistic/mesoscale systems ...
Docking...
Conformers search...
Build supercells...
Build surfaces...
Substitutional search...
Merge...
Stack layers...
Random substitutions...
Split into Molecules
(FeCu4PbBiS6)2 (Pb21m setting of Pmc2_1)
K6Fe24CuS26Cl (Pm-3m) ~ (COD #9010632
~ Fe0.5 Cu0.5 Cr2 S4
(Fe5Cu4S8)12 (P222) ~ (COD #9011156)
(FeCuS2)4 (I-42d) ~ (COD #2104753)
~ (COD #9012061)
Fe2Cu6SnS8 (P-4m2) ~ (COD #9004107)
Fe9Cu8S16 (P-42m) ~ (COD #9011145)

Random substitution

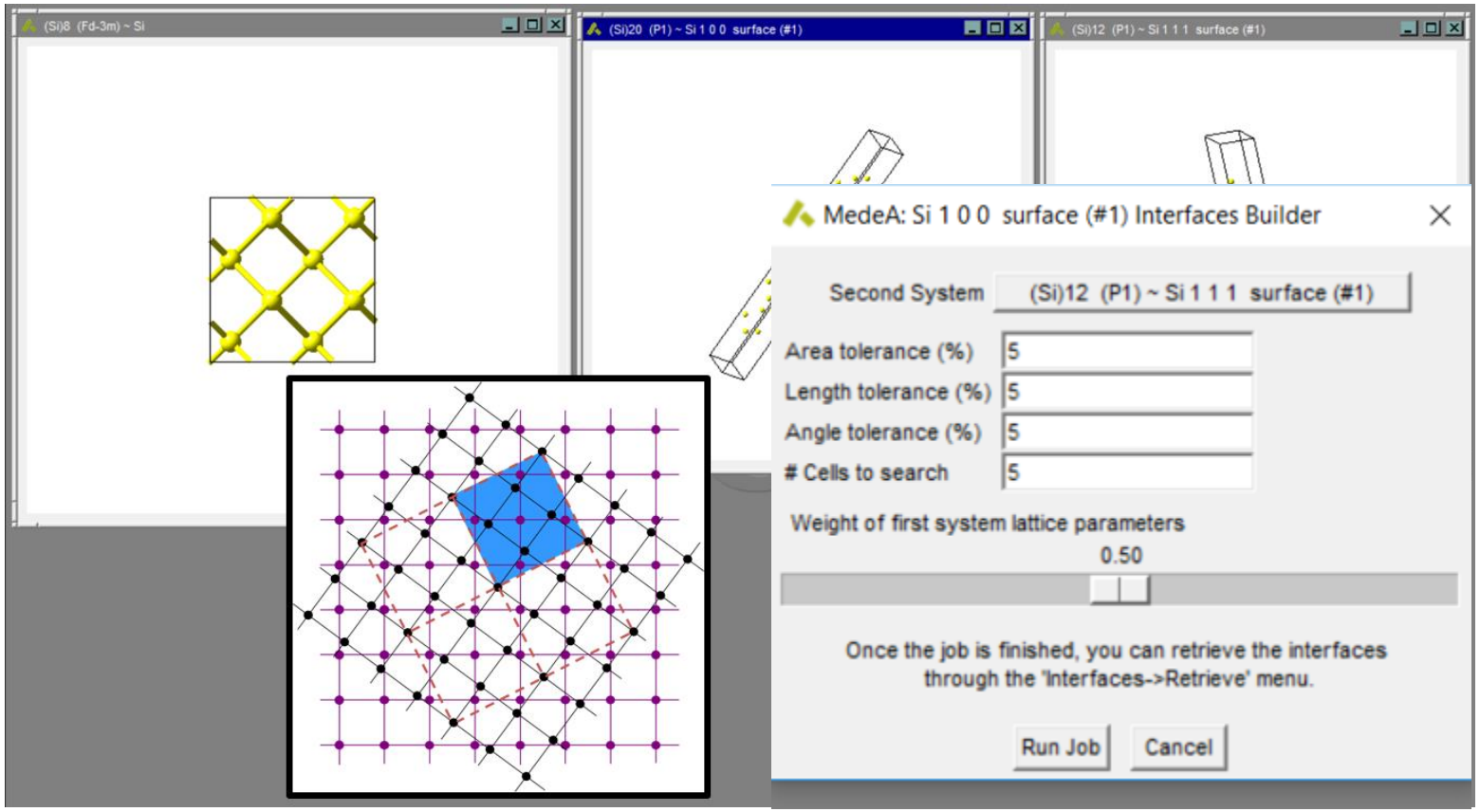


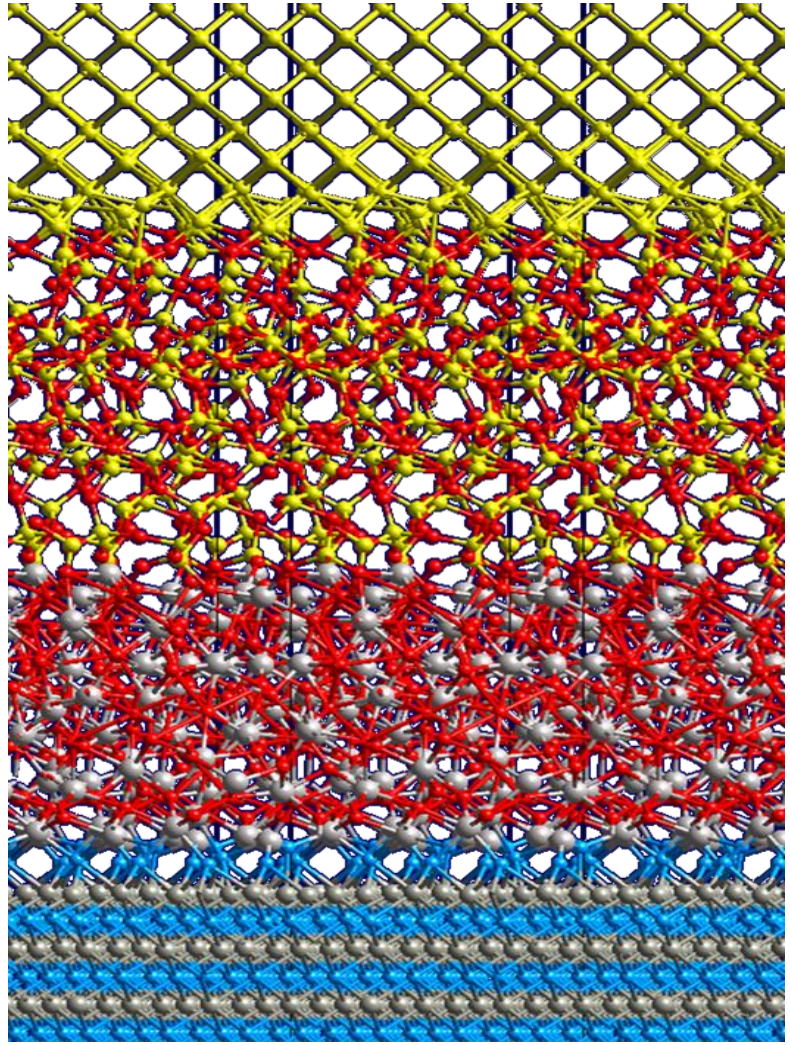
Surface



materials design

Interface builder





https://www.materialsdesign.com/datasheet/InterfaceBuilder

materials design

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

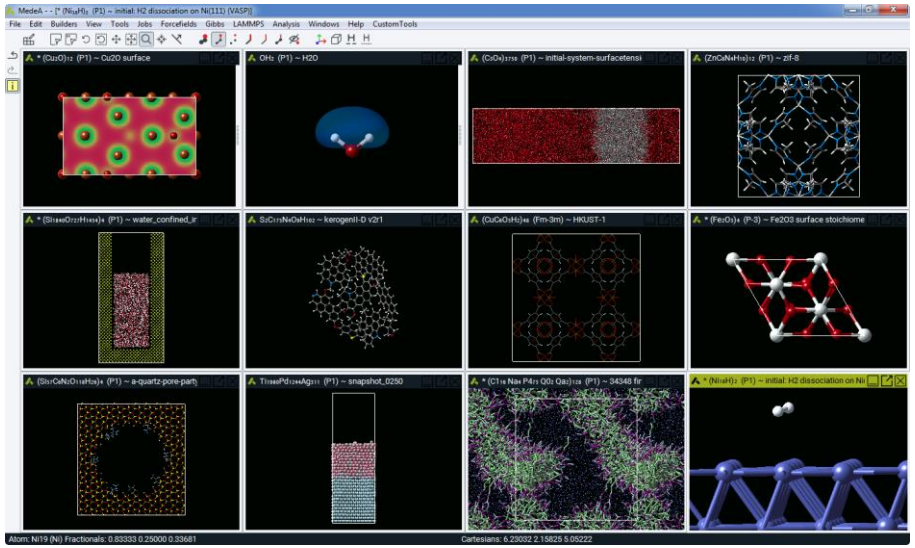
Analysis Tools

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

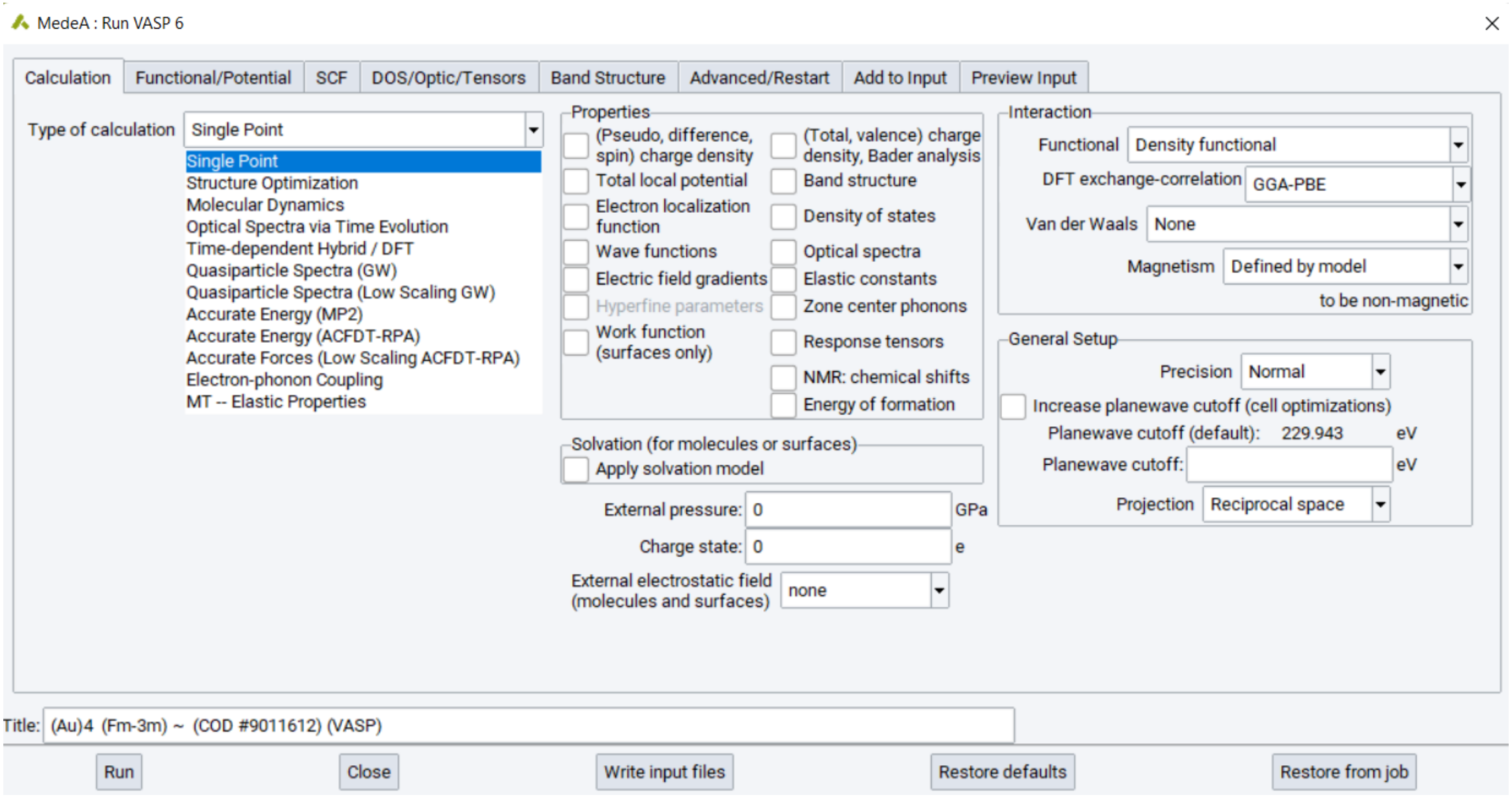
JobServer & TaskServer

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

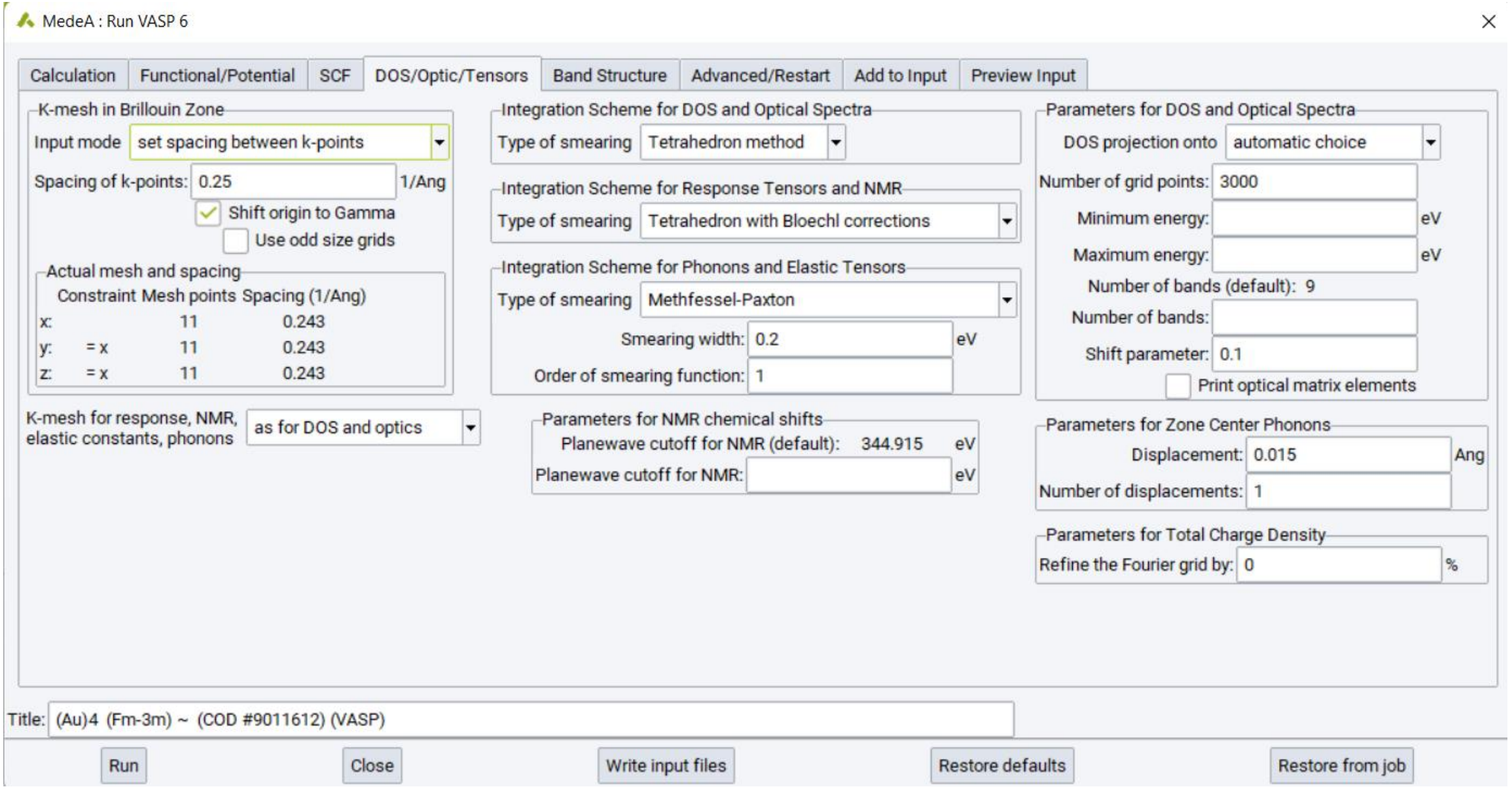
MedeA environment



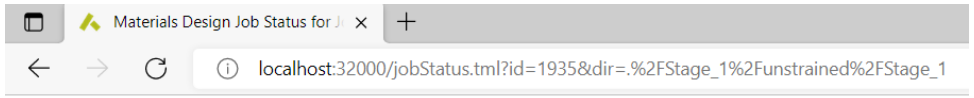
MedeA® VASP GUI



MedeA® VASP GUI



MedeA® VASP Output



- Trajectory

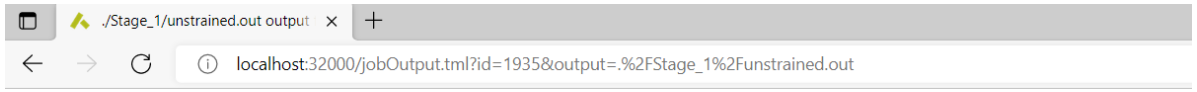
Available Output Files in ./Stage_1/unstrained/Stage_1

File	Size	Download
OSZICAR.out	1.1 kB	as plain text
OUTCAR.out	61.6 kB	as plain text
VASP.out	2.2 kB	as plain text

Other Files in ./Stage_1/unstrained/Stage_1 (caution: may be binary!)

File	Size	Download
CONTCAR	536 B	as plain text
EIGENVAL	12.0 kB	as plain text
IBZKPT	1.4 kB	as plain text
INCAR	584 B	as plain text
Job.xml	1.5 kB	as plain text
KPOINTS	51 B	as plain text
POSCAR	259 B	as plain text
POTCAR	451.7 kB	as plain text
PROCAR	57.2 kB	as plain text
XDATCAR	306 B	as plain text
initial.sci	1.5 kB	as plain text
minimized.sci	1.5 kB	as plain text
script	2.5 kB	as plain text
stdout	1.7 kB	as plain text

Follow this link for direct access to the directory, which is useful for downloading files




```
VASP 6 CALCULATION PROTOCOL:
============================
1. Geometry optimization (atom positions)


VASP parameters
===============
This is a calculation based on density functional theory and the GGA-PBE exchange-correlation functional for describing the interactions.

Since no magnetic moments are in the model, this is a non-magnetic calculation using 'normal' precision
and a default planewave cutoff energy of 295.446 eV.

The electronic iterations convergence is 1.00E-005 eV using the Normal (blocked Davidson) algorithm
and reciprocal space projection operators.

The requested k-spacing is 0.5 per Angstrom, which leads to a 5x5x4 mesh.
This corresponds to actual k-spacings of 0.449 x 0.449 x 0.428 per Angstrom.
The k-mesh is forced to be centered on the gamma point.

Using first order Methfessel-Paxton smearing with a width of 0.2 eV.
=========================================

Using version 4.0 GGA-PBE / PAW potentials:
        Au                  PAW_PBE Au 04Oct2007
        Cu                  PAW_PBE Cu 22Jun2005

There are 18 symmetry-unique k-points
The plane wave cutoff is 295.45 eV

   VASP energy:              -7.145475 eV for AuCu cell

   Initial VASP energy:      -7.145475 eV for AuCu cell
   Relaxation energy:         0.000000 eV gained after 1 optimization steps.

Electronic contributions:
                           Empirical Formula          Cell
                                   AuCu             AuCu
                           ----------------- -----------------
                VASP Energy          -7.145475       -7.145475 eV
                          =        -689.433        -689.433 kJ/mol

Cell parameters:
 Parameter    Value
---------- ------------
         a     2.800000
         b     2.800000
         c     3.670000
     alpha    90.000000
      beta    90.000000
     gamma    90.000000
```

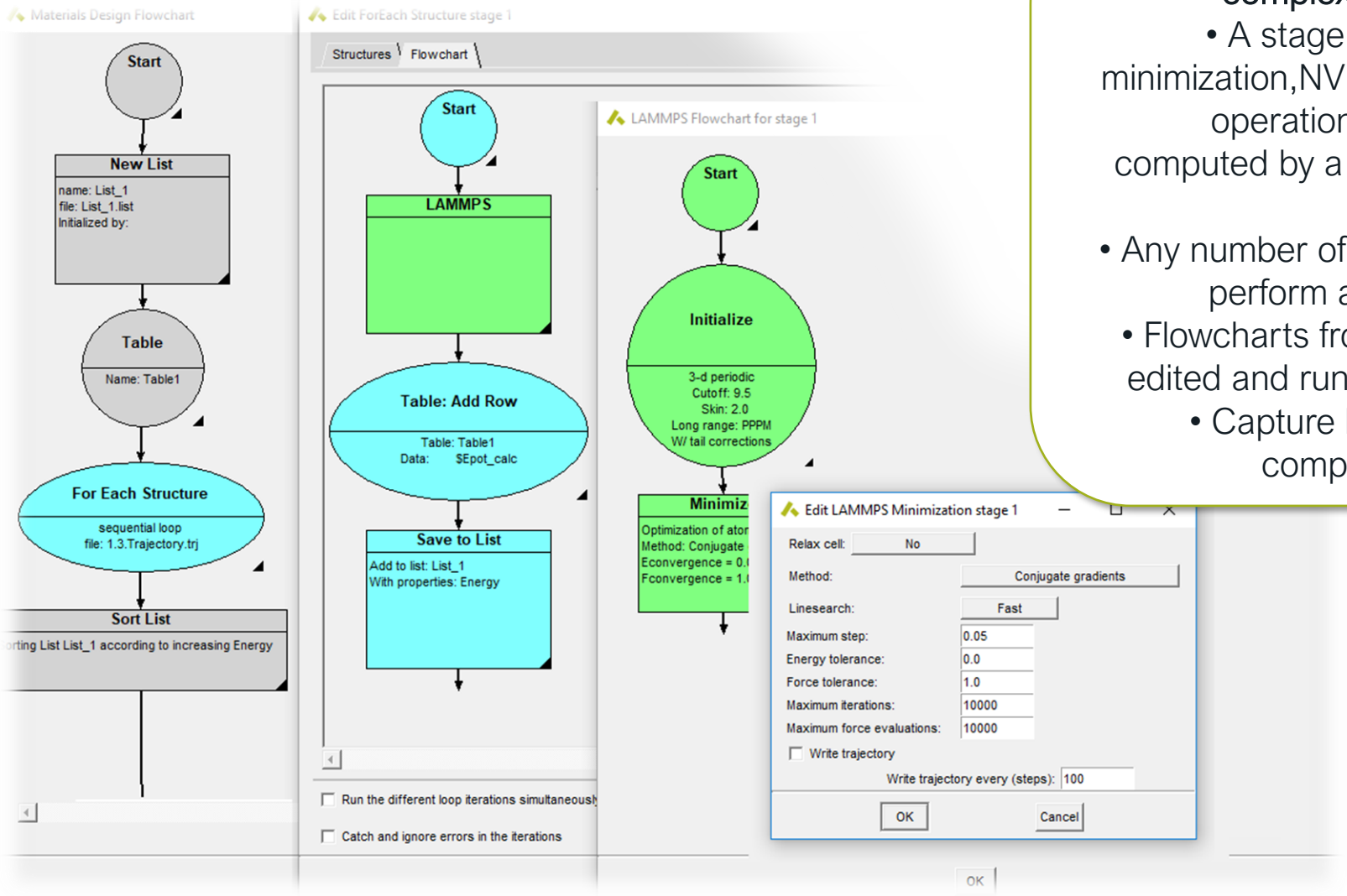
materials design

MedeA® VASP Ressources

- Tutorials:
  - Introduction to MedeA VASP: Learn how to set up and run VASP first principles calculations with MedeA
  - Introduction to MedeA MT: Elastic Properties of TaN: Learn how to calculate the mechanical properties of crystals with MedeA MT and MedeA VASP
  - Introduction to MedeA Phonon: Vibrational Properties of Silicon: Learn how to calculate the vibrational spectrum of silicon using MedeA Phonon with VASP and LAMMPS
  - Introduction to MedeA UNCLE: Cluster expansion calculation of Au/Cu alloy: Learn how to set up cluster expansion calculations with MedeA UNCLE for Au/Cu alloy
  - Introduction to MedeA FFO: Optimizing Buckingham Forcefield for LiNbO3: Learn how to optimize a Buckingham forcefield for LiNbO3 with MedeA Forcefield Optimizer
  - Thermoelectrics: Seebeck Coefficient of Bismuth Chalcogenides: This tutorial describes how to calculate the Seebeck coefficient of the material Bi2Te3 with MedeA Electronics and MedeA VASP
  - Calculate the Color of Cadmium Selenide and Cadmium Sulfide: Learn how to calculate the optical properties, such as color, of materials using an ab initio approach with MedeA VASP
  - Electron-Phonon Coupling: Phonon Induced Change of the GaAs Band Gap as a Function of Temperature: Learn how to use the single displacement approach by Zacharias and Giustino to calculate the phonon-induced temperature-dependent change of the GaAs band gap with MedeA VASP 6
  - Obtain Accurate Heat of Formation for SiC with ACFDT RPA: Learn how to calculate the heat of formation of silicon carbide using ACFDT RPA with MedeA VASP 6
  - Thermal Expansion of ZnO: Learn how to calculate the thermal expansion of materials with MedeA
- Webinars:
  - VASP in MedeA: A Fast Way- From Models to Reliable Results: http://my.materialsdesign.com/webinar-31
  - The Color of Materials: Value from Computed Optical Properties: http://my.materialsdesign.com/webinar-25
  - Atomistic Simulations as a Driver of Industrial Innovation: http://my.materialsdesign.com/webinar-18
  - Predicting Elastic Properties Using Ab Initio and Forcefield Based Simulations: http://my.materialsdesign.com/webinar-15

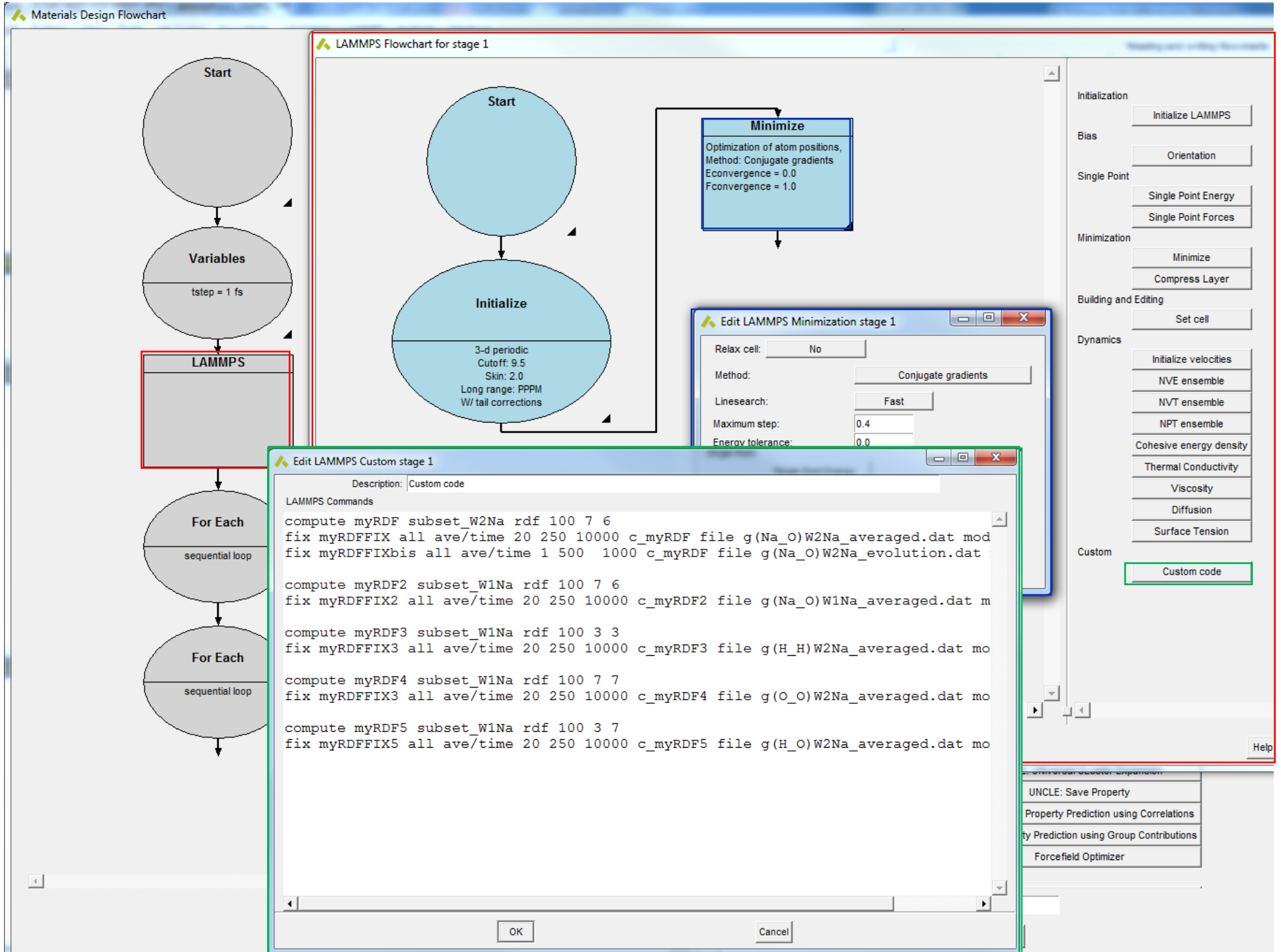
and more..

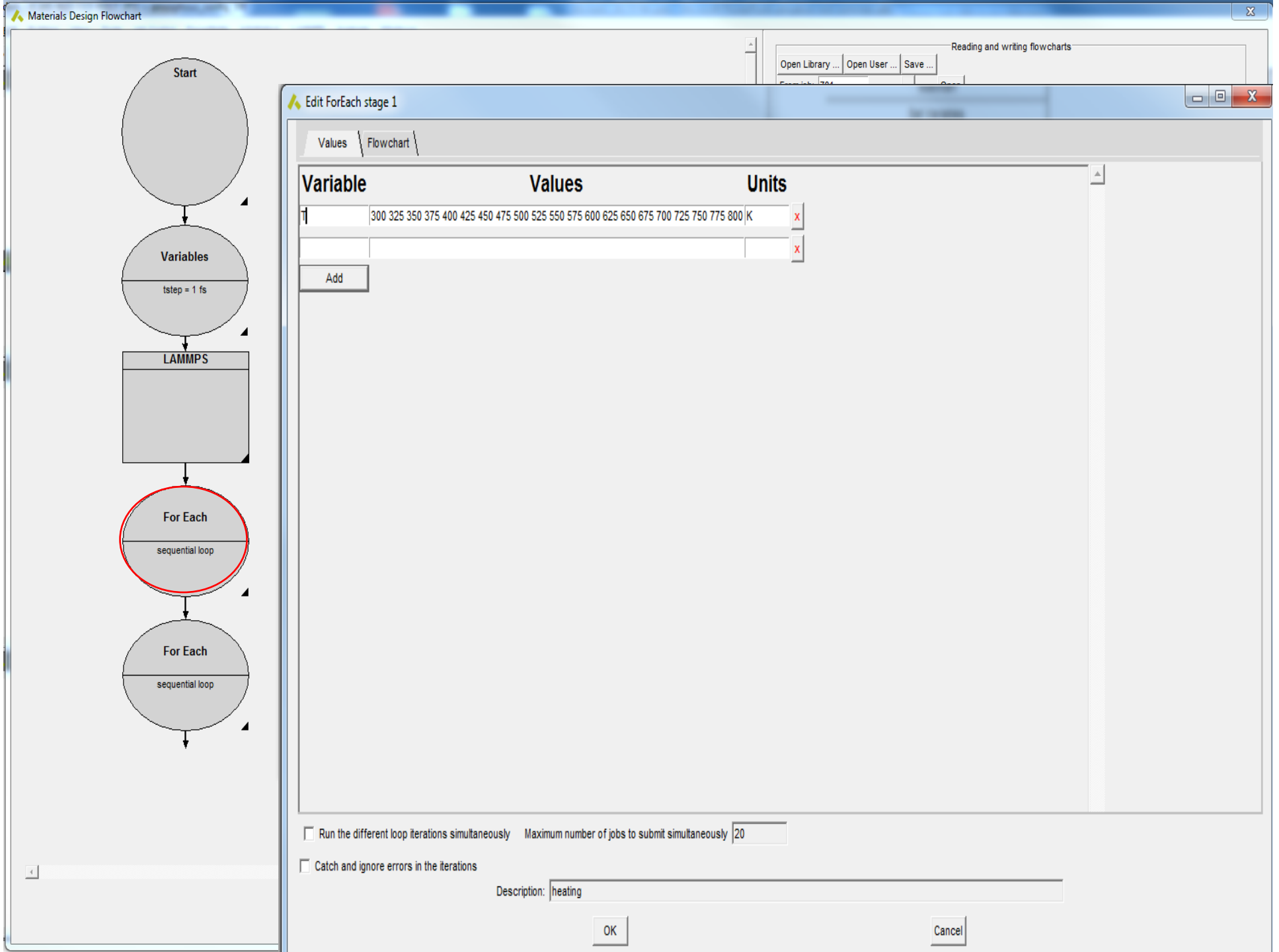
LAMMPS GUI and Flowcharts

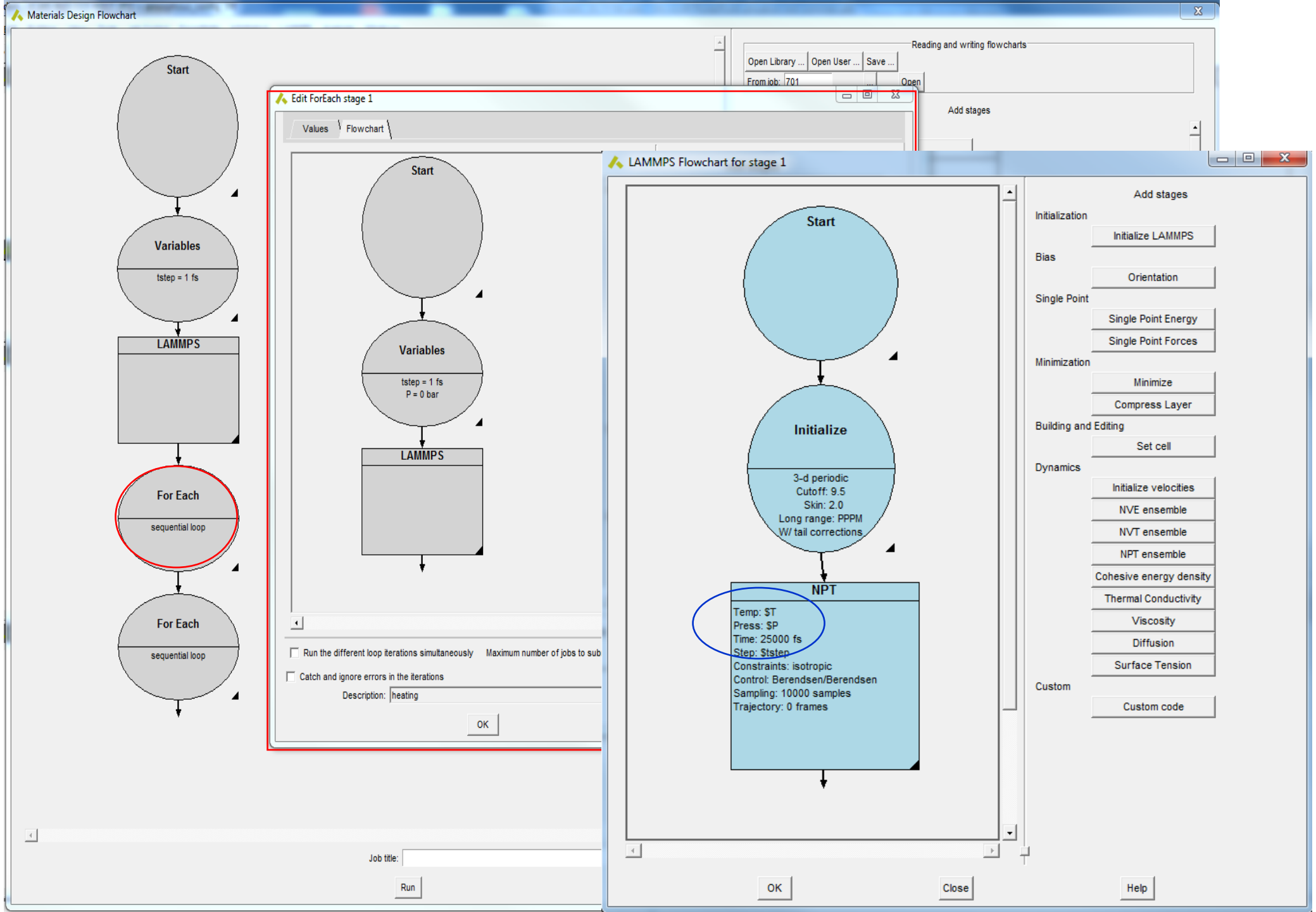


- Powerful flowchart interface lets you easily set up complex calculations by connecting stages
- A stage can be a computation, e.g. energy minimization,NVT and NPT dynamics, as well as an operation such as setting the density to that computed by a previous stage, or building a larger simulation box
- Any number of stages can be chained together to perform a detailed, reproducible calculation.
- Flowcharts from any previous calculation can be edited and run again, even on different molecules
- Capture best practices, and share validated computational strategies with colleagues

Custom Stage available for LAMMPS advances users


Materials Design Flowchart
Start
Variables
tstep = 1 fs
LAMMPS
For Each
sequential loop
For Each
sequential loop
LAMMPS Flowchart for stage 1
Start
Initialize
3-d periodic
Cutoff: 9.5
Skin: 2.0
Long range: PPPM
W/ tail corrections
Minimize
Optimization of atom positions,
Method: Conjugate gradients
Econvergence = 0.0
Fconvergence = 1.0
Edit LAMMPS Minimization stage 1
Relax cell: No
Method: Conjugate gradients
Linesearch: Fast
Maximum step: 0.4
Energy tolerance: 0.0
Edit LAMMPS Custom stage 1
Description: Custom code
LAMMPS Commands
compute myRDF subset_W2Na rdf 100 7 6
fix myRDFFIX all ave/time 20 250 10000 c_myRDF file g(Na_O)W2Na_averaged.dat mod
fix myRDFFIXbis all ave/time 1 500 1000 c_myRDF file g(Na_O)W2Na_evolution.dat
compute myRDF2 subset_W1Na rdf 100 7 6
fix myRDFFIX2 all ave/time 20 250 10000 c_myRDF2 file g(Na_O)W1Na_averaged.dat m
compute myRDF3 subset_W1Na rdf 100 3 3
fix myRDFFIX3 all ave/time 20 250 10000 c_myRDF3 file g(H_H)W2Na_averaged.dat mo
compute myRDF4 subset_W1Na rdf 100 7 7
fix myRDFFIX3 all ave/time 20 250 10000 c_myRDF4 file g(O_O)W2Na_averaged.dat mo
compute myRDF5 subset_W1Na rdf 100 3 7
fix myRDFFIX5 all ave/time 20 250 10000 c_myRDF5 file g(H_O)W2Na_averaged.dat mo
OK
Cancel
Initialization
Initialize LAMMPS
Bias
Orientation
Single Point
Single Point Energy
Single Point Forces
Minimization
Minimize
Compress Layer
Building and Editing
Set cell
Dynamics
Initialize velocities
NVE ensemble
NVT ensemble
NPT ensemble
Cohesive energy density
Thermal Conductivity
Viscosity
Diffusion
Surface Tension
Custom
Custom code
Help
UNCLE: Save Property
Property Prediction using Correlations
ty Prediction using Group Contributions
Forcefield Optimizer


Materials Design Flowchart
Start
Variables
tstep = 1 fs
LAMMPS
For Each
sequential loop
For Each
sequential loop
Reading and writing flowcharts
Open Library ...
Open User ...
Save ...
Edit ForEach stage 1
Values
Flowchart
Variable
Values
Units
T
300 325 350 375 400 425 450 475 500 525 550 575 600 625 650 675 700 725 750 775 800
K
Add
Run the different loop iterations simultaneously
Maximum number of jobs to submit simultaneously
20
Catch and ignore errors in the iterations
Description:
heating
OK
Cancel

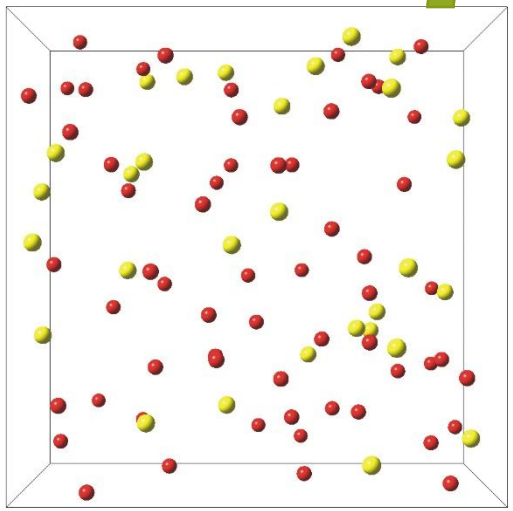

Materials Design Flowchart
Start
Variables
tstep = 1 fs
LAMMPS
For Each
sequential loop
For Each
sequential loop
Reading and writing flowcharts
Open Library ...
Open User ...
Save ...
From job: 701
Open
Add stages
Edit ForEach stage 1
Values
Flowchart
Start
Variables
tstep = 1 fs
P = 0 bar
LAMMPS
Run the different loop iterations simultaneously
Maximum number of jobs to sub
Catch and ignore errors in the iterations
Description: heating
OK
LAMMPS Flowchart for stage 1
Start
Initialize
3-d periodic
Cutoff: 9.5
Skin: 2.0
Long range: PPPM
W/ tail corrections
NPT
Temp: $T
Press: $P
Time: 25000 fs
Step: $tstep
Constraints: isotropic
Control: Berendsen/Berendsen
Sampling: 10000 samples
Trajectory: 0 frames
Add stages
Initialization
Initialize LAMMPS
Bias
Orientation
Single Point
Single Point Energy
Single Point Forces
Minimization
Minimize
Compress Layer
Building and Editing
Set cell
Dynamics
Initialize velocities
NVE ensemble
NVT ensemble
NPT ensemble
Cohesive energy density
Thermal Conductivity
Viscosity
Diffusion
Surface Tension
Custom
Custom code
Job title:
Run
OK
Close
Help

MedeA® LAMMPS Ressources

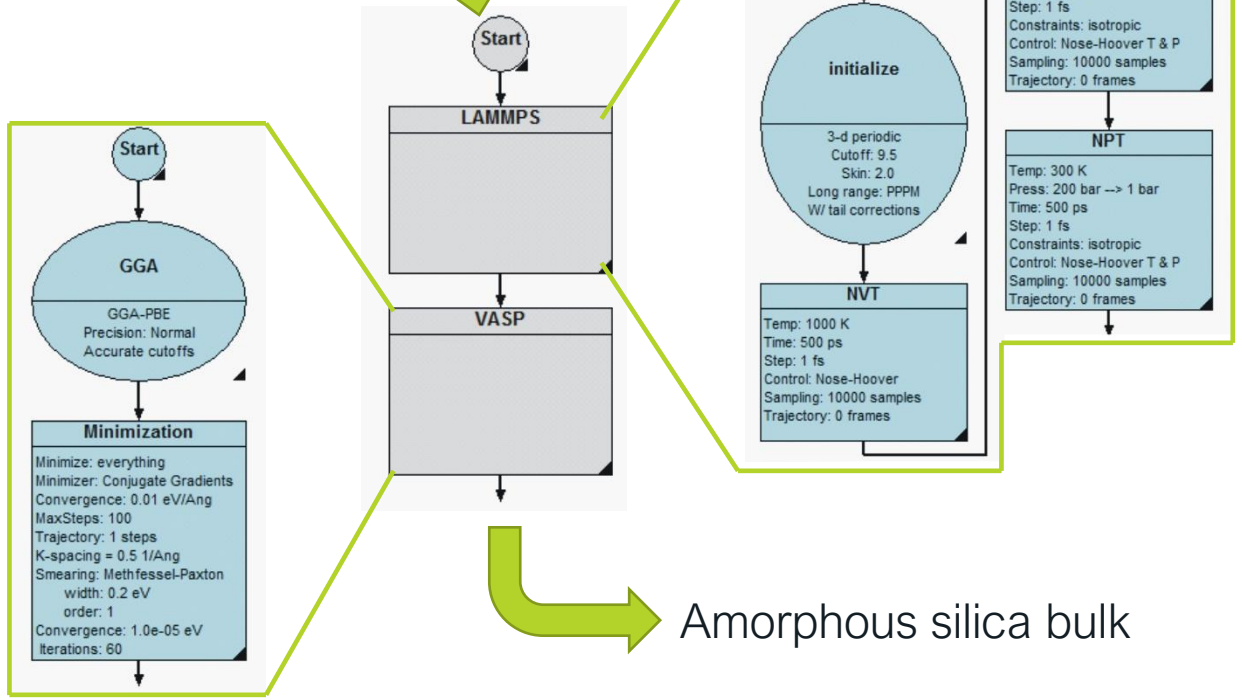
- Tutorials:
  - Introduction to MedeA LAMMPS: Learn how to set up and run LAMMPS molecular dynamics simulations with MedeA
  - Importing External Potential Parameters into MedeA: Learn how to import external potential parameters and files into MedeA
  - Deposition of O2 on a Si Surface with Reactive 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

Interoperability

1. Create 30(Si O2) cell at low density with Amorphous Builder – Forcefield is cvff_aug



2. NVT dynamic annealing with LAMMPS followed by NPT equilibration and VASP geometry optimization



Amorphous silica bulk

and repeat the procedure

materials design

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…

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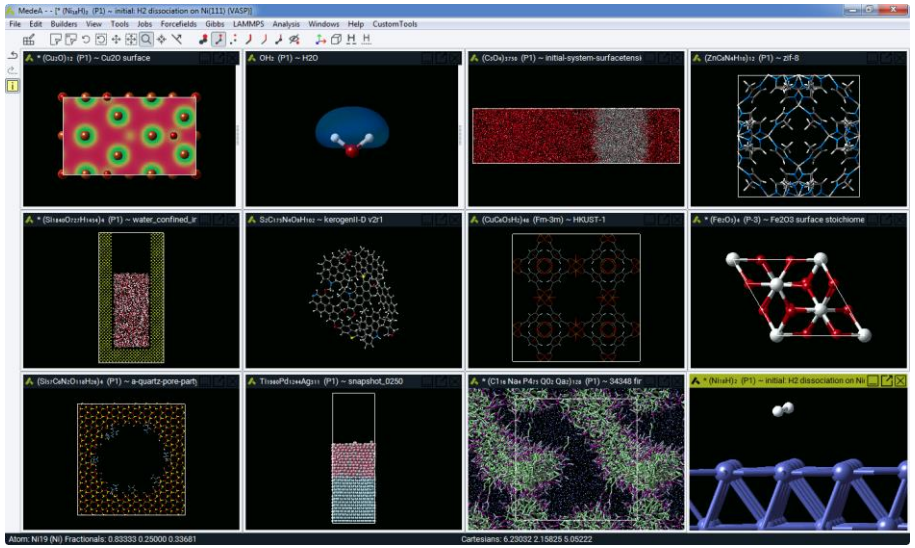
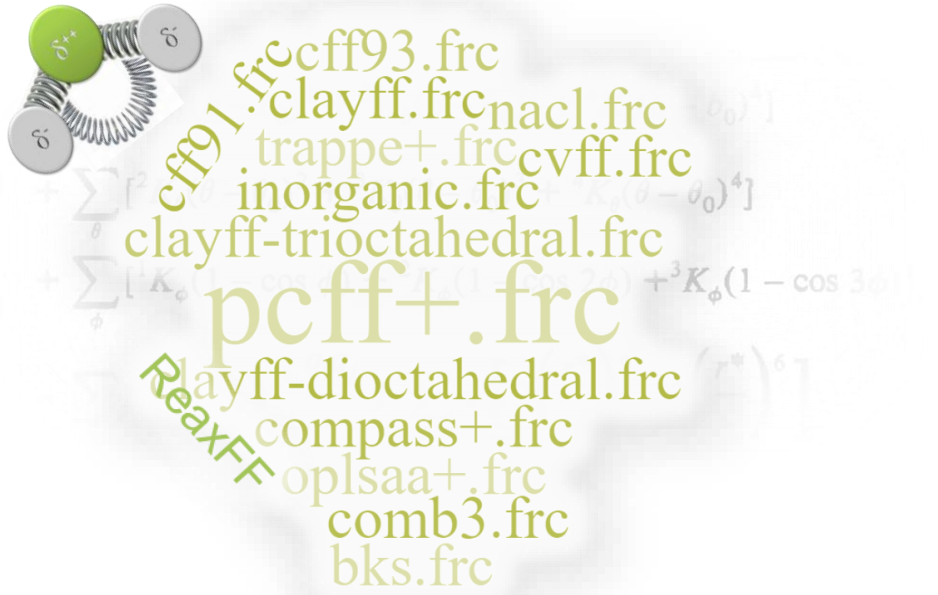
MedeA environment



Potentials - Forcefields

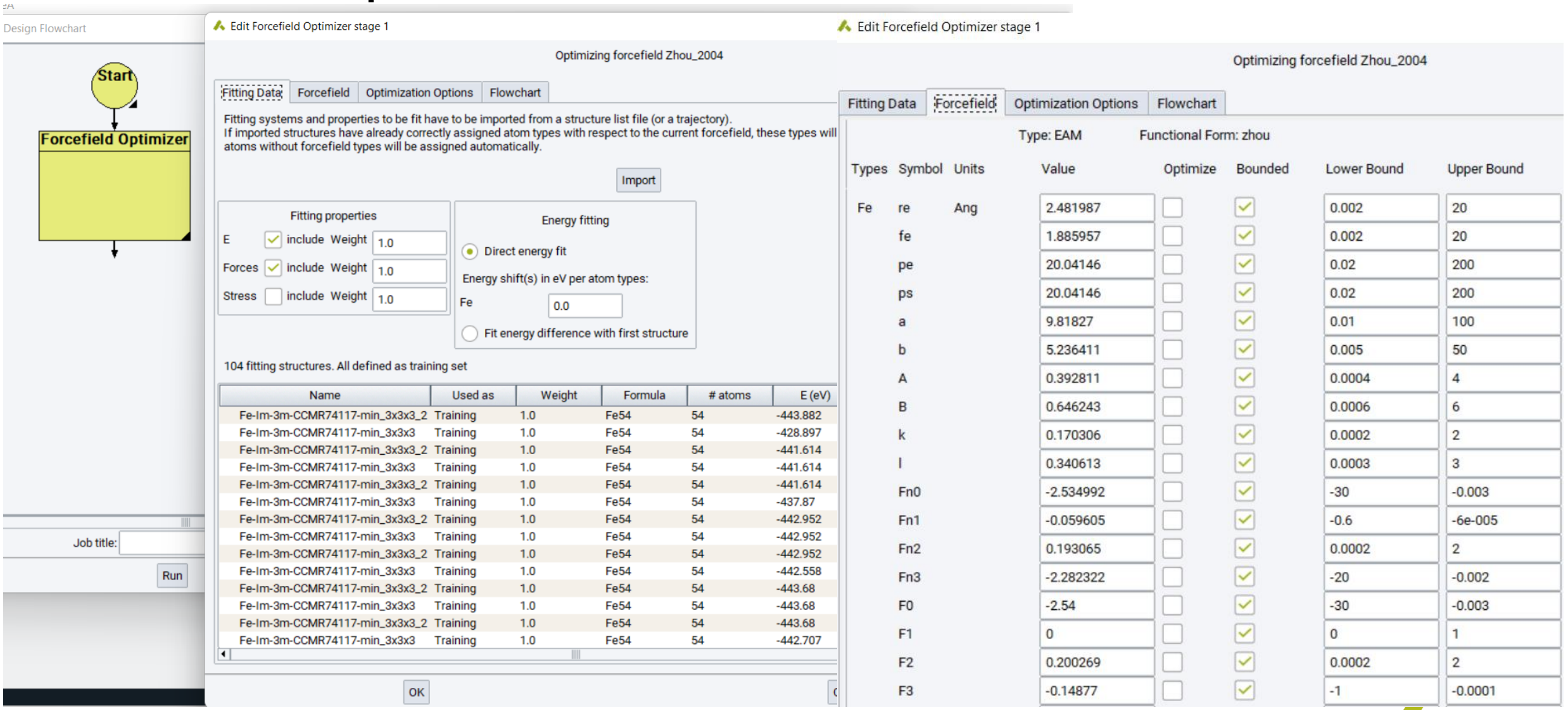


- Metallic forcefields:
  - EAM
    - All LAMMPS eam, eam/fs…
  - MEAM
- Inorganic forcefields:
  - Buckingham
  - BKS
  - Clay-FF
  - CVFF_aug
- Semiconductor forcefields:
  - Tersoff
  - Stillinger-Weber
- Organic (valence) forcefields:
  - PCFF/PCFF+*
  - Compass/Compass+
  - OPLS-AA/OPLS-AA+*
  - AUA/AUA+ *
  - Trappe+ *
- Reactive forcefields
  - COMB3
  - ReaxFF
- Mesoscale
  - Martini
  - Shinoda

- Increased simulation coverage and accuracy from the state of art forcefields for molecular dynamics and Monte Carlo
- **Automatic assignment of atom types and charges**
- **Customizable forcefields**: safely add and change parameters when needed, changes are kept separate and not overwritten by updates; version tracking to keep all modifications accessible for evaluation and comparison
- Materials Design's experts provide industrial level support of forcefields shipped
- The complexities of developing and tuning forcefields requires a reliable and powerful computing platform. MedeA's architecture with the JobServer/TaskServer is the right environment to get things done.

materials design

Forcefield Optimizer

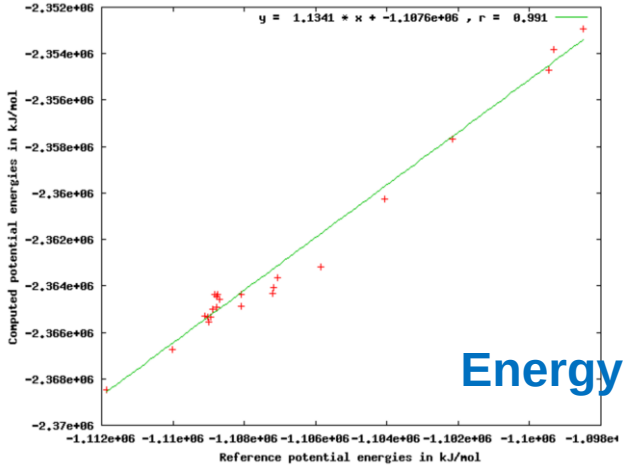


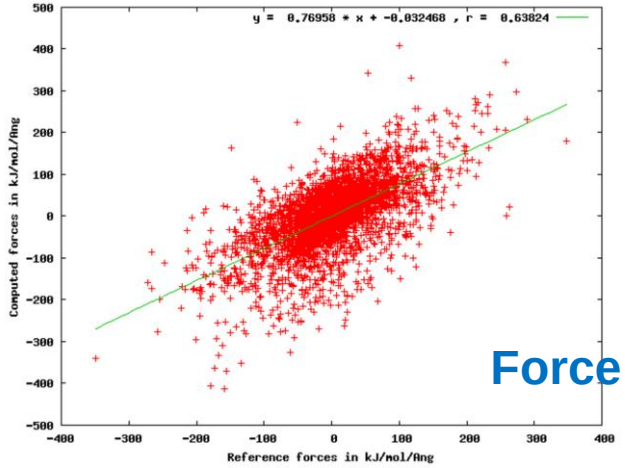
materials design

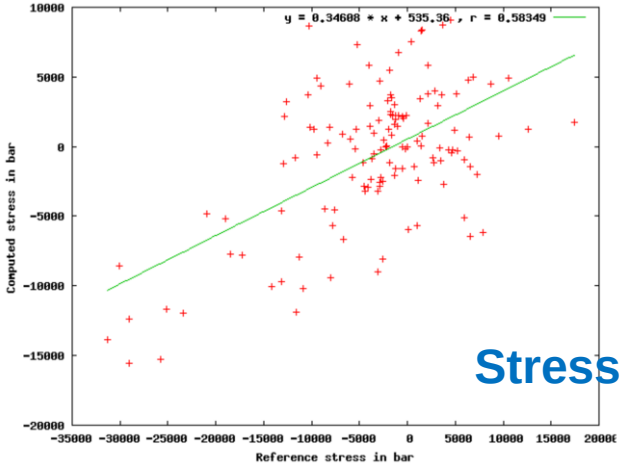
Forcefield Optimizer

- Examine fitting output graphs

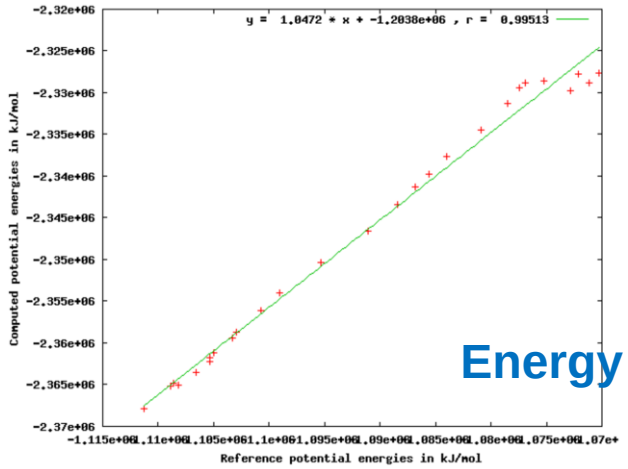
Training

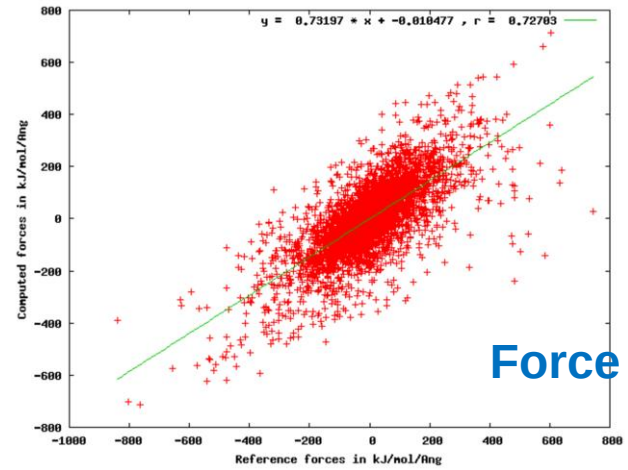


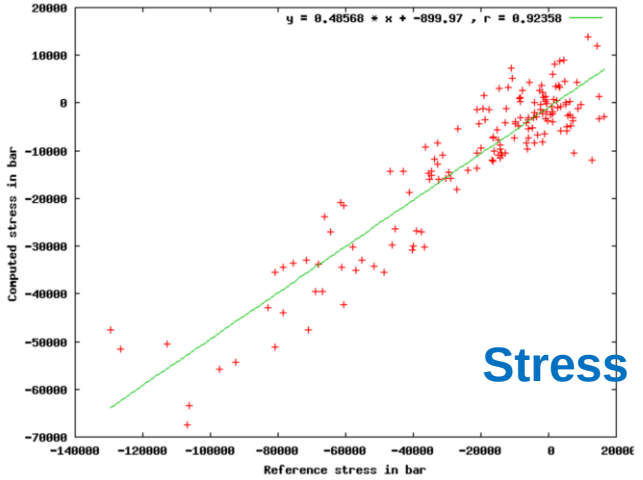




Validation







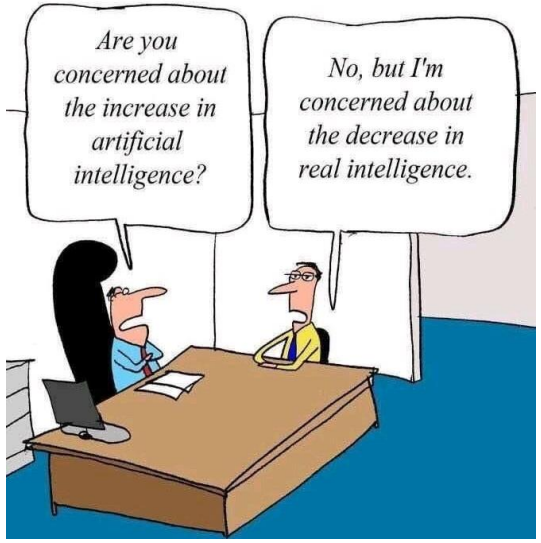
materials design

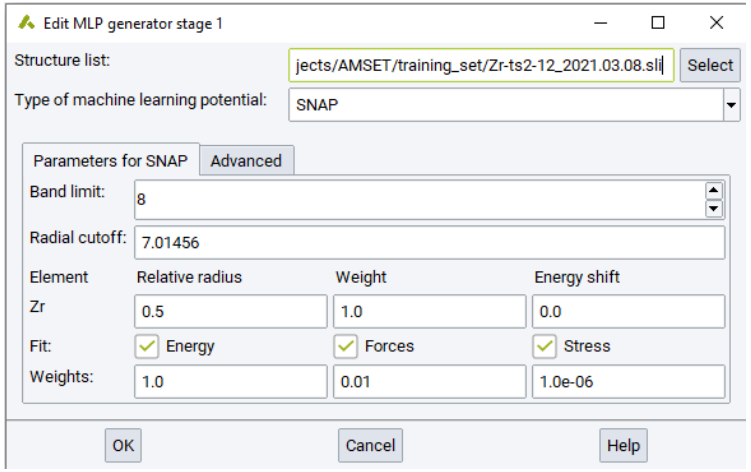
Machine Learning Potential

Build a model

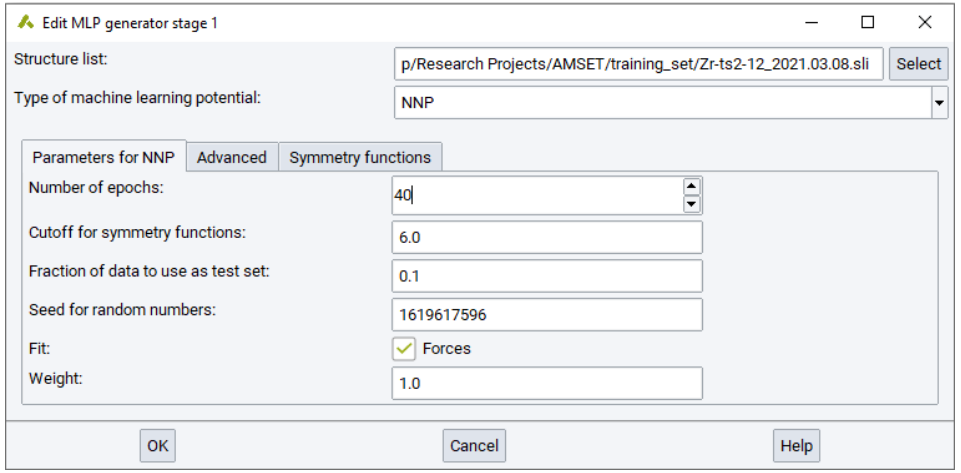
Use VASP to run an ab initio MD simulation

Use the MD trajectory to train a SNAP MLP





- Spectral Neighbor Analysis Potential (SNAP)



- Neural Network Potential (NNP)

materials design

Databases

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

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

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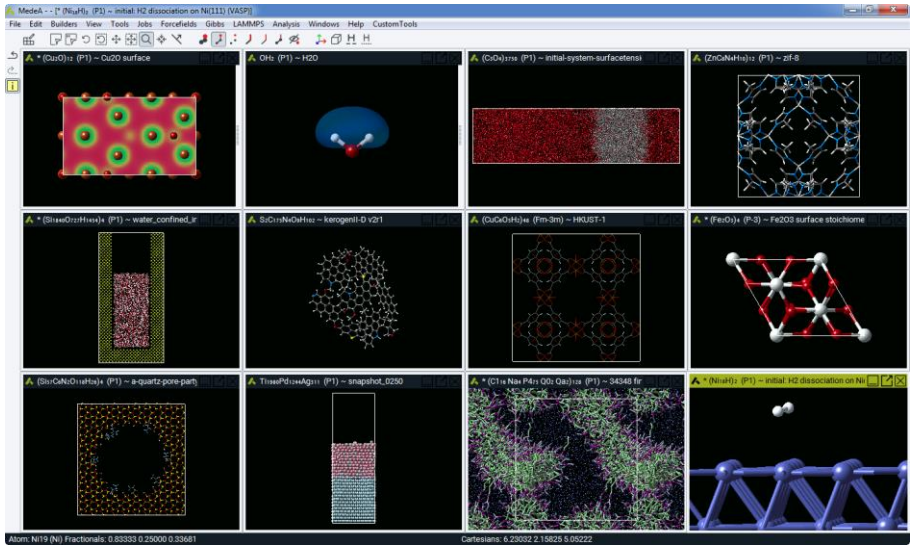
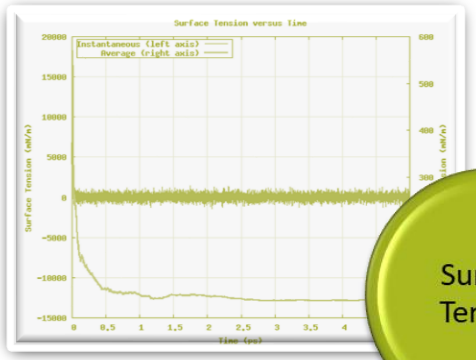
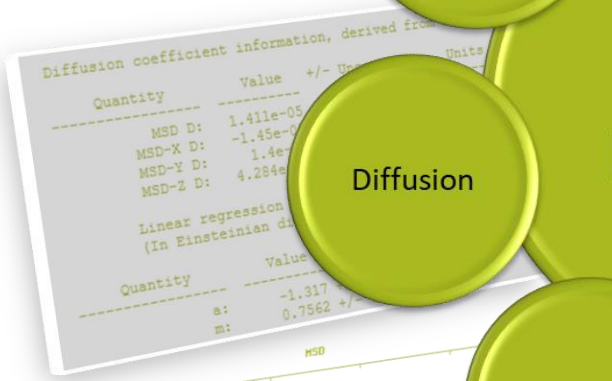


Properties Modules





Cohesive energy density

Surface Tension

Mechanical properties

MedeA®

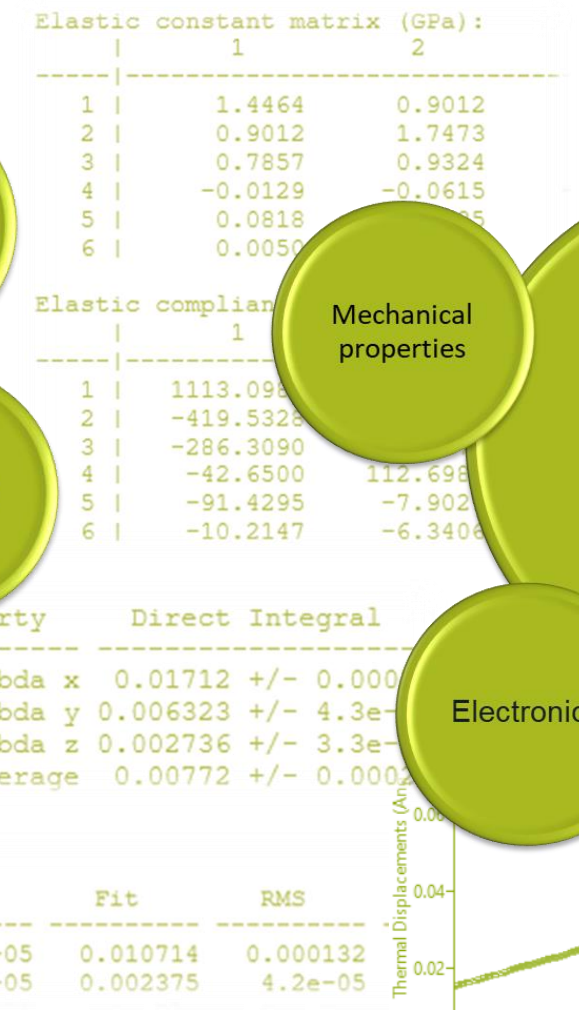
LAMMPS

Diffusion

Hill Wallpole bounds

Viscosity

Thermal conductivity



Automated convergence

Mechanical properties

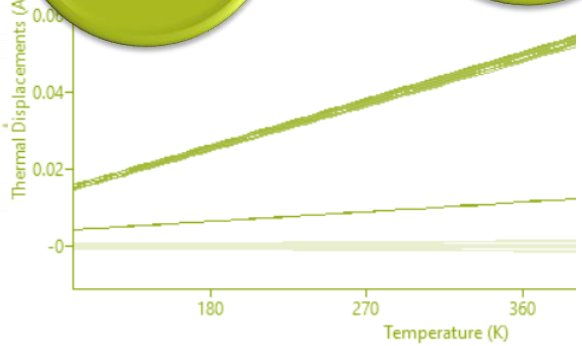
MedeA®

VASP

Phonon

Electronics

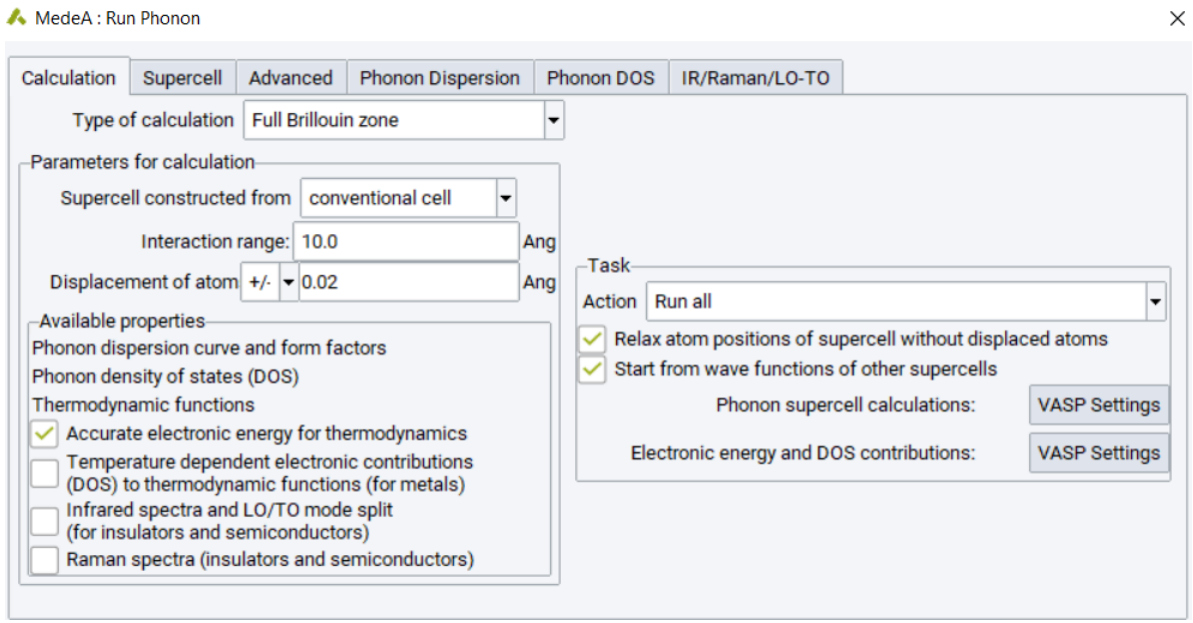
TSS

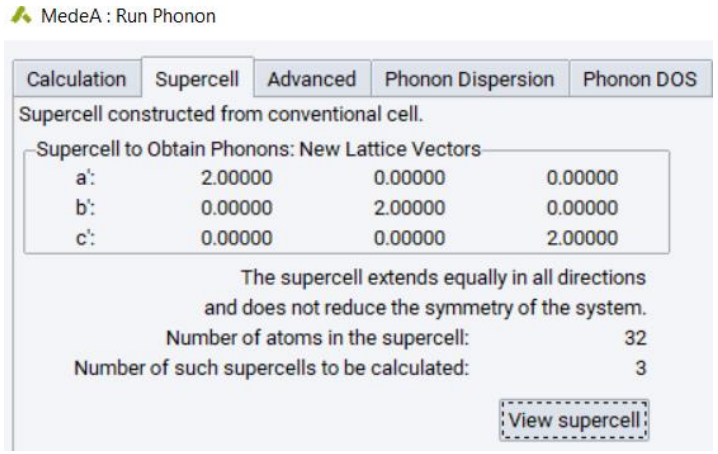


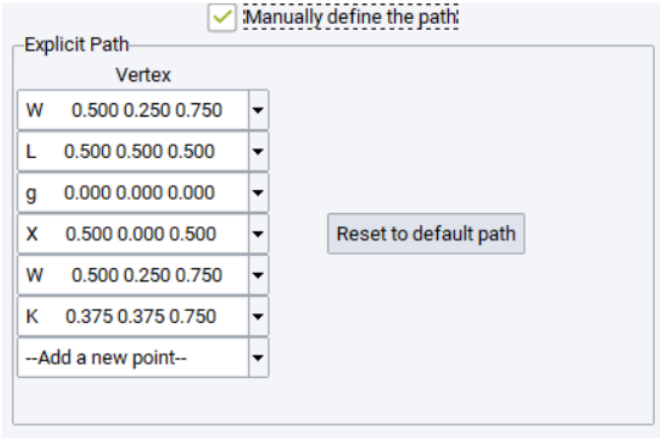
materials design

Phonon Module

- MedeA Phonon is based on the PHONON program authored by Prof. Krzysztof Parlinski2,3
- Automatic detection and use of the space-group symmetry of the phase
- Fully automatic determination of supercell and the necessary atomic displacements
- Fully automated setup, execution, and processing of VASP jobs
- Uses forces computed with VASP, MOPAC, and LAMMPS.
- The use of Phonons with VASP includes the ability to utilize GGA+U, meta-GGA, van der Waals, hybrid functionals, spin-polarization, and fully relativistic Hamiltonians
- Partial freezing of atoms possible.
- Applicable to transition state geometries
- Restart capabilities in case of hardware or communication failures.







materials design

Phonon module

Available Results

- PhononDensityOfStates
- PhononDispersion
- ThermodynamicFunctions

Available Output Files

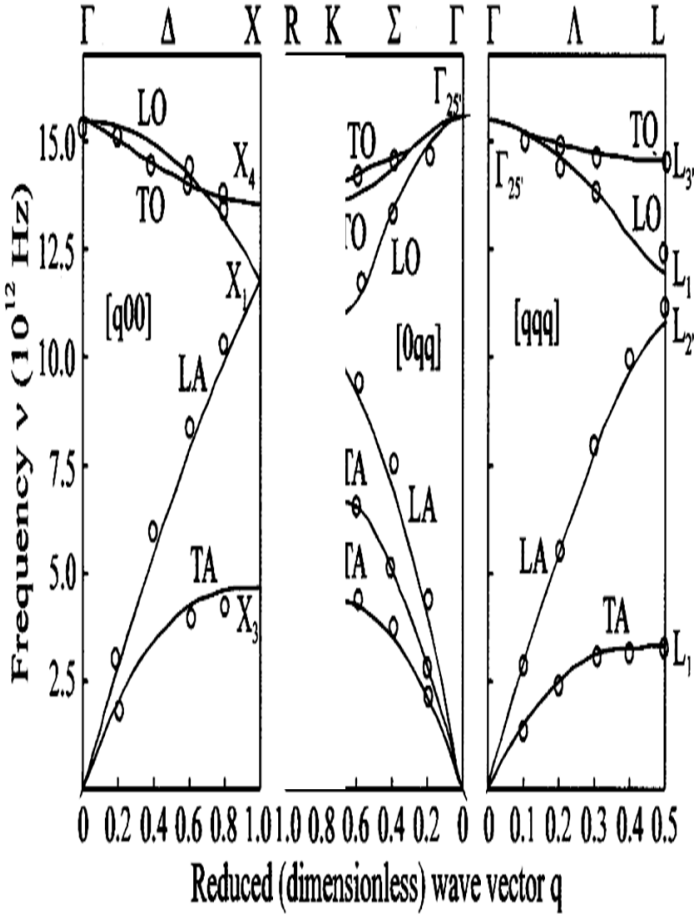
File	Size	Download
Job.out	23.2 kB	as plain text
OSZICAR.out	1.1 kB	as plain text
OUTCAR.out	84.3 kB	as plain text
VASP.out	1.6 kB	as plain text
displaced_Mg_a OSZICAR.out	1.1 kB	as plain text
displaced_Mg_a OUTCAR.out	111.6 kB	as plain text
displaced_Mg_a VASP.out	1.9 kB	as plain text
displaced_Mg_b OSZICAR.out	1.1 kB	as plain text
displaced_Mg_b OUTCAR.out	113.5 kB	as plain text
displaced_Mg_b VASP.out	2.0 kB	as plain text
displaced_O_a OSZICAR.out	1.3 kB	as plain text
displaced_O_a OUTCAR.out	117.3 kB	as plain text
displaced_O_a VASP.out	2.2 kB	as plain text
displaced_O_b OSZICAR.out	1.3 kB	as plain text
displaced_O_b OUTCAR.out	117.3 kB	as plain text
displaced_O_b VASP.out	2.2 kB	as plain text
undisplaced OSZICAR.out	1.4 kB	as plain text
undisplaced OUTCAR.out	110.0 kB	as plain text
undisplaced VASP.out	2.2 kB	as plain text

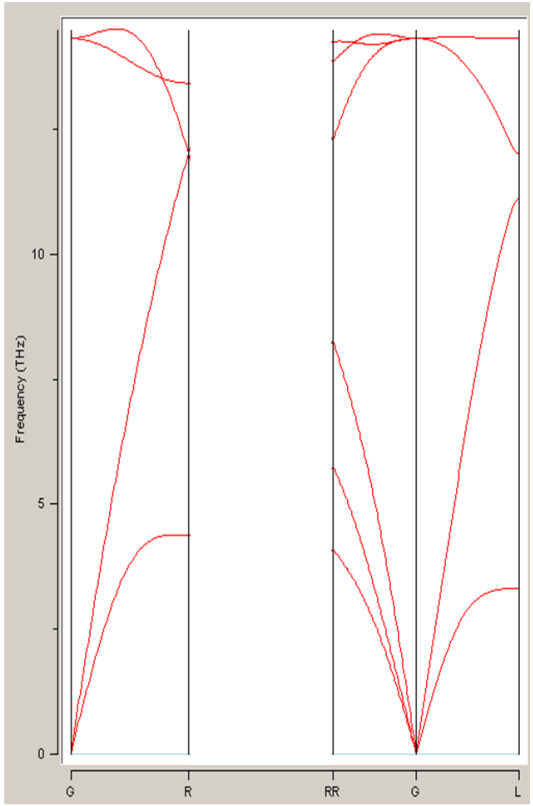
phonon0.HFF	20.1 kB	as plain text
phonon0.cpu	276 B	as plain text
phonon0.d00	567 B	as plain text
phonon0.d01	1.2 kB	as plain text
phonon0.d02	400 B	as plain text
phonon0.d03	1.1 kB	as plain text
phonon0.d05	736 B	as plain text
phonon0.d07	63.2 kB	as plain text
phonon0.d08	231.5 kB	as plain text
phonon0.d10	434 B	as plain text
phonon0.d11	434 B	as plain text
phonon0.d12	100 B	as plain text
phonon0.d13	506 B	as plain text
phonon0.d14	6.9 kB	as plain text
phonon0.d16	12.7 kB	as plain text
phonon0.d17	236 B	as plain text
phonon0.d18	41.9 kB	as plain text
phonon0.d19	29.1 kB	as plain text
phonon0.d20	3.0 kB	as plain text
phonon0.d21	3.1 kB	as plain text
phonon0.d22	4.7 kB	as plain text
phonon0.d23	4.7 kB	as plain text
phonon0.d34	47.7 kB	as plain text
phonon0.d44	331 B	as plain text
phonon0.d73	15.5 kB	as plain text
phonon0.d92	400 B	as plain text

*.d22	atomic positions used by viewer to show supercell (format as VASP POSCAR).
*.d23	POSCAR file containing positions of particles in the supercell. It can be used directly by the VASP software . POSCAR is generated if VASP POSCAR is selected at **Supercell for Atoms**.
*.d24	content of **Comments Editor**.
*.d25	data of cummulant total and partial phonon density of states selected by **Plot Partial DOS**.
*.d26	file **Plot Internal Energy** as a function of temperature.
*.d27	file **Plot Free Energy** as a function of temperature.
*.d28	file **Plot Entropy** as a function of temperature.
*.d29	file **Plot Heat Capacity** as a function of temperature.
*.d30	file **Plot Thermal Displacements** $< U^2 >$ as a function of temperature. One column format.
*.d32	thermal displacements $< U^2 >$: XX, XY,XZ,YX,YY,YZ,ZX,ZY,ZZ as a function of temperature. Six columns format. Input.
*.d33	thermal displacements $< U^2 >$: XX,YY,ZZ,YZ,ZX,XY as a function of temperature. One column format. Output.
*.d34	diagonal and off-diagonal density of states for neutron and x-rays scattering.
*.d37	data for incoherent inelastic neutron scattering on monocrystal.
*.d38	incoherent inelastic neutron scattering on monocrystal. Total and cummulant contributions.
*.d39	x-ray nuclear inelastic scattering on monocrystals. Total and cummulant contributions.
*.d40	incoherent inelastic neutron scattering on polycrystal. Total and cummulant contributions.
*.d44	DISCAR file which contains required displacements to calculate Hellmann-Feynman forces. It can be used to generate sequence of POSCAR's files for VASP.

materials design

Phonon module





The following thermodynamic functions are obtained from the phonon
density of states within the harmonic approximation. The results are
meaningful only below the melting point, which lies well below 3000 K
for most materials.
Definitions:

Cv	: vibrational heat capacity at constant volume
E_vib(T)=E(T)-E(0)	: the change in vibrational internal energy from 0 K, where E(0) = E_elec + ZPE is the electronic energy of formation E_elec plus the zero point energy ZPE
S(T)	: the vibrational entropy at temperature T
-(A(T)-E(0))	: the change in the vibrational Helmholtz free energy from 0 K
E(T)	: the electronic energy of formation plus the vibrational internal energy, so this term is E_elec + ZPE + E_vib(T)
A(T)	: the electronic plus vibrational Helmholtz free energy, E(T) - T.S(T)

Note that the electronic energy, which is part of the enthalpy and free energies,
is set to zero because the reference energies of the elements in their standard state are unavailable.

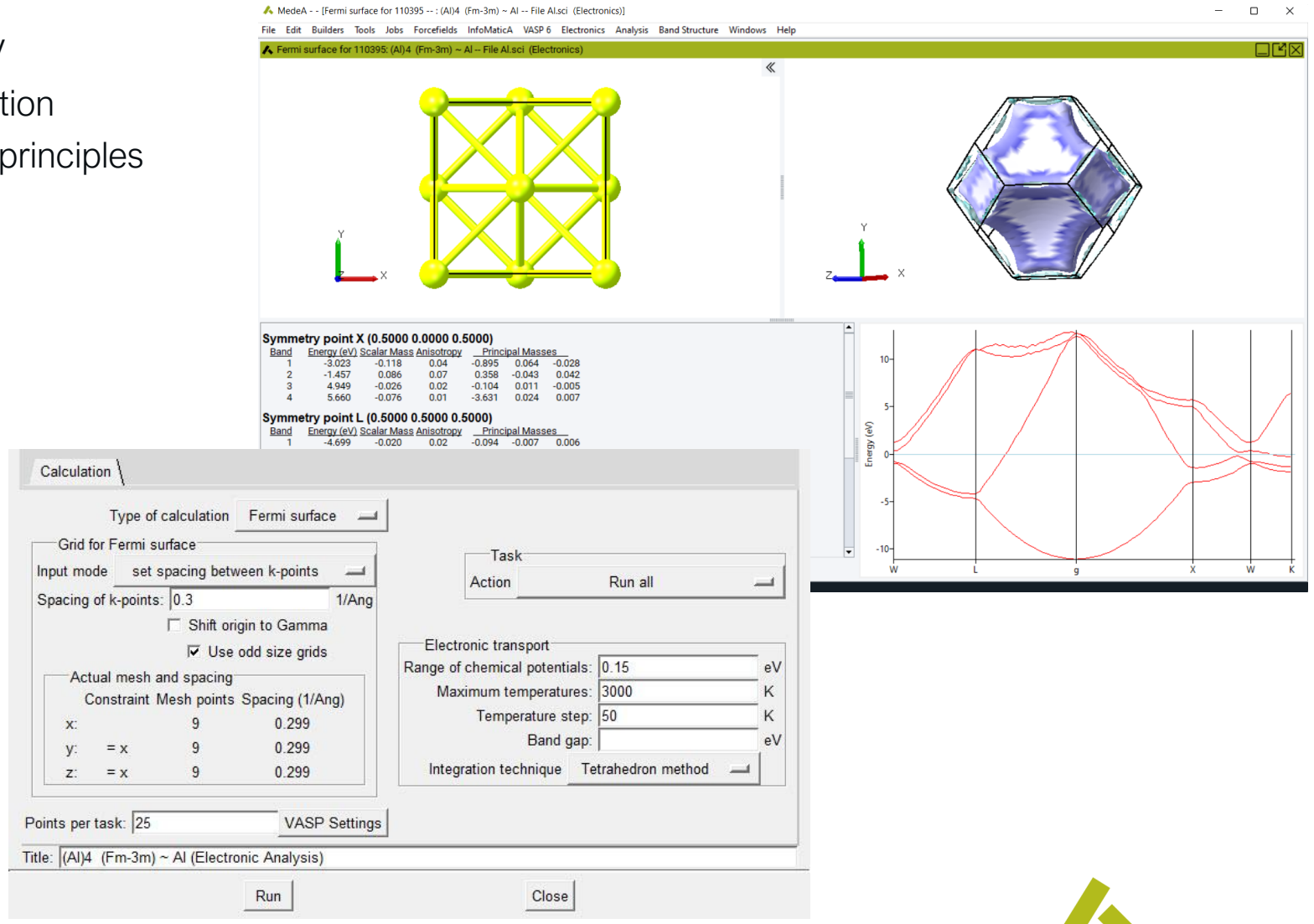
Electronic energy = 0.00 kJ/mol (set to zero since reference energies are unavailable)
PV term = 0.35 kJ/mol
Zero-point energy = 13.52 kJ/mol

T K	Cv J/K/mol	E(T)-E(0) kJ/mol	S(T) J/K/mol	-(A(T)-E(0)) kJ/mol	E(T) kJ/mol	A(T) kJ/mol
0	0.0000	0.0000	0.0000	-0.0000	13.5163	13.5163
1	0.0000	0.0000	0.0000	-0.0000	13.5163	13.5163
2	0.0000	0.0000	0.0000	-0.0000	13.5163	13.5163
3	0.0000	0.0000	0.0000	-0.0000	13.5163	13.5163
4	0.0002	0.0000	0.0000	-0.0000	13.5163	13.5163
5	0.0006	0.0000	0.0001	-0.0000	13.5163	13.5163
10	0.0097	0.0000	0.0026	-0.0000	13.5163	13.5163
15	0.0320	0.0001	0.0103	0.0000	13.5164	13.5163
20	0.0716	0.0004	0.0245	0.0001	13.5167	13.5162
30	0.2312	0.0018	0.0791	0.0006	13.5181	13.5157
40	0.5855	0.0056	0.1880	0.0019	13.5220	13.5144
50	1.2480	0.0145	0.3834	0.0047	13.5308	13.5117
60	2.2771	0.0318	0.6962	0.0099	13.5481	13.5064
70	3.6651	0.0613	1.1471	0.0190	13.5776	13.4973
80	5.3605	0.1062	1.7441	0.0334	13.6225	13.4829
90	7.2889	0.1692	2.4850	0.0544	13.6856	13.4619
100	9.3709	0.2524	3.3597	0.0835	13.7688	13.4328
125	14.7935	0.5544	6.0326	0.1996	14.0707	13.3167
150	19.9395	0.9897	9.1925	0.3892	14.5060	13.1271
175	24.4535	1.5461	12.6142	0.6614	15.0624	12.8549
200	28.2614	2.2064	16.1358	1.0207	15.7227	12.4956
225	31.4179	2.9537	19.6527	1.4682	16.4700	12.0481

materials design

Electronics module

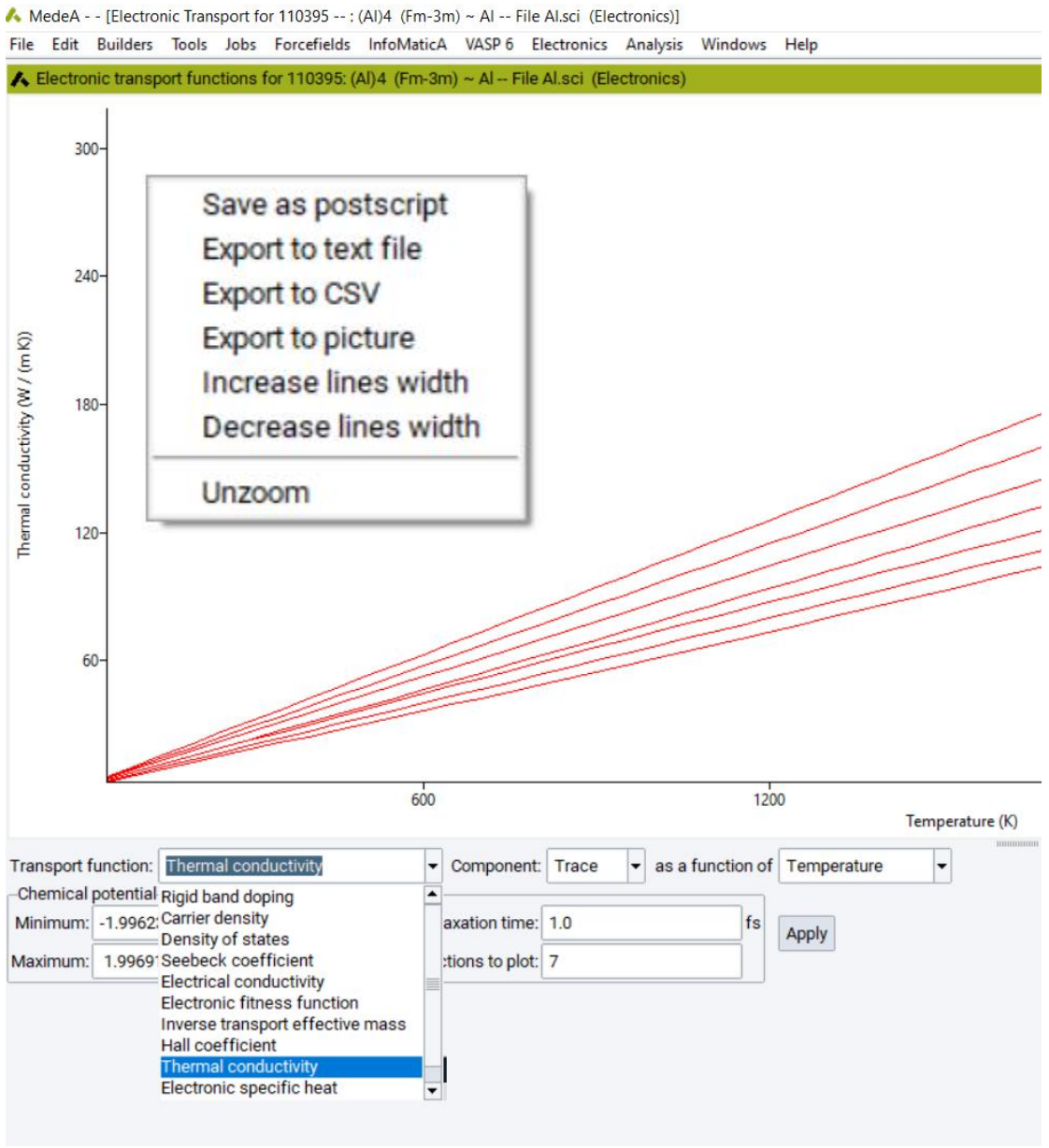
- Boltzmann theory: semiclassical theory
  - electrons follow classical equations of motion
  - electron velocity/effective mass from first principles
  - results depend on relaxation time
- calculated properties
  - electrical conductivity
  - thermopower (Seebeck coefficient)
  - thermal conductivity (electronic part)
  - electronic specific heat
  - Pauli paramagnetic susceptibility
  - Hall conductivity
- results vs. temperature or doping



materials design

Electronics Module

- Three-dimensional isosurfaces of electronic energies (Fermi surfaces) in k-space
- Interactive analysis of effective masses for each band at any point in k-space
- Interpolated electronic band structure displayed for orientation
- Highly accurate effective mass tensors for selected electron or hole bands at requested points in k-space
- Electrical conductivity, thermal conductivity
- Thermoelectric power (Seebeck coefficient)
- Electronic specific heat
- Pauli paramagnetic susceptibility
- Hall coefficient



Examples

DOI: 10.1039/C8MH01069B (Communication) *Mater. Horiz.*, 2019, **6**, 182-191

Direct probe of the nuclear modes limiting charge mobility in molecular semiconductors†

Thomas F. Harrelson [a], Varuni Dantanarayana [b], Xiaoyu Xie [c], Correy Koshnick [d], Dingqi Nai [a], Ryan Fair [e], Sean A. Nuñez [f], Alan K. Thomas [g], Tucker L. Murrey [d], Michael A. Hickner [f], John K. Grey [g], John E. Anthony [h], Enrique D. Gomez [e], Alessandro Troisi [c], Roland Faller [a] and Adam J. Moulé *[ab]

Applied Surface Science
Volume 521, 15 August 2020, 146256

Full Length Article

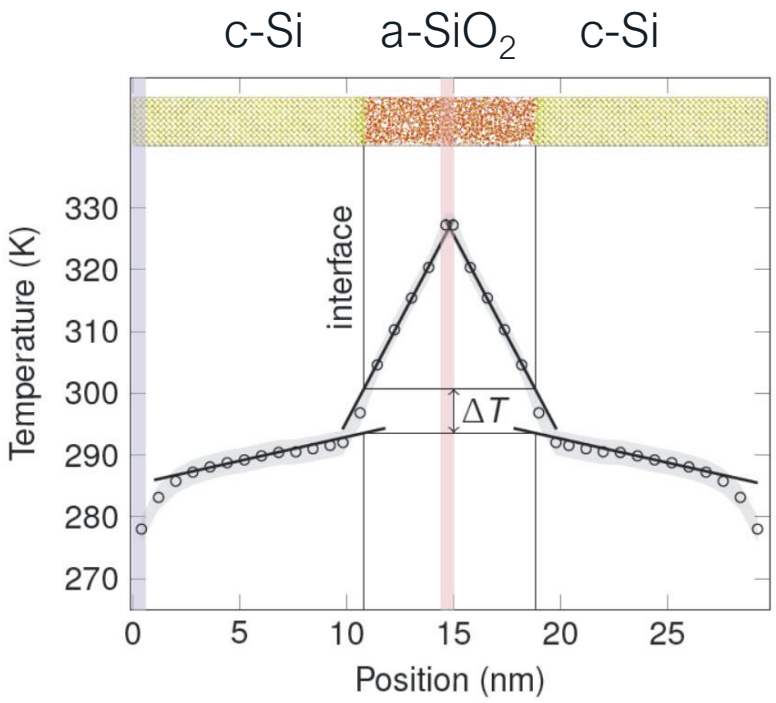
Enhancing thermoelectric properties of monolayer GeSe via strain-engineering: A first principles study

Yu Li [a], Kuan Ma [a], Xing Fan [a, b], Fusheng Liu [a], Junqin Li [a], Heping Xie [a]

Thermal Conductivity

Reverse non-equilibrium molecular dynamics

Sharp interface between crystalline Si and amorphous SiO_2



A. France-Lanord, P. Soukiassian, C. Glattli, and E. Wimmer, J. Chem. Phys. **144**, 104705 (2016)

Green-Kubo Approach

To examine isotope effects, 300K thermal conductivities for isotopically pure and 'natural' isotopic mixtures of pure Si and Ge were calculated (units: $Wm^{-1}K^{-1}$)

	Isotopically Pure	Isotopic Mixture	Expt(*)
Si	272	128	130
Ge	98	37	58

* http://www.ioffe.rssi.ru/SVA/NSM/Semicond/SiGe/thermal.htm

materials design

Example

THE JOURNAL OF CHEMICAL PHYSICS **144**, 104705 (2016)

Ab initio parameterization of a charge optimized many-body forcefield for Si–SiO_2: Validation and thermal transport in nanostructures

Arthur France-Lanord,[1,2,a)] Patrick Soukiassian,[2] Christian Glattli,[2] and Erich Wimmer[1]
[1]*Materials Design SARL, 92120 Montrouge, France*
[2]*SPEC, CEA, CNRS, Université Paris-Saclay, CEA Saclay, 91191 Gif-sur-Yvette, France*

JOURNAL OF APPLIED PHYSICS **117**, 214303 (2015)

Thermal conductivity of nanostructured Si_xGe_{1-x} in amorphous limit by molecular dynamics simulation

Payam Norouzzadeh,[1,2] Amin Nozariasbmarz,[1] Jerzy S. Krasinski,[2] and Daryoosh Vashaee[1,a)]
[1]*Monteith Research Center, Electrical and Computer Engineering Department, North Carolina State University, Raleigh, North Carolina 27606, USA*
[2]*School of Electrical and Computer Engineering, Helmerich Advanced Technology Research Center, Oklahoma State University, Tulsa, Oklahoma 74106, USA*

materials design

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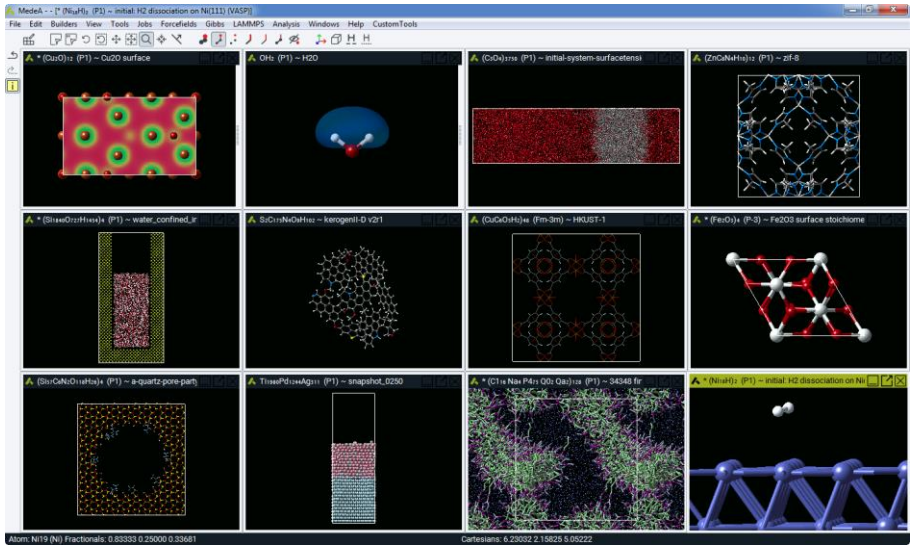
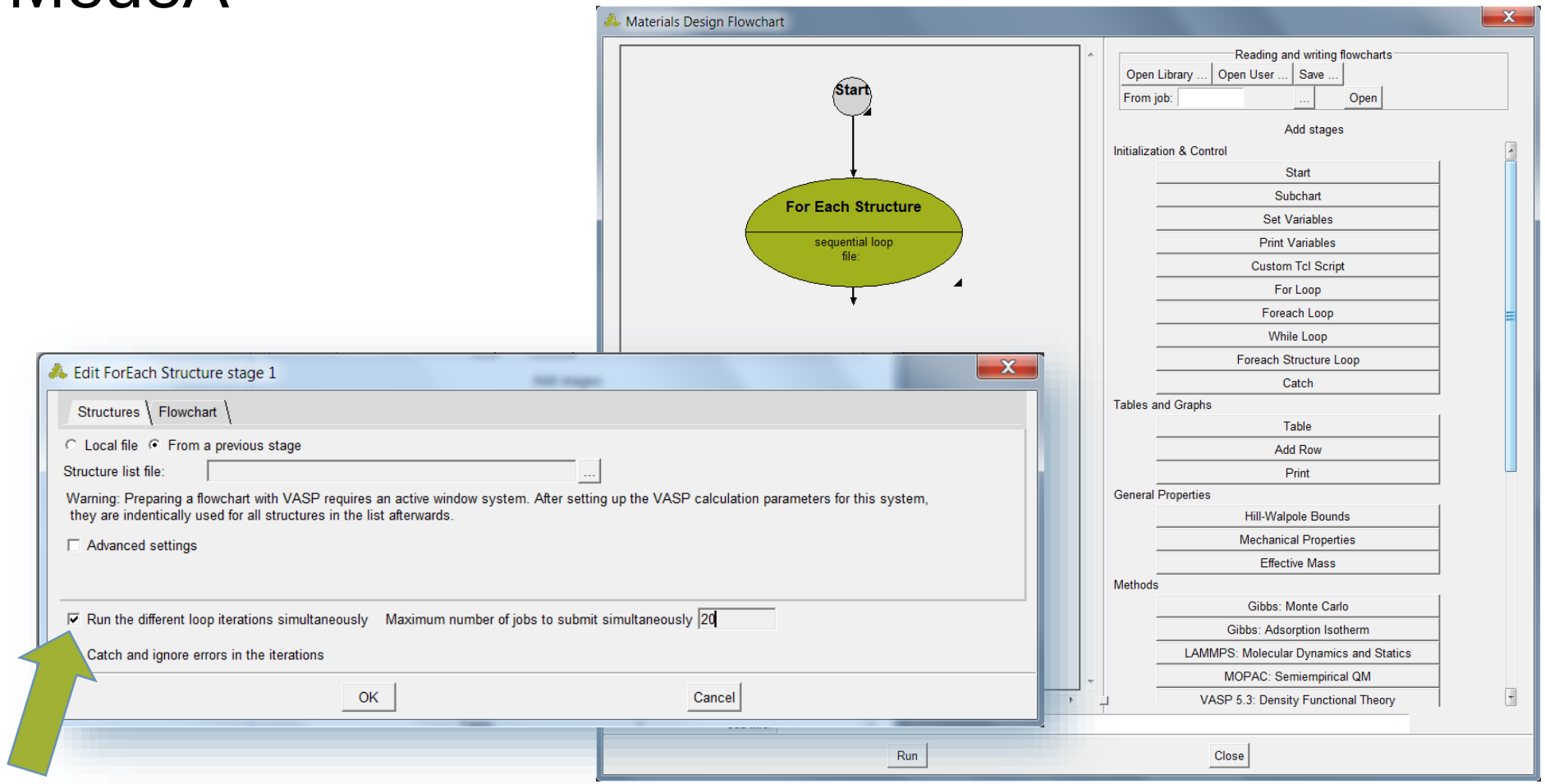


HT in MedeA



- Value: Highly efficient screening of large number of compounds

materials design

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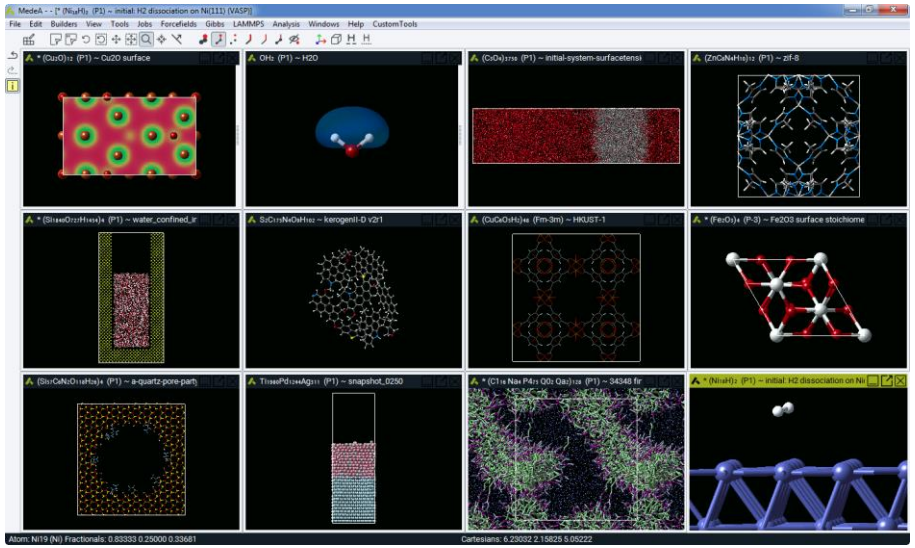


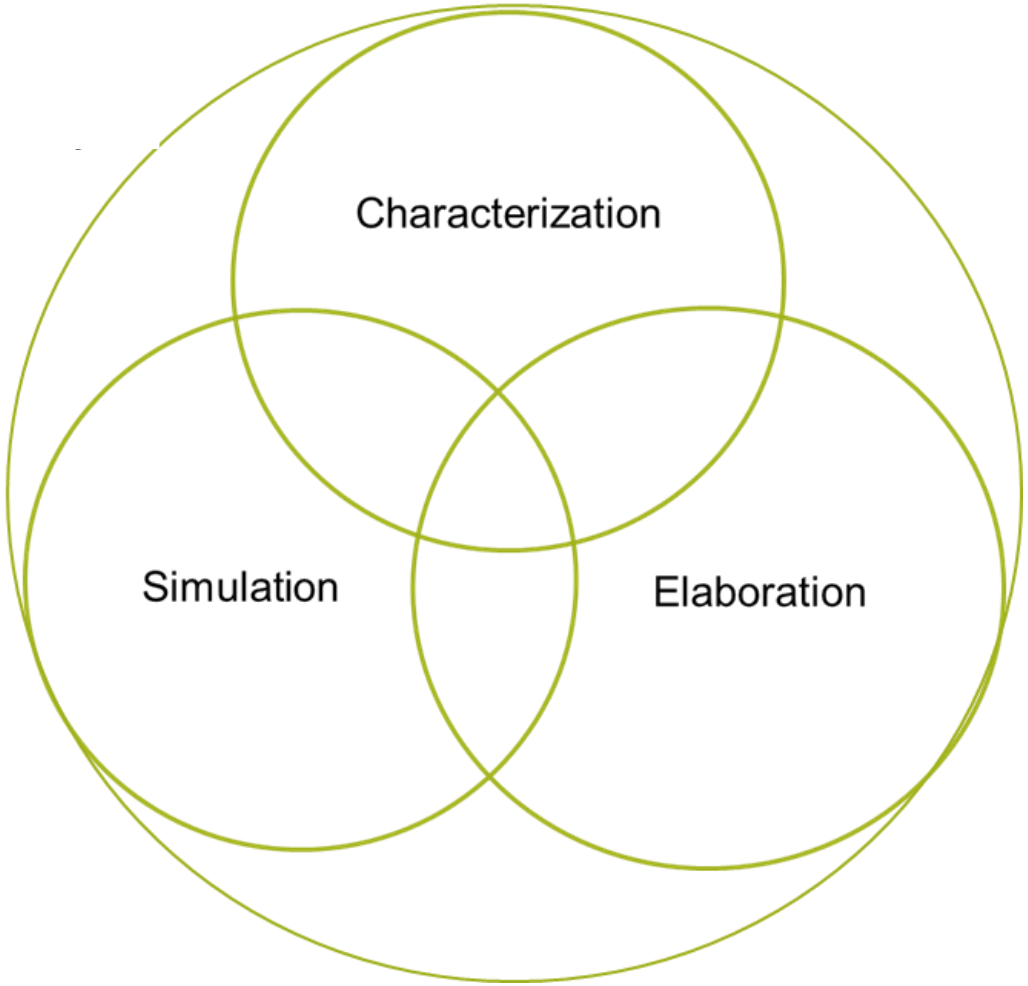
MedeA's 3-Tier Architecture

- MedeA's **three-tier architecture** lets you submit compute jobs to local or remote compute resources.
- Parallel task processing and MedeA's high-throughput job control guarantee optimal performance on workstations and HPC platforms under Windows and Linux alike.
- Submit your workflow, turn off your workstation or laptop and take a break! – Or join a meeting!
- MedeA's tier architecture takes care of the entire workflow, in serial mode, or parallel, or running through structure list with hundreds of entries in high-throughput mode.
- Workflows may include multiple stages involving several solvers, intermediate analysis and building, and even on-the-fly graphical analysis. - Though you still need to write the report or paper yourself. ☺

The JobServer interprets the flowchart…
…and automates the process.

materials design

Conclusion



MedeA helps focus on key objectives such as materials screening, design of experiment and scientific analysis, rather than dealing with shell programming, file formats, command lines and syntax issues.

Over 500 customers in Industry, Universities, and Government Laboratories

"Computational material science tools have revolutionized the evaluation of neutron thermal scattering laws. All of the new thermal scattering laws including in the new US national ENDF/B-VIII.0 nuclear data library were developed using DFT or MD simulations. ***The vast majority were developed by MedeA users using VASP, PHONON, and LAMMPS.****"*

-Michael L. Zerkle, Ph.D.
Senior Advisor, Reactor Physics Methods Development,
Naval Nuclear Laboratory

materials design

Materials Design: Technical Teams

Development Team


Clive Freeman
President & CEO


Benoit LeBlanc
Software Architect


Dave Rigby
Senior Scientist


Marianna Yiannourakou
Research Scientist


Walter Wolf
Senior Scientist


Jason Aubry
Development Engineer

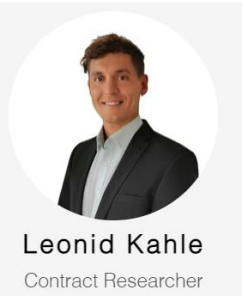

Jörg-Rüdiger Hill
Senior Software Engineer in Contract Research & Development

Research Team


Erich Wimmer
Chief Scientific Officer & Chairman of the Board


Mikael Christensen
Research Scientist

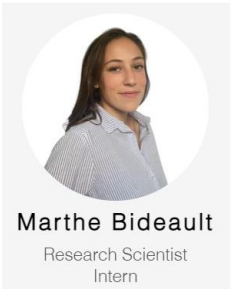

Volker Eyert
Senior Scientist


Leonid Kahle
Contract Researcher


Xavier Rozanska
Research Scientist


Benoit Minisini
Pre-Sales Application Scientist


Boris Belin
Research Scientist in Contract Research & Development

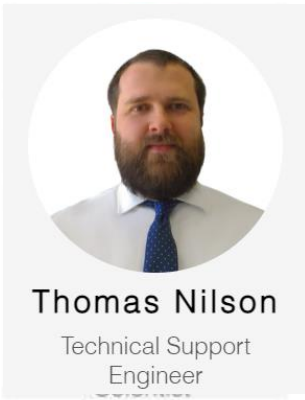

Marthe Bideault
Research Scientist Intern

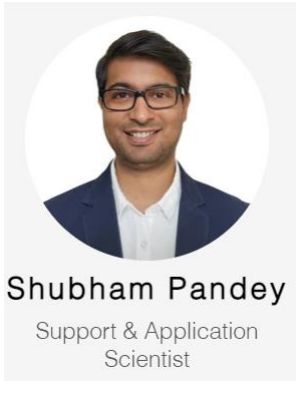
Support Team


Ray Shan
Director of Support


Rene Windiks
Senior Scientist, Battery Specialist


David Reith
Application & Research Scientist


Thomas Nilson
Technical Support Engineer


Shubham Pandey
Support & Application Scientist

materials design