



materials design

Monacoste 2022

Computational Materials Science in MedeA[®] environment

B. Minisini, J. Coll

11th May 2022

bminisini@materialsdesign.com


DFT

$$\hat{H}\psi = E\psi \rightarrow \hat{h}_{\text{eff}}\phi_i = \epsilon_i\phi_i$$
$$E[\rho(r)] = T + \int V_{\text{eff}}(r)\rho(r)dr$$

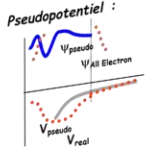
Plane wave basis

$$\phi_i(r) = \sum C_i(\mathbf{G})e^{i\mathbf{G}\cdot\mathbf{r}}$$

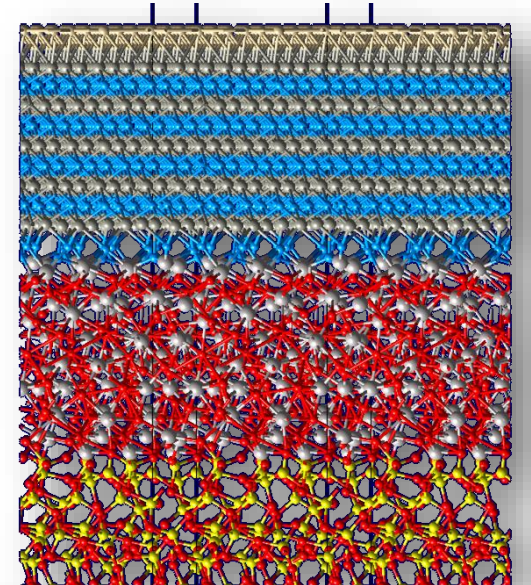
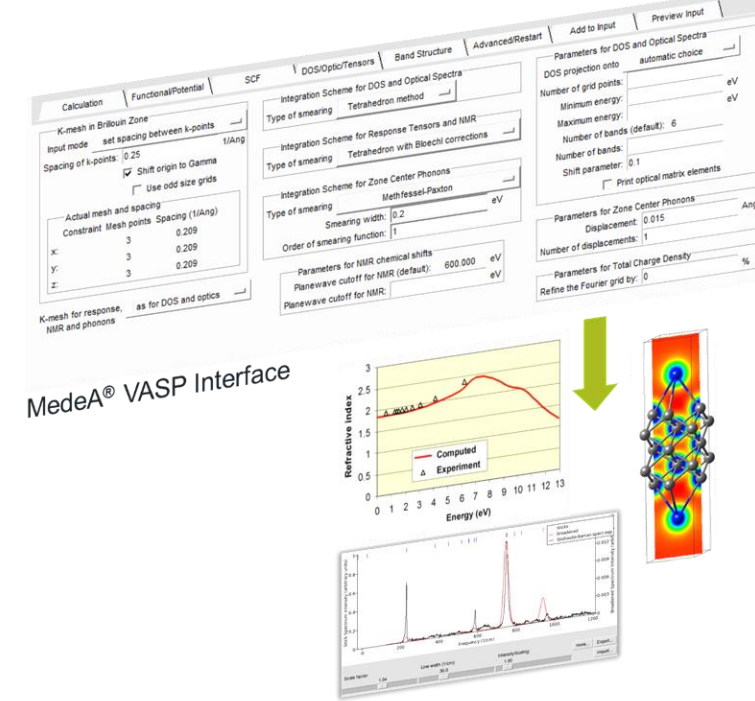
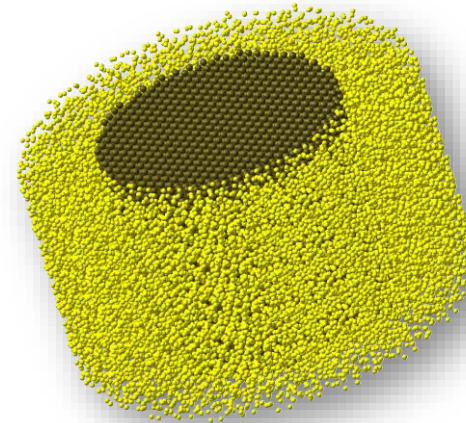
K-points :



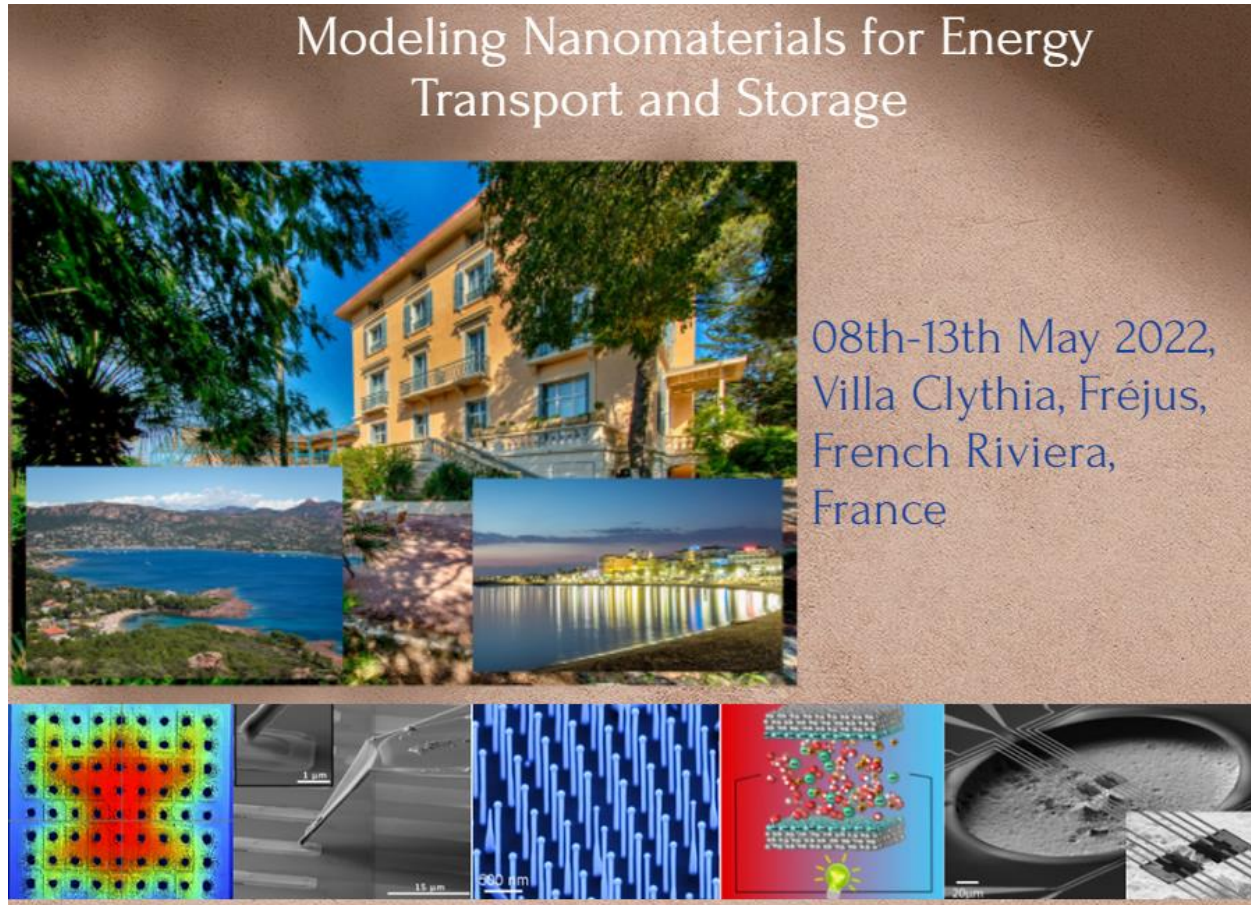
Pseudopotential :


$$\frac{\hbar^2}{2m}|G|^2 \leq E_{\text{truncature}}$$

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 $0.01 \text{ eV } \text{\AA}^{-1}$, 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

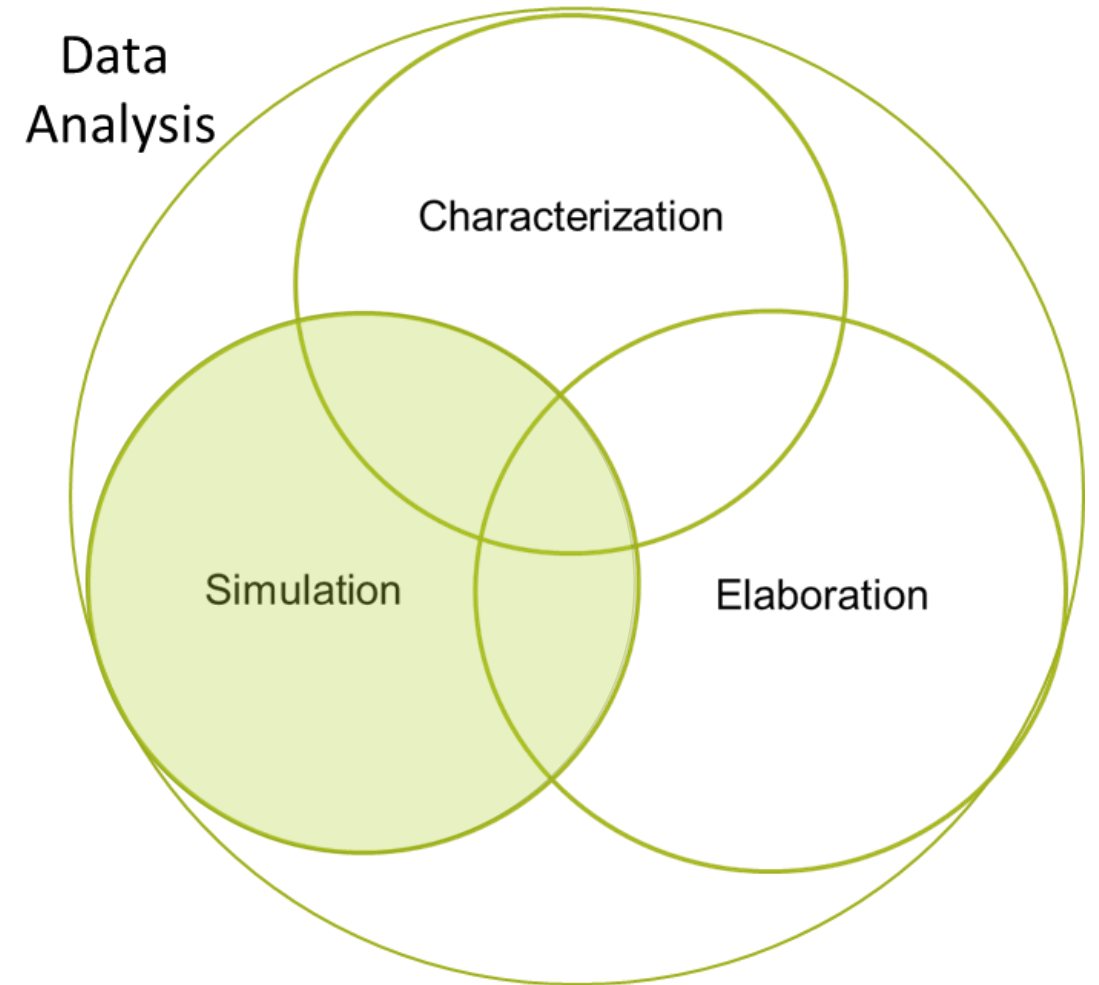


Introduction



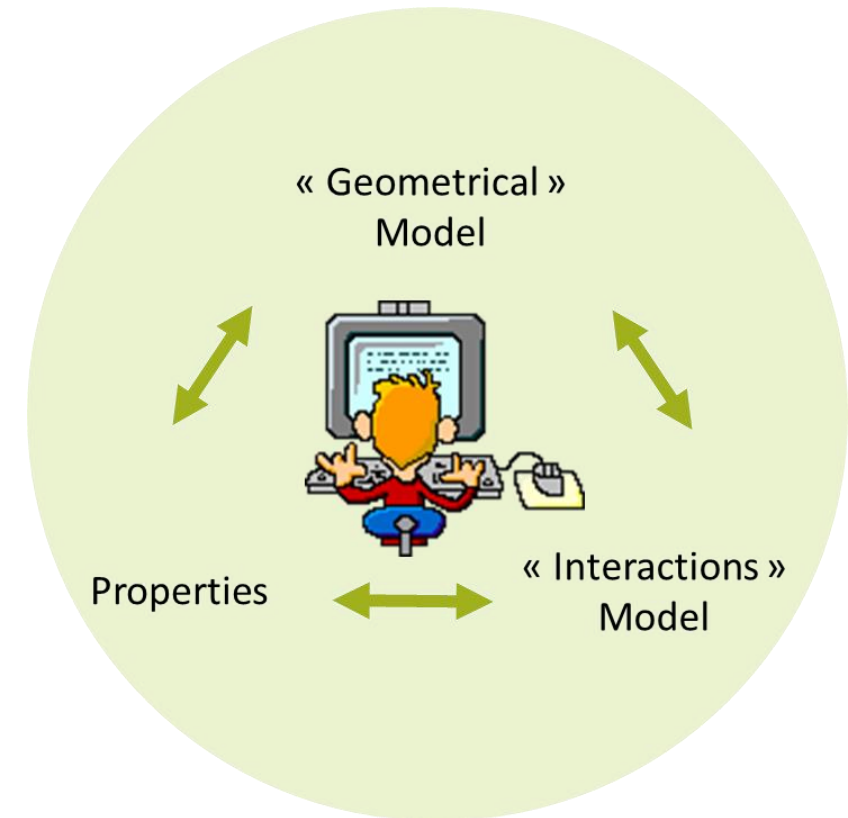
DATA :

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



Introduction

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



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 »

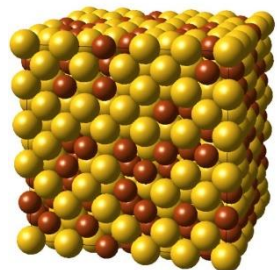
R.J QUANN (Exxon Mobil), , Oil & Gas Sci. Tech. 68, 110-1113, 2013

« ...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. »

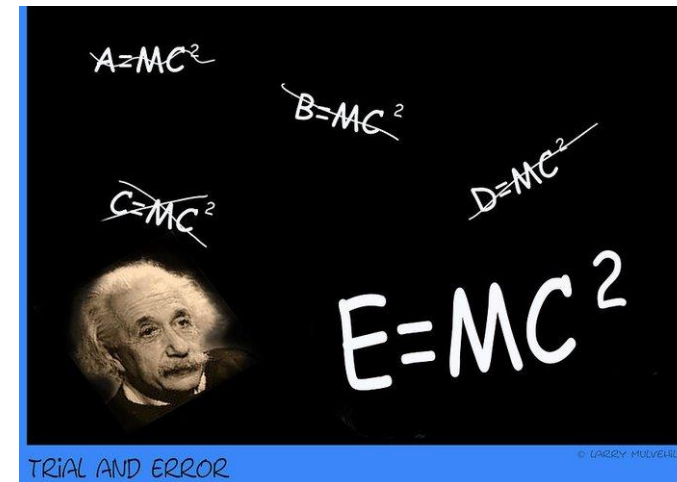
THORTON et al JOM, 61, 12-17, 2009



Introduction



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



Introduction

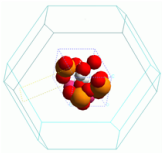
$$\hat{H}\psi = E\psi \xrightarrow{\text{DFT}} \hat{h}_{\text{eff}}\varphi_i = \varepsilon_i\varphi_i$$

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

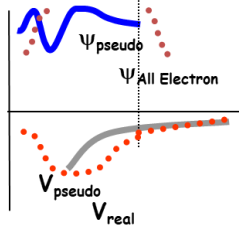
Plane wave basis

$$\varphi_i(r) = \sum C_i(\mathbf{G})e^{i\mathbf{G}\cdot\mathbf{r}}$$

K-points :



Pseudopotential :



$$\frac{\hbar^2}{2m}|\mathbf{G}|^2 \leq E_{\text{ionization}}$$

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 $0.01 \text{ eV } \text{\AA}^{-1}$, 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

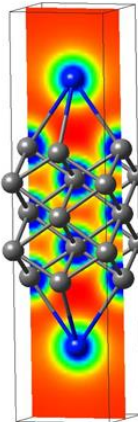
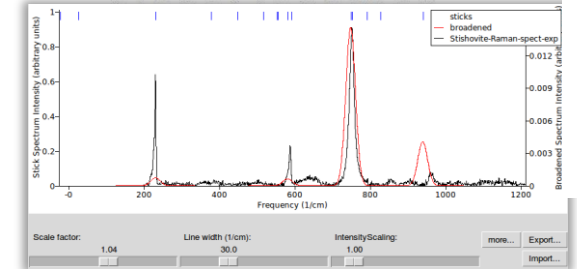
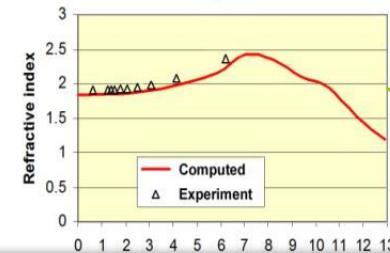
- [NGX, NGY, NGZ and NGXF, NGYF, NGZF-tags](#)
- [KSPACING-tag and KGAMMA-tag](#)
- [NBANDS-tag](#)
- [NBLK-tag](#)
- [SYSTEM-tag](#)
- [NWRITE-tag](#)
- [ENCUT-tag](#)
- [ENAUG-tag](#)
- [PREC-tag](#)
- [ISPIN-tag](#)
- [MAGMOM-tag](#)
- [ISTART-tag](#)
- [ICHARG-tag](#)
- [INIWAV-tag](#)
- [NELM, NELMIN 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_...
' 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
```

INCAR
KPOINTS



Introduction

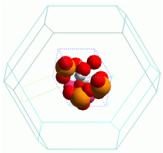
$$\hat{H}\psi = E\psi \xrightarrow{\text{DFT}} \hat{h}_{\text{eff}}\varphi_i = \varepsilon_i\varphi_i$$

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

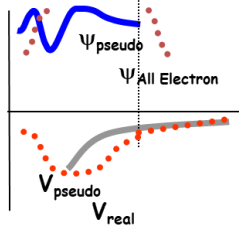
Plane wave basis

$$\varphi_i(\mathbf{r}) = \sum C_i(\mathbf{G})e^{i\mathbf{G}\cdot\mathbf{r}}$$

K-points :



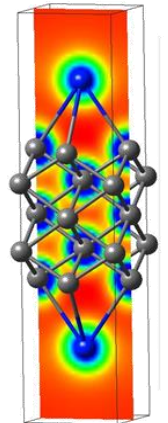
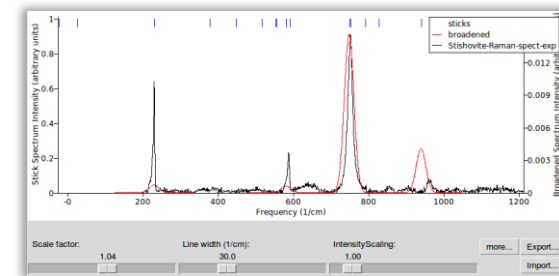
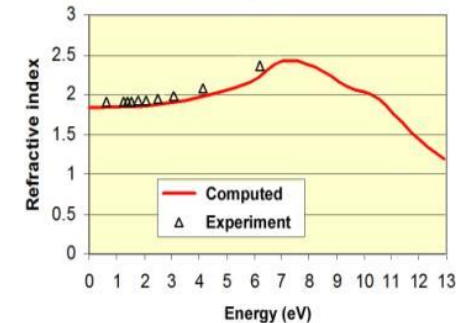
Pseudopotential :



$$\frac{\hbar^2}{2m}|\mathbf{G}|^2 \leq E_{\text{truncature}}$$

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 $0.01 \text{ eV } \text{\AA}^{-1}$, 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

MedeA[®] VASP Interface



Introduction

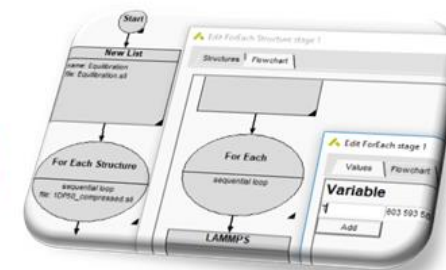
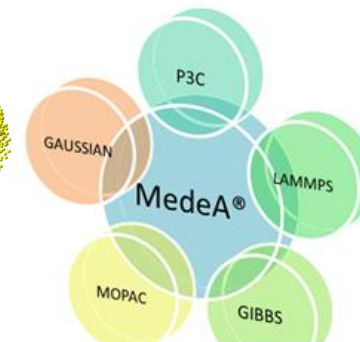
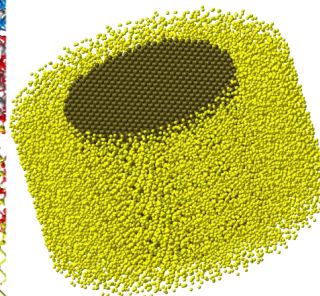
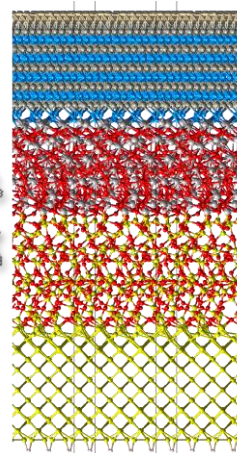
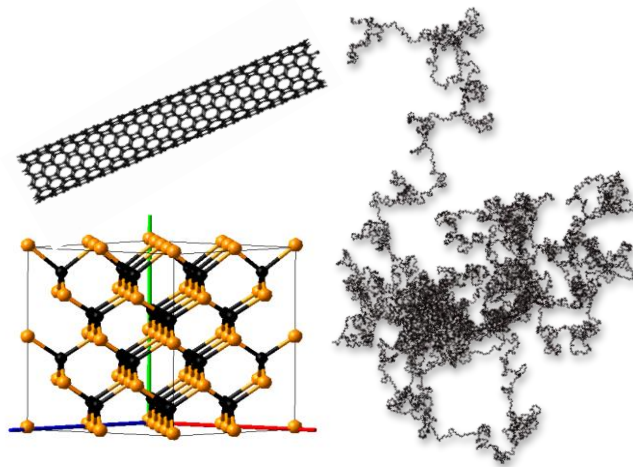
“I like MedeA, it gives me more time to think.”

-Ryoji Asahi

Toyota Central Research and Development Laboratories, Nagoya, Japan

Introduction

Atomic-scale
Simulations

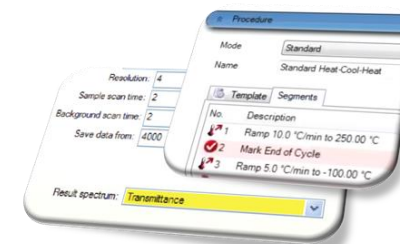
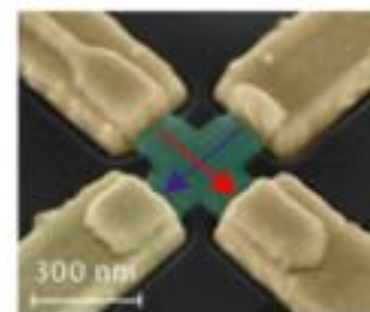
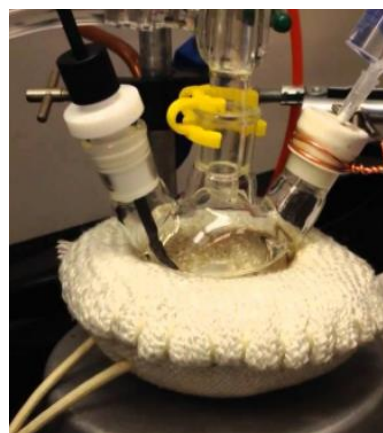


Formulation

Synthesis

Characterization

Laboratory
Work



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

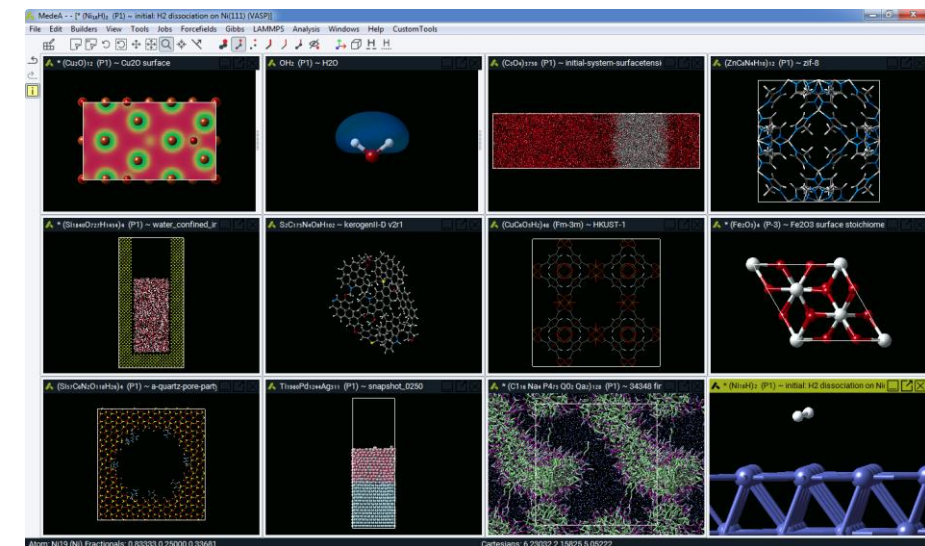
Analysis Tools

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

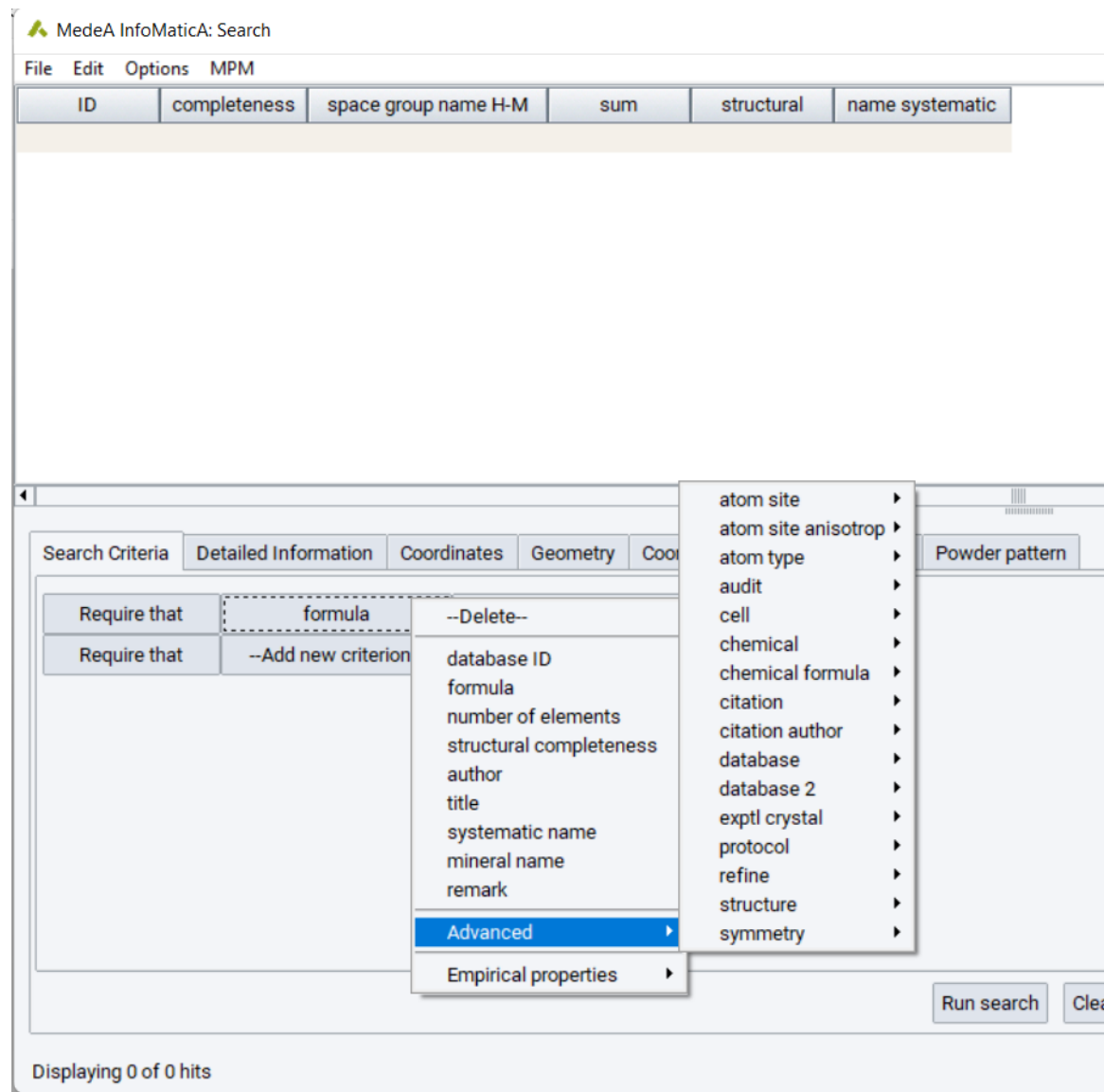


Databases

over 1.1 million entries



<https://www.materialsdesign.com/databases>

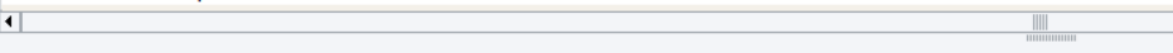


Databases

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.1521718	Complete	F-43m	Cr2 Cu0.5 Fe0.5 S4	Cr2 Cu0.5 Fe0.5 S4	Fe0.5 Cu0.5 Cr2 S4
COD.9003726	Complete	F-43m	Cu2 Fe S2	Cu2 Fe S2	
COD.9003726	Complete	F-43m	Cu2 Fe S2	Cu2 Fe S2	
COD.9012061	Complete	I-42m	Cu2 Fe Ge S4	Cu2 Fe Ge S4	
COD.9003726	Complete	F-43m	Cu2 Fe S2	Cu2 Fe S2	
COD.9003726	Complete	F-43m	Cu2 Fe S2	Cu2 Fe S2	
COD.9000061	Complete	Pcmn	Cu Fe2 S3	Cu Fe2 S3	
COD.9008201	Complete	Pcmn	Cu Fe2 S3	Cu Fe2 S3	
COD.9004101	Complete	P-4m2	Cu6 Fe2 S8 Sn	Cu6 Fe2 S8 Sn	
COD.9008201	Complete	Pcmn	Cu Fe2 S3	Cu Fe2 S3	



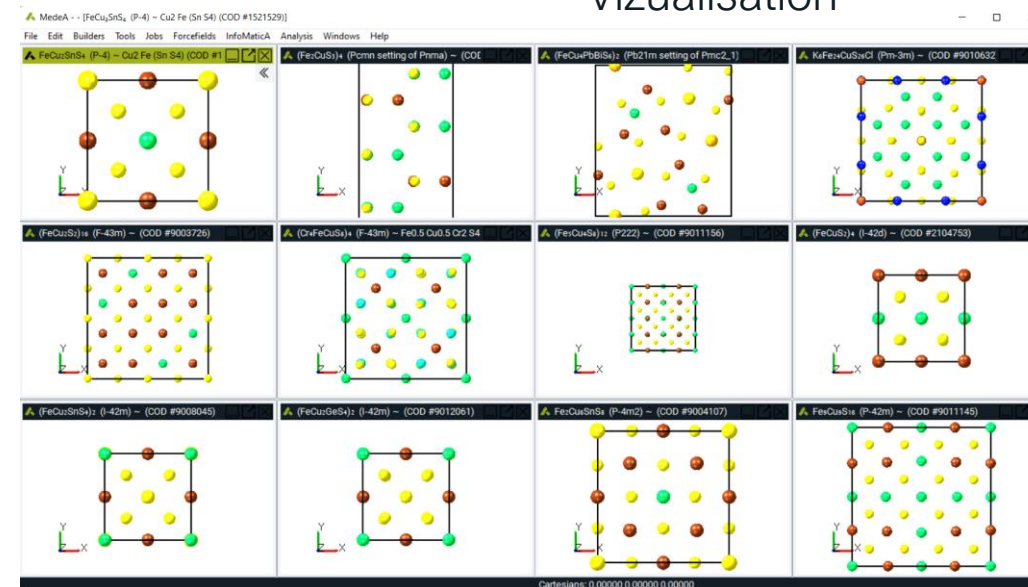
Search Criteria Detailed Information Coordinates Geometry Coordination Pair Correlation Powder pattern

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



MedeA: structure list editor

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

SQLite structure list file (30720 bytes): C:/Users/BenoitMinisini/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

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



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

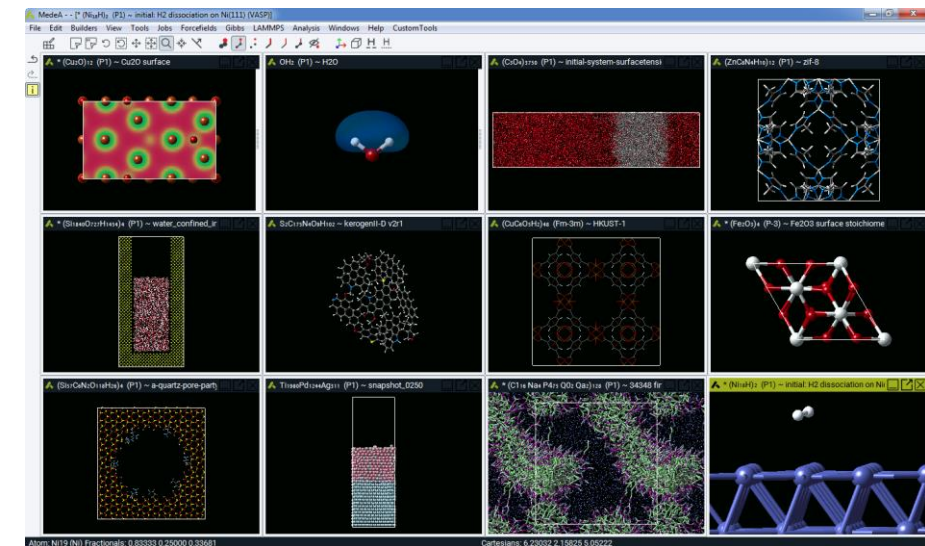
Analysis Tools

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



Builders

MedeA -- [FeCu₂SnS₄ (P-4) ~ Cu₂ Fe (Sn S₄) (COD #1521529)]

File Edit Builders Tools Jobs Forcefields InfoMaticA Analysis Windows Help

FeCu₂S₄ (P-4) ~ (COD #1521529)

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

(FeCu₂SnS₄)₂ (Pb21m setting of Pmc2_1) ~ (COD #9010632)

K₆Fe₂₄Cu₂₄Sn₂₄Cl (Pm-3m) ~ (COD #9010632)

(FeCu₂SnS₄)₂ (P-4) ~ (COD #1521529)

Fe_{0.5}Cu_{0.5}Cr₂S₄ ~ (COD #9011156)

(Fe₃Cu₄Sn₄)₁₂ (P222) ~ (COD #9011156)

(FeCu₂SnS₄)₄ (I-42d) ~ (COD #2104753)

(FeCu₂SnS₄)₂ (P-4) ~ (COD #9012061)

Fe₂Cu₈Sn₈S₈ (P-4m2) ~ (COD #9004107)

Fe₉Cu₉Sn₉S₉ (P-42m) ~ (COD #9011145)



Random substitution

The screenshot displays the MedeaA software interface, specifically the 'Random substitutions' dialog box. The dialog is titled 'MedeaA: random substitutions' and contains the following elements:

- Instructions:** A text block explaining that multiple substitution rules can be added and applied consecutively in a top-down order. It also notes that if no matching atoms are found for a rule, the user can choose to ignore it or dismiss the whole substitution, resulting in no structure being created. It mentions that users can ask for several draws to generate new random structures.
- Options:**
 - ☐ Stop on unmatched rules
 - ☐ For microporous materials, obey Lowenstein's rule, if possible (requires bonds)
 - ☒ Create new structures as new windows
 - ☐ Append to structure list
- Substitution Rule Configuration:**
 - A button labeled 'Create' followed by a text input field containing '1' and the label 'random structure(s)'.
 - A rule configuration area showing:
 - Substitute:** A dropdown menu with 'all' selected.
 - atoms of:** A dropdown menu with 'atoms of' selected, and a list of categories: 'all', 'exactly', 'percent of', 'atoms of', 'atoms whose name', 'atoms whose subset', 'atoms from group', 'atoms from period', 'alkali metals', 'alkaline earths', 'halogens', 'transition metals', and 'lanthanides'.
 - Cu** (element symbol) followed by a 'with' button.
 - atoms of:** A dropdown menu with 'atoms of' selected, and a list of categories: 'atoms of', 'atoms of', and 'vacancies'.
 - Si** (element symbol) followed by an 'isotope:' button.
 - Average mass:** A dropdown menu with 'Average mass' selected, and a list of values: 'Average mass', 'Natural mix', '28', '29', and '30'.

The background of the interface shows a 3D model of a crystal structure, likely a perovskite, with atoms represented by colored spheres (yellow, green, red, blue) and bonds shown as lines. The model is displayed in a 3D perspective view with axes labeled X, Y, and Z.

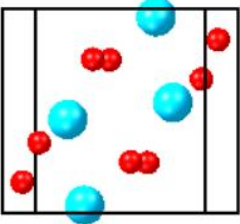


Surface

MedeA - - [* (HfO₂)₁₃₂ (P1) ~ system#12]

File Edit Builders Tools Jobs Forcefields InfoMaticA Analysis Windows Help

(HfO₂)₄ (P121/c1 setting of P2_1/c) ~ (COD #9013470)



Y
Z X

Miller indices

h: 1
k: 1
l: 1

Search

Surface parameter

Repeats: 1
Gap (Ang): 10.0
Angular tolerance (deg): 1.0


Create

Found a (1 1 1) oriented cell with a repeat distance of 93.2468 Ang.

The angular deviation of the new c axis from the (1 1 1) plane normal is 0.97 deg. This will create a slight distortion of the original interatomic distances, in order to keep the new c axis exactly perpendicular to the surface plane.

Please provide the thickness of the slab in terms of the number of repeats and the gap between slabs, and press 'Create'.

(HfO₂)₁₃₂ (P-1) ~ (COD #9013470) (1 1 1) surface



Z Y
X

X

(COD #9013470) (1 1 1) surface, symmetry = P-1
slab thickness: 93.2468 Ang
total thickness: 103.247 Ang

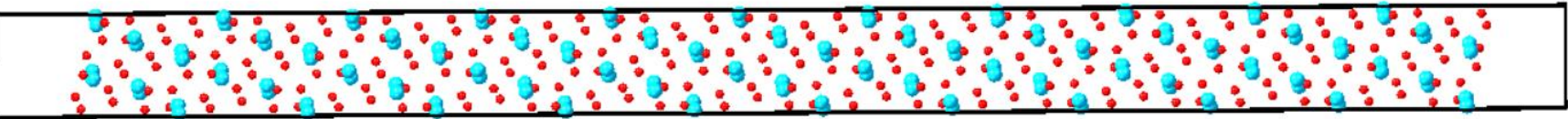
Lower plane altitude 5.0
Upper plane altitude 98.246795

New Symmetry: P-1 Formula: (Hf O2)132 Update


Create as ☒ P1 ☐ Symmetric ☐ Centered P1
☐ Bottom P1

with a surface normal in z-direction

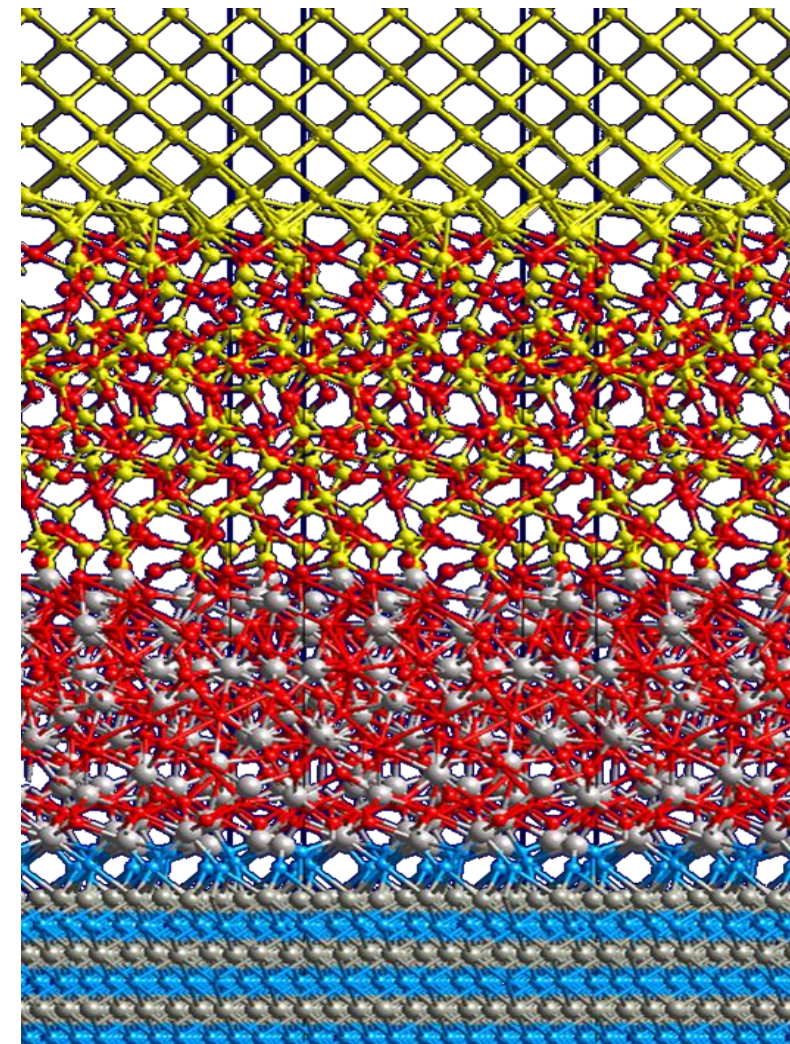
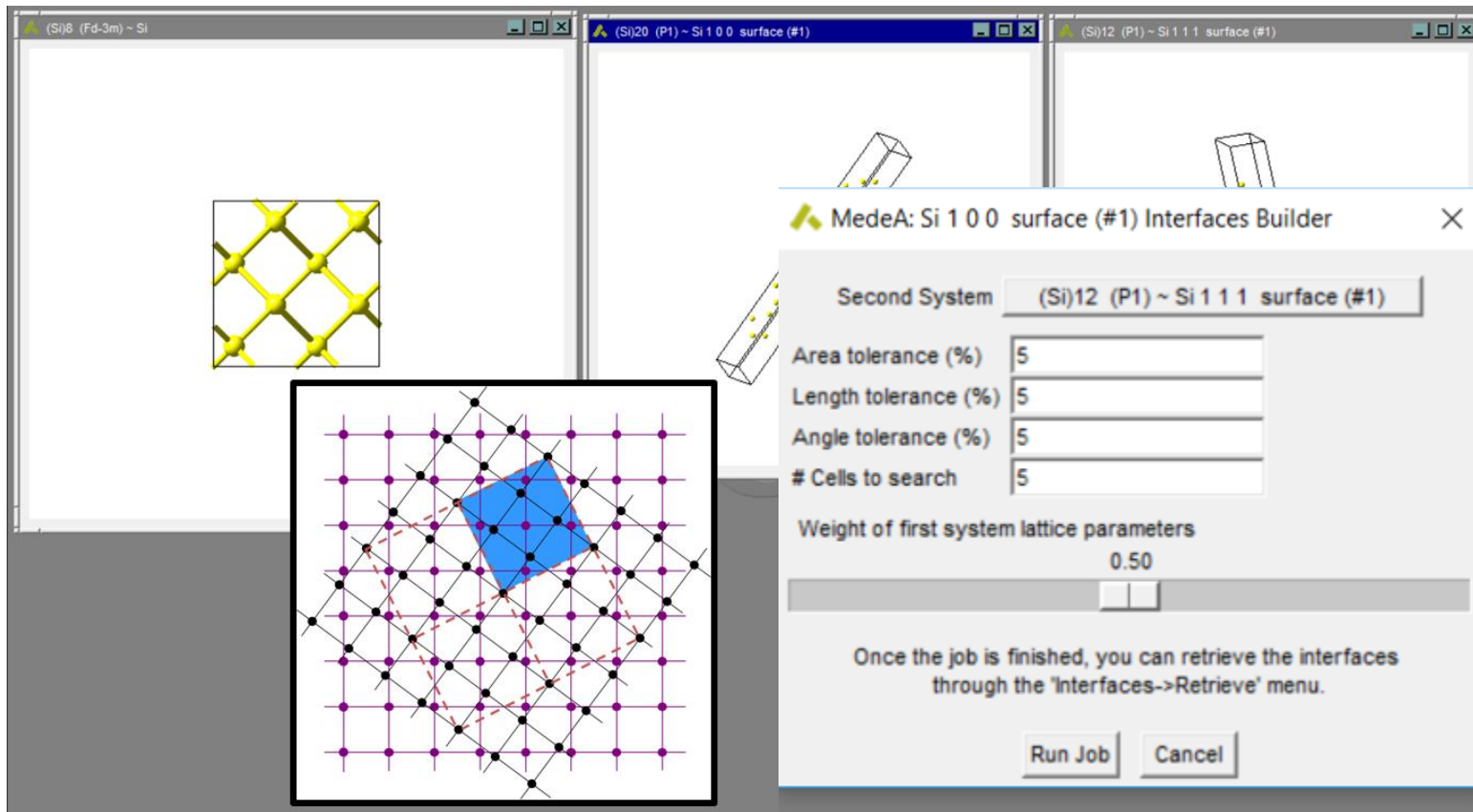
* (HfO₂)₁₃₂ (P1) ~ system#12



Y
Z X

 **materials design**

Interface builder



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

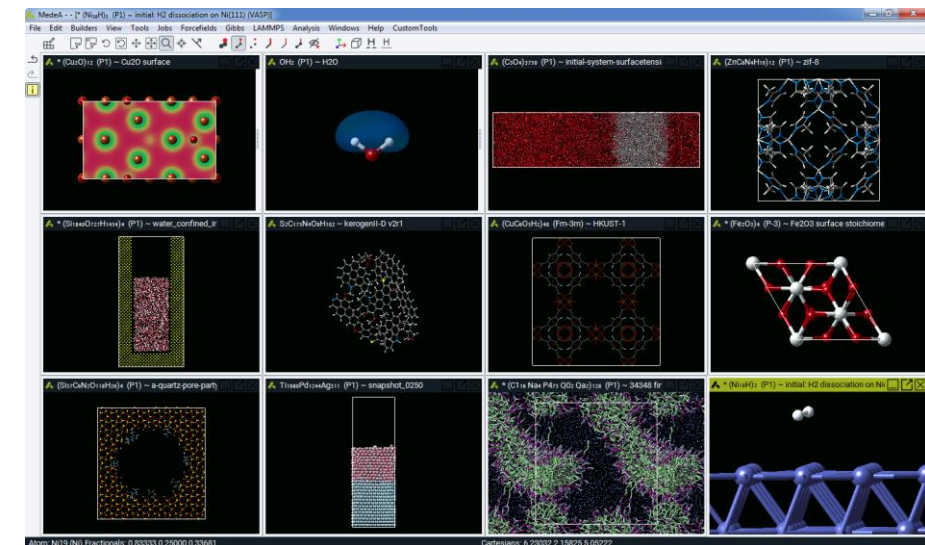
Analysis Tools

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 : 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

Optical Spectra via Time Evolution

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

☐ Elastic constants

☐ Zone center phonons

☐ Response tensors

☐ NMR: chemical shifts

☐ Energy of formation

☐ Solvation (for molecules or surfaces)

☐ Apply solvation model

External pressure: 0 GPa

Charge state: 0 e

External electrostatic field (molecules and surfaces) 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): 229.943 eV

Planewave cutoff:

Projection

Reciprocal space

Title: (Au)4 (Fm-3m) ~ (COD #9011612) (VASP)

Run

Close

Write input files

Restore defaults

Restore from job



MedeA[®] VASP GUI

MedeA : Run VASP 6

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

K-mesh in Brillouin Zone

Input mode: set spacing between k-points

Spacing of k-points: 0.25 1/Ang

☒ Shift origin to Gamma

☐ Use odd size grids

Actual mesh and spacing

	Constraint	Mesh points	Spacing (1/Ang)
x:		11	0.243
y:	= x	11	0.243
z:	= x	11	0.243

K-mesh for response, NMR, elastic constants, phonons: as for DOS and optics

Integration Scheme for DOS and Optical Spectra

Type of smearing: Tetrahedron method

Integration Scheme for Response Tensors and NMR

Type of smearing: Tetrahedron with Bloechl corrections

Integration Scheme for Phonons and Elastic Tensors

Type of smearing: Methfessel-Paxton

Smearing width: 0.2 eV

Order of smearing function: 1

Parameters for DOS and Optical Spectra

DOS projection onto: automatic choice

Number of grid points: 3000

Minimum energy: eV

Maximum energy: eV

Number of bands (default): 9

Number of bands:

Shift parameter: 0.1

☐ Print optical matrix elements

Parameters for NMR chemical shifts

Planewave cutoff for NMR (default): 344.915 eV

Planewave cutoff for NMR: eV

Parameters for Zone Center Phonons

Displacement: 0.015 Ang

Number of displacements: 1

Parameters for Total Charge Density

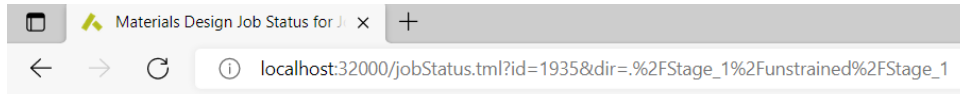
Refine the Fourier grid by: 0 %

Title: (Au)4 (Fm-3m) ~ (COD #9011612) (VASP)

Run Close Write input files Restore defaults Restore from job



MedeA[®] VASP Output



- Trajectory

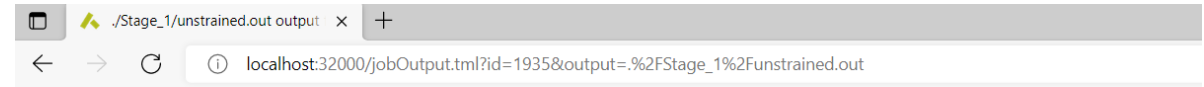
Available Output Files in ./Stage_1/unstrained/Stage_1

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 plane-wave 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
```

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

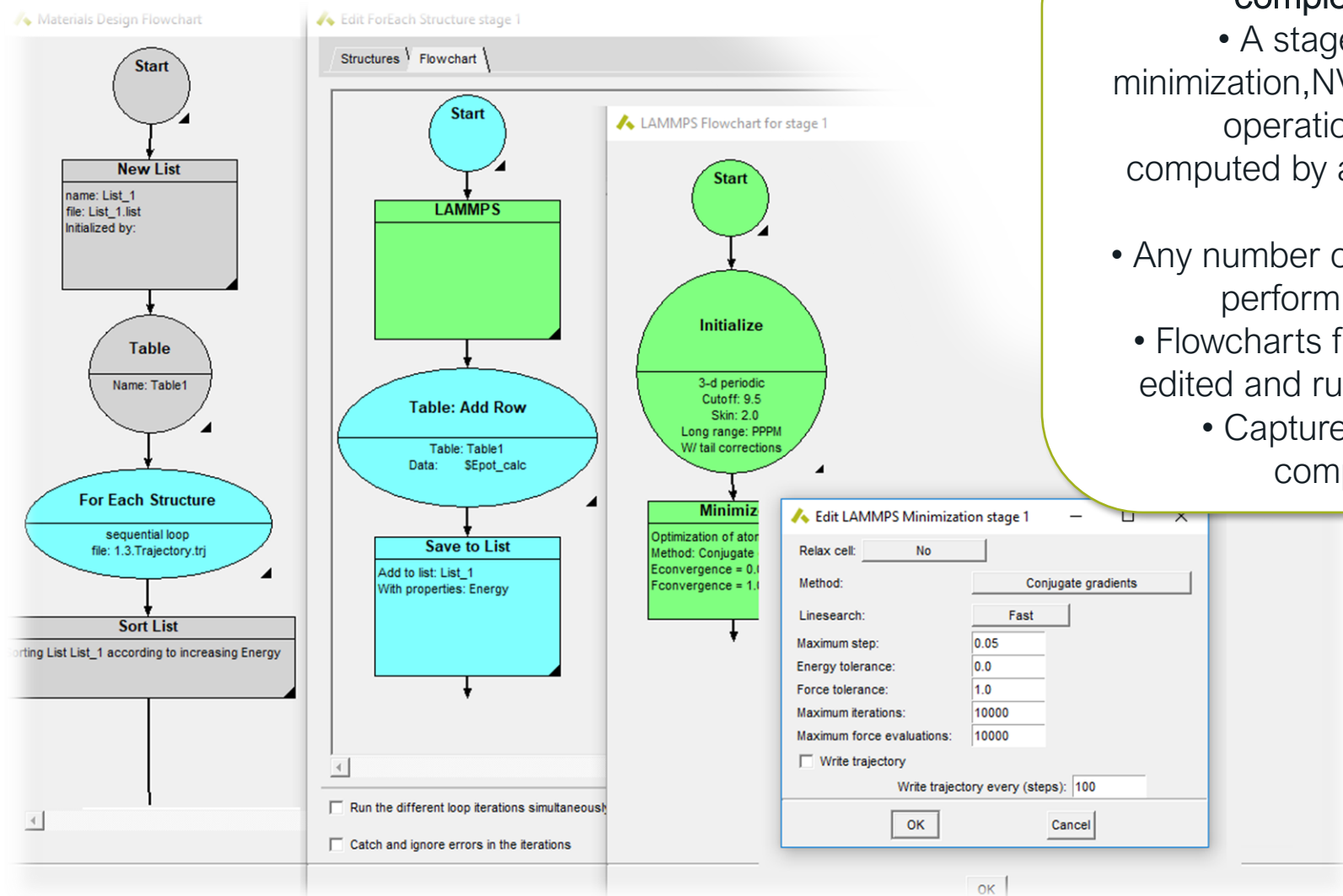
► Webinars:

- 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..



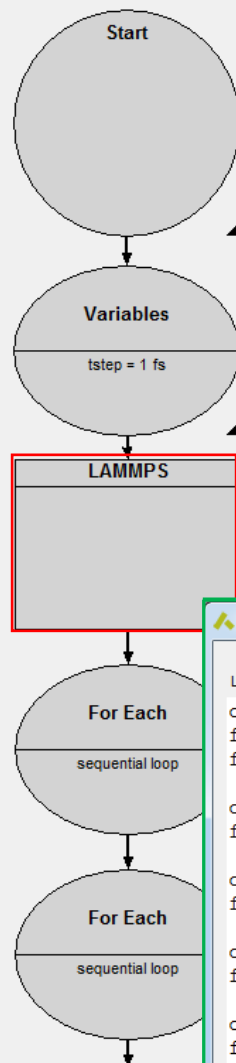
LAMMPS GUI and Flowcharts



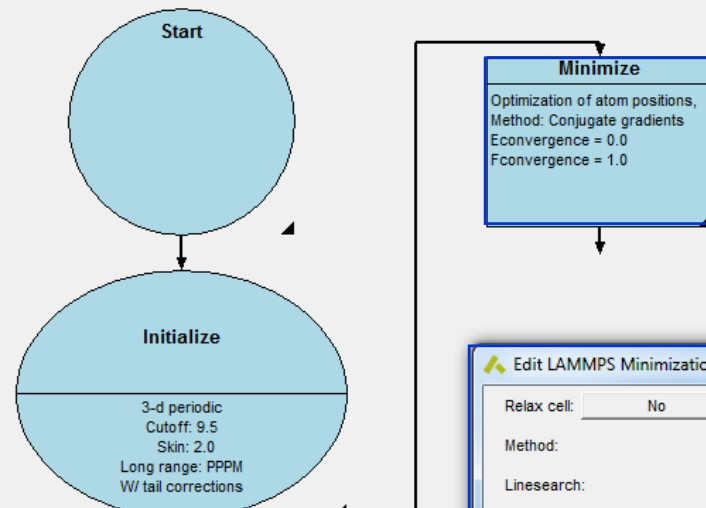
- Powerful flowchart interface lets you easily set up complex calculations by connecting stages
 - A stage can be a computation, e.g. energy minimization, NVT and NPT dynamics, as well as an operation such as setting the density to that computed by a previous stage, or building a larger simulation box
- 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
advanced
users





LAMMPS Flowchart for stage 1



Edit LAMMPS Minimization stage 1

Relax cell:

Method:

Linesearch:

Maximum step:

Energy tolerance:

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

Bias

Single Point

Minimization

Building and Editing

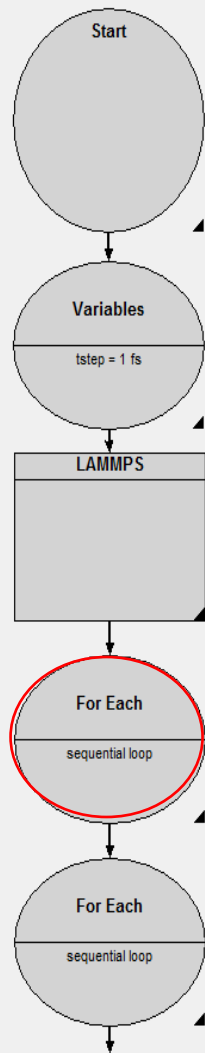
Dynamics

Custom

Help

LAMMPS Command Line Explanation





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

Reading and writing flowcharts

Open Library ... Open User ... Save ...

From job: 701

Add stages

Edit ForEach stage 1

Values Flowchart

Start

Variables

tstep = 1 fs

LAMMPS

For Each

sequential loop

For Each

sequential loop

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

Variables

tstep = 1 fs
P = 0 bar

LAMMPS

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

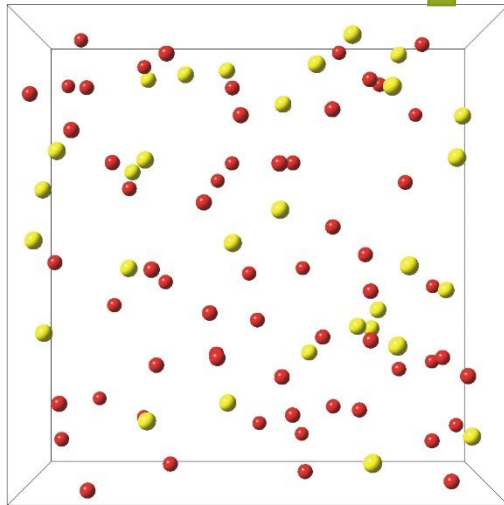
► Webinars:

- 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>

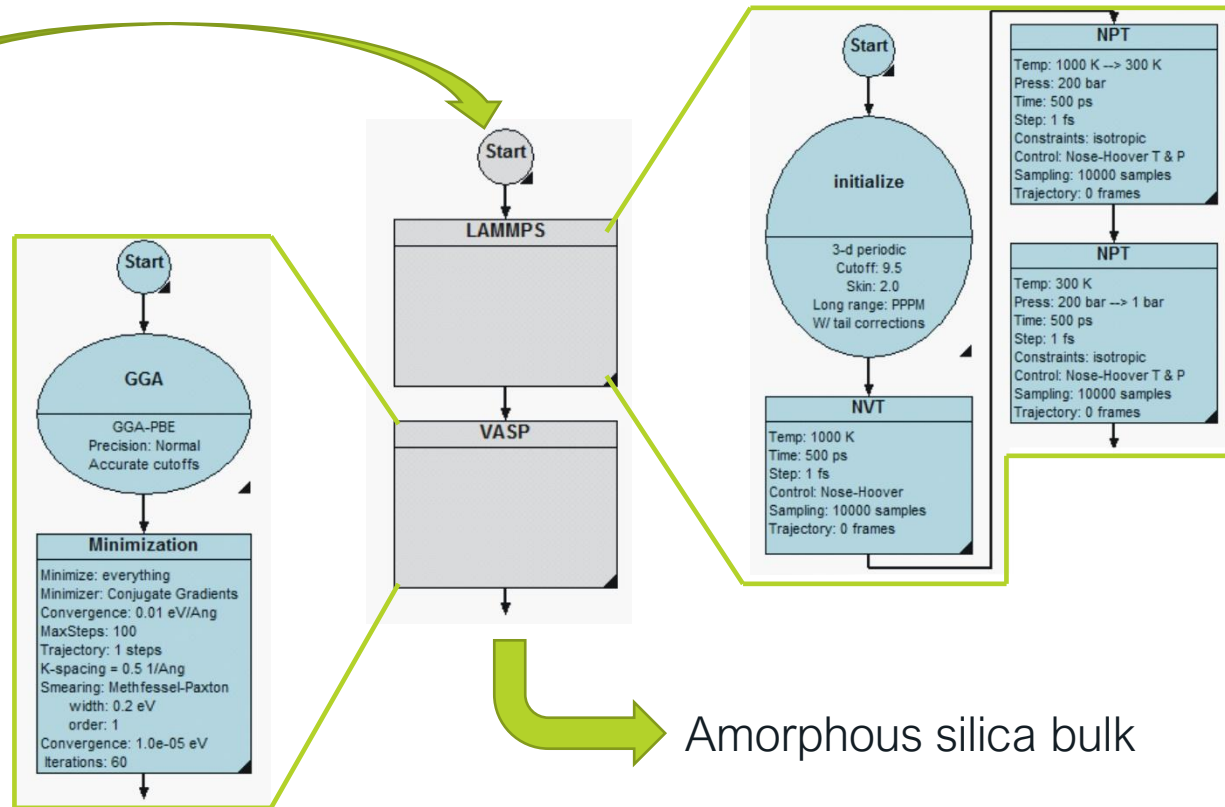


Interoperability

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



and repeat the procedure

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** Machine Learning Potential Generator

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

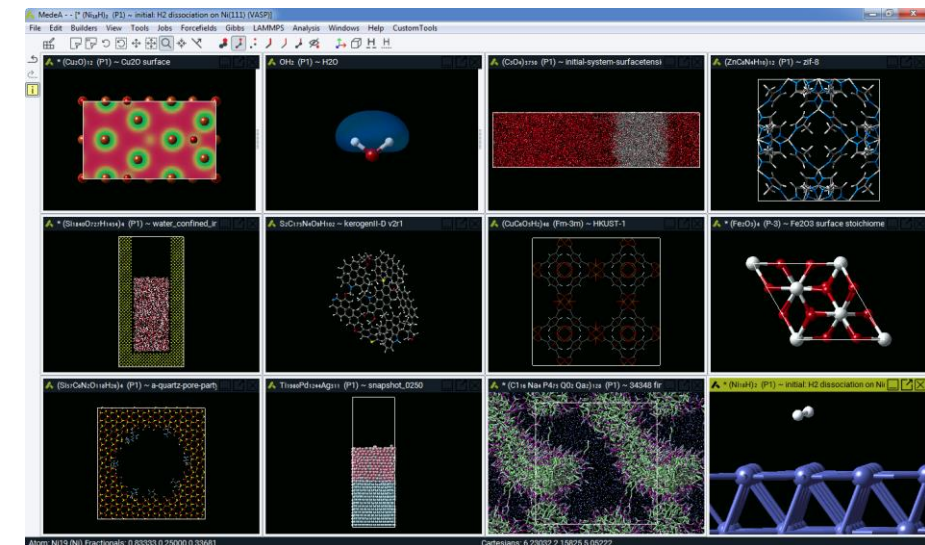
Analysis Tools

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



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

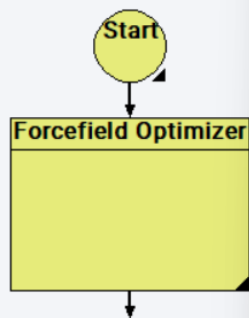
- Martini
- Shinoda

- 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.

Forcefield Optimizer

2A

Design Flowchart



Edit Forcefield Optimizer stage 1

Edit Forcefield Optimizer stage 1

Optimizing forcefield Zhou_2004

Optimizing forcefield Zhou_2004

Fitting Data Forcefield Optimization Options Flowchart

Fitting systems and properties to be fit have to be imported from a structure list file (or a trajectory).
If imported structures have already correctly assigned atom types with respect to the current forcefield, these types will
atoms without forcefield types will be assigned automatically.

Import

Fitting properties

E ☒ include Weight 1.0
Forces ☒ include Weight 1.0
Stress ☐ include Weight 1.0

Energy fitting

☒ Direct energy fit
Energy shift(s) in eV per atom types:
Fe 0.0
☐ Fit energy difference with first structure

104 fitting structures. All defined as training set

Name	Used as	Weight	Formula	# atoms	E (eV)
Fe-Im-3m-CCMR74117-min_3x3x3_2	Training	1.0	Fe54	54	-443.882
Fe-Im-3m-CCMR74117-min_3x3x3	Training	1.0	Fe54	54	-428.897
Fe-Im-3m-CCMR74117-min_3x3x3_2	Training	1.0	Fe54	54	-441.614
Fe-Im-3m-CCMR74117-min_3x3x3	Training	1.0	Fe54	54	-441.614
Fe-Im-3m-CCMR74117-min_3x3x3_2	Training	1.0	Fe54	54	-441.614
Fe-Im-3m-CCMR74117-min_3x3x3	Training	1.0	Fe54	54	-437.87
Fe-Im-3m-CCMR74117-min_3x3x3_2	Training	1.0	Fe54	54	-442.952
Fe-Im-3m-CCMR74117-min_3x3x3	Training	1.0	Fe54	54	-442.952
Fe-Im-3m-CCMR74117-min_3x3x3_2	Training	1.0	Fe54	54	-442.952
Fe-Im-3m-CCMR74117-min_3x3x3	Training	1.0	Fe54	54	-442.558
Fe-Im-3m-CCMR74117-min_3x3x3_2	Training	1.0	Fe54	54	-443.68
Fe-Im-3m-CCMR74117-min_3x3x3	Training	1.0	Fe54	54	-443.68
Fe-Im-3m-CCMR74117-min_3x3x3_2	Training	1.0	Fe54	54	-443.68
Fe-Im-3m-CCMR74117-min_3x3x3	Training	1.0	Fe54	54	-442.707

OK

Fitting Data Forcefield Optimization Options Flowchart

Type: EAM

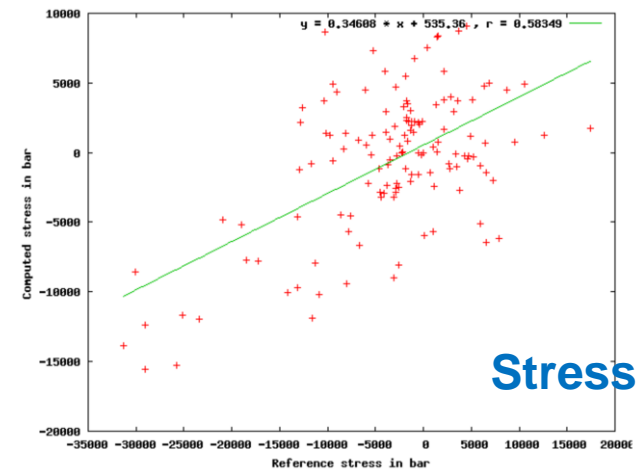
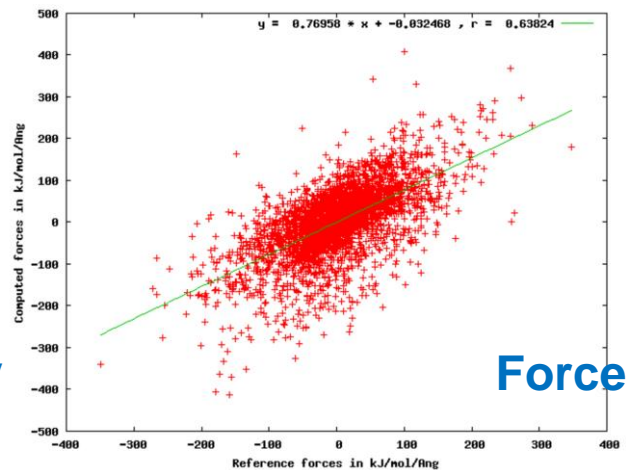
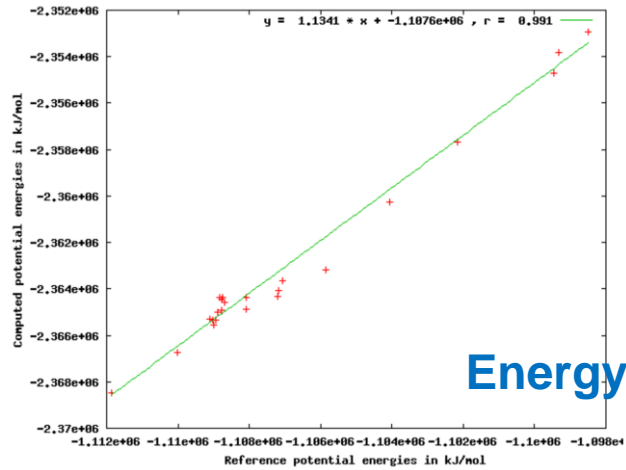
Functional Form: zhou

Types	Symbol	Units	Value	Optimize	Bounded	Lower Bound	Upper Bound
Fe	re	Ang	2.481987	<input type="checkbox"/>	<input checked="" type="checkbox"/>	0.002	20
	fe		1.885957	<input type="checkbox"/>	<input checked="" type="checkbox"/>	0.002	20
	pe		20.04146	<input type="checkbox"/>	<input checked="" type="checkbox"/>	0.02	200
	ps		20.04146	<input type="checkbox"/>	<input checked="" type="checkbox"/>	0.02	200
	a		9.81827	<input type="checkbox"/>	<input checked="" type="checkbox"/>	0.01	100
	b		5.236411	<input type="checkbox"/>	<input checked="" type="checkbox"/>	0.005	50
	A		0.392811	<input type="checkbox"/>	<input checked="" type="checkbox"/>	0.0004	4
	B		0.646243	<input type="checkbox"/>	<input checked="" type="checkbox"/>	0.0006	6
	k		0.170306	<input type="checkbox"/>	<input checked="" type="checkbox"/>	0.0002	2
	l		0.340613	<input type="checkbox"/>	<input checked="" type="checkbox"/>	0.0003	3
	Fn0		-2.534992	<input type="checkbox"/>	<input checked="" type="checkbox"/>	-30	-0.003
	Fn1		-0.059605	<input type="checkbox"/>	<input checked="" type="checkbox"/>	-0.6	-6e-005
	Fn2		0.193065	<input type="checkbox"/>	<input checked="" type="checkbox"/>	0.0002	2
	Fn3		-2.282322	<input type="checkbox"/>	<input checked="" type="checkbox"/>	-20	-0.002
	F0		-2.54	<input type="checkbox"/>	<input checked="" type="checkbox"/>	-30	-0.003
	F1		0	<input type="checkbox"/>	<input checked="" type="checkbox"/>	0	1
	F2		0.200269	<input type="checkbox"/>	<input checked="" type="checkbox"/>	0.0002	2
	F3		-0.14877	<input type="checkbox"/>	<input checked="" type="checkbox"/>	-1	-0.0001

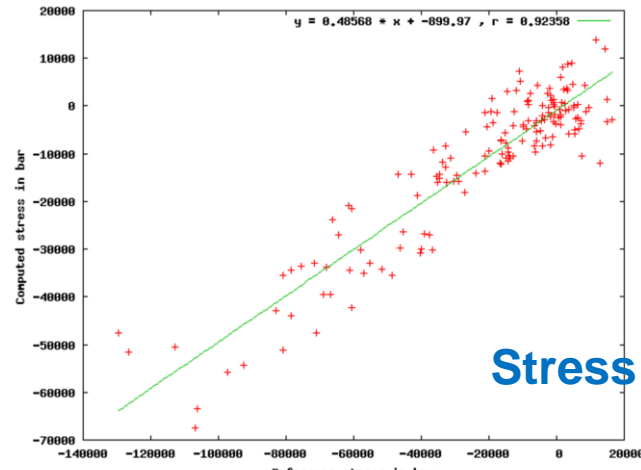
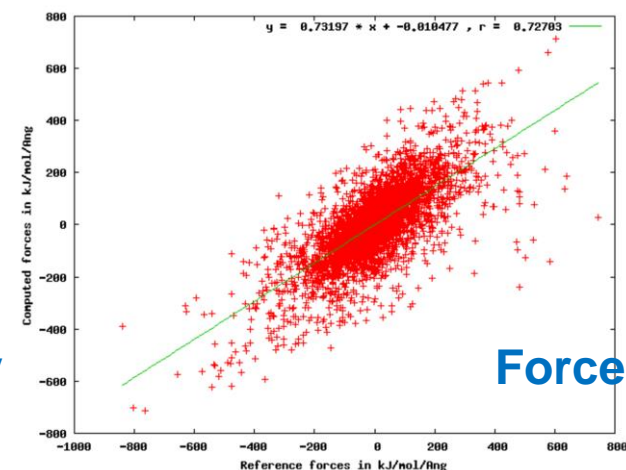
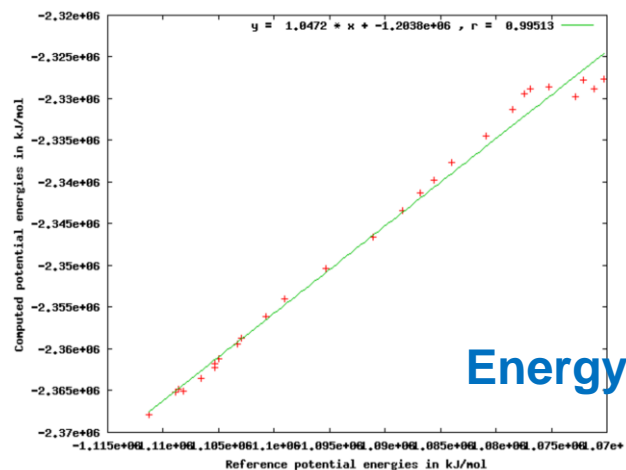
Forcefield Optimizer

- Examine fitting output graphs

Training



Validation

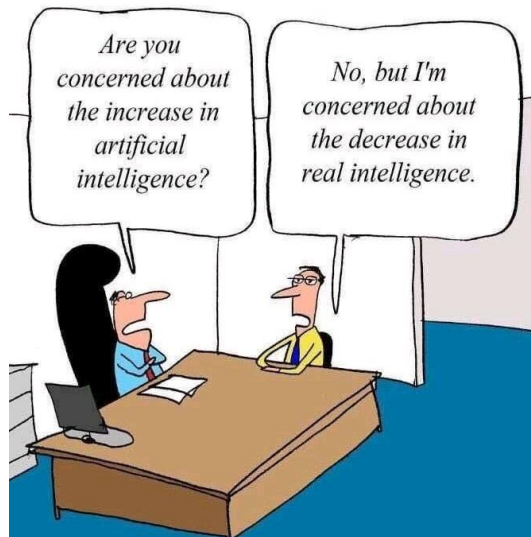


Machine Learning Potential

Build a model

Use VASP to run an ab initio MD simulation

Use the MD trajectory to train a SNAP MLP



Edit MLP generator stage 1

Structure list:

Type of machine learning potential: SNAP

Parameters for SNAP

Band limit:

Radial cutoff:

Element	Relative radius	Weight	Energy shift
Zr	<input type="text" value="0.5"/>	<input type="text" value="1.0"/>	<input type="text" value="0.0"/>
Fit:	<input checked="" type="checkbox"/> Energy	<input checked="" type="checkbox"/> Forces	<input checked="" type="checkbox"/> Stress
Weights:	<input type="text" value="1.0"/>	<input type="text" value="0.01"/>	<input type="text" value="1.0e-06"/>

► Spectral Neighbor Analysis Potential (SNAP)

Edit MLP generator stage 1

Structure list:

Type of machine learning potential: NNP

Parameters for NNP

Number of epochs:

Cutoff for symmetry functions:

Fraction of data to use as test set:

Seed for random numbers:

Fit: ☒ Forces

Weight:

► Neural Network Potential (NNP)

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** Machine Learning Potential Generator

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

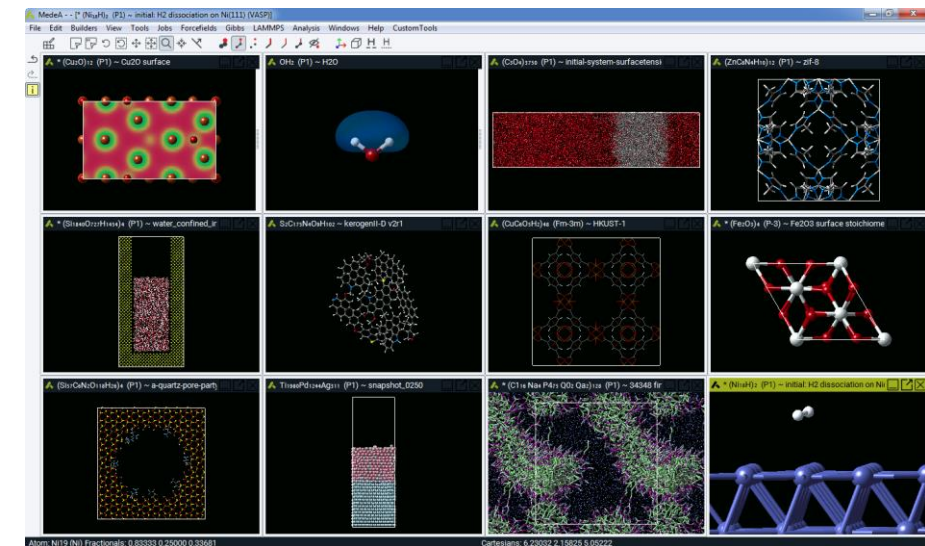
Analysis Tools

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

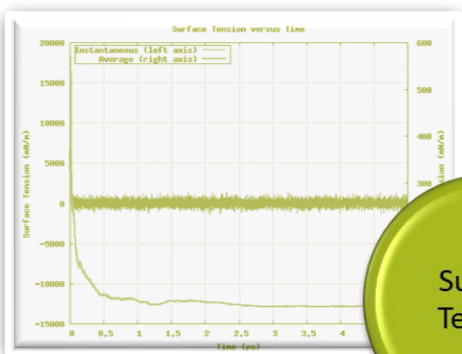
JobServer & TaskServer

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

MedeA environment



Properties Modules

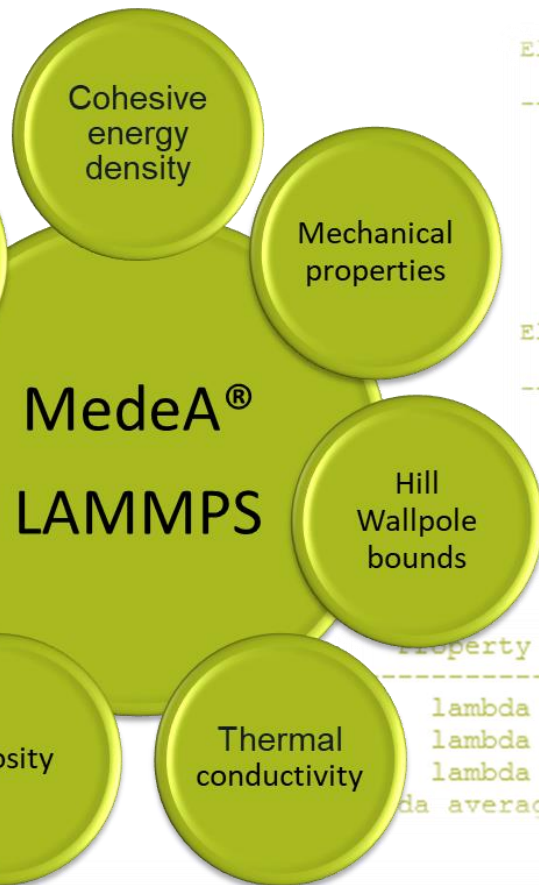


Diffusion coefficient information, derived from

Quantity	Value	+/-	Units
MSD D:	1.411e-05		
MSD-X D:	-1.45e-05		
MSD-Y D:	1.4e-05		
MSD-Z D:	4.284e-05		

Linear regression
(In Einsteinian d)

Quantity	Value
a:	-1.317
m:	0.7562 +/-



Elastic constant matrix (GPa):

	1	2
1	1.4464	0.9012
2	0.9012	1.7473
3	0.7857	0.9324
4	-0.0129	-0.0615
5	0.0818	0.085
6	0.0050	0.0050

Elastic complian

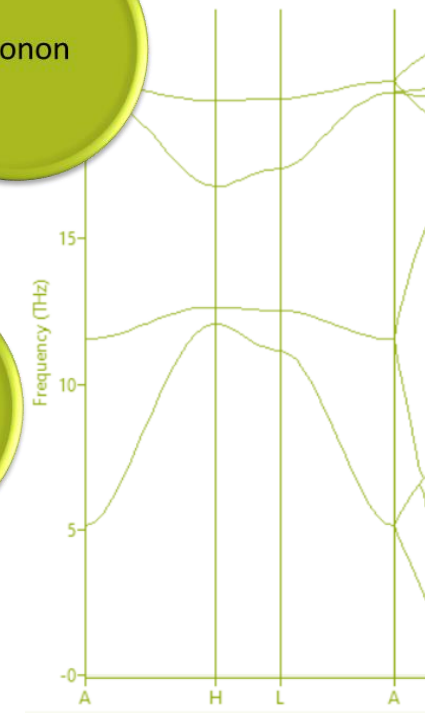
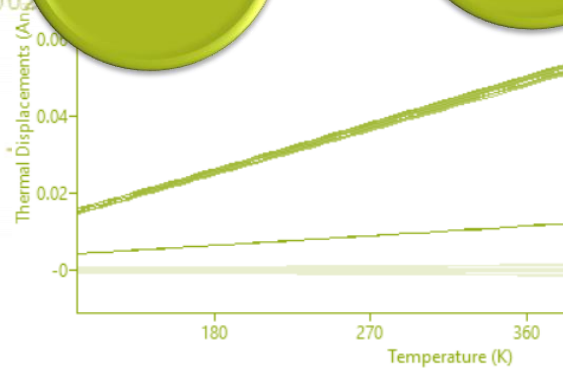
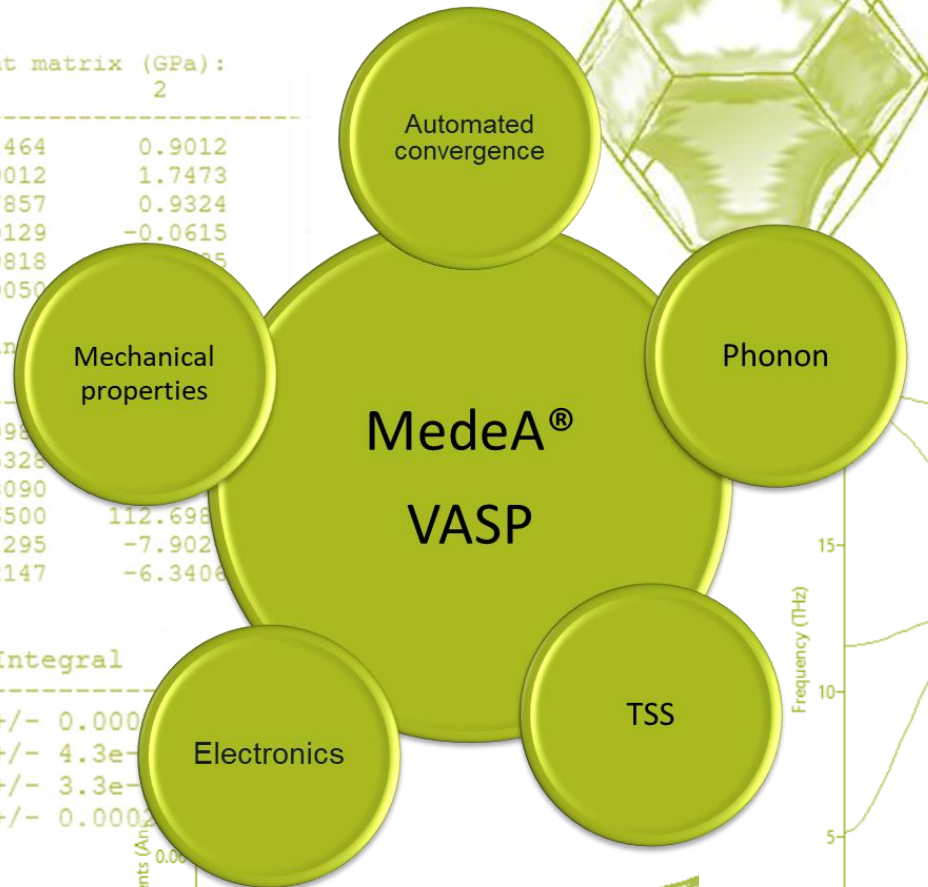
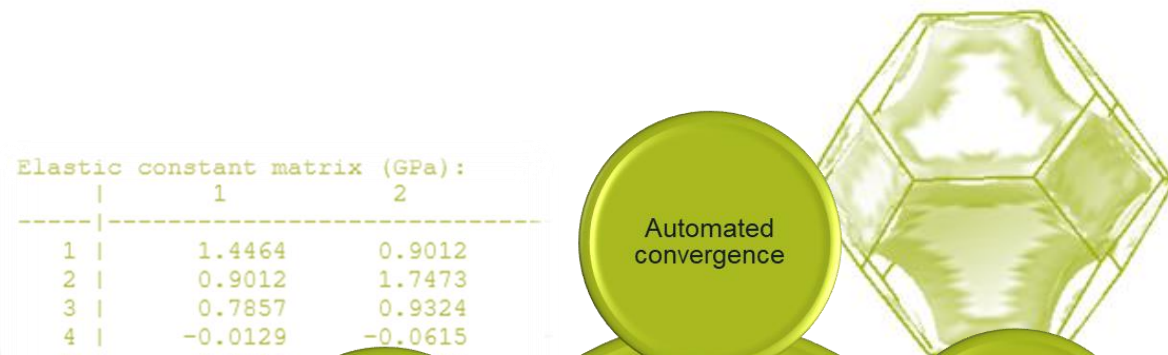
	1	2
1	1113.098	
2	-419.5328	
3	-286.3090	
4	-42.6500	112.698
5	-91.4295	-7.902
6	-10.2147	-6.3406

Property Direct Integral

lambda x	0.01712 +/- 0.000
lambda y	0.006323 +/- 4.3e-
lambda z	0.002736 +/- 3.3e-
lambda average	0.00772 +/- 0.000

Property	Direct Integral	Fit	RMS
eta x	0.010428 +/- 9.1e-05	0.010714	0.000132
eta y	0.004432 +/- 9.1e-05	0.002375	4.2e-05

© Materials Design, Inc. 2022



Phonon Module

- MedeA Phonon is based on the PHONON program authored by Prof. Krzysztof Parlinski^{2,3}
- 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.

MedeA : Run Phonon

Calculation Supercell Advanced Phonon Dispersion Phonon DOS IR/Raman/LO-TO

Type of calculation: Full Brillouin zone

Parameters for calculation

Supercell constructed from: conventional cell

Interaction range: 10.0 Ang

Displacement of atom: +/- 0.02 Ang

Available properties

Phonon dispersion curve and form factors

Phonon density of states (DOS)

Thermodynamic functions

☒ Accurate electronic energy for thermodynamics

☐ Temperature dependent electronic contributions (DOS) to thermodynamic functions (for metals)

☐ Infrared spectra and LO/TO mode split (for insulators and semiconductors)

☐ Raman spectra (insulators and semiconductors)

Task

Action: Run all

☒ Relax atom positions of supercell without displaced atoms

☒ Start from wave functions of other supercells

Phonon supercell calculations: VASP Settings

Electronic energy and DOS contributions: VASP Settings

MedeA : Run Phonon

Calculation Supercell Advanced Phonon Dispersion Phonon DOS

Supercell constructed from conventional cell.

Supercell to Obtain Phonons: New Lattice Vectors

a:	2.00000	0.00000	0.00000
b:	0.00000	2.00000	0.00000
c:	0.00000	0.00000	2.00000

The supercell extends equally in all directions and does not reduce the symmetry of the system.

Number of atoms in the supercell: 32

Number of such supercells to be calculated: 3

View supercell

☒ Manually define the path

Explicit Path

Vertex

W	0.500 0.250 0.750
L	0.500 0.500 0.500
g	0.000 0.000 0.000
X	0.500 0.000 0.500
W	0.500 0.250 0.750
K	0.375 0.375 0.750
--Add a new point--	

Reset to default path

Phonon module

Available Results

- PhononDensityOfStates
- PhononDispersion
- ThermodynamicFunctions

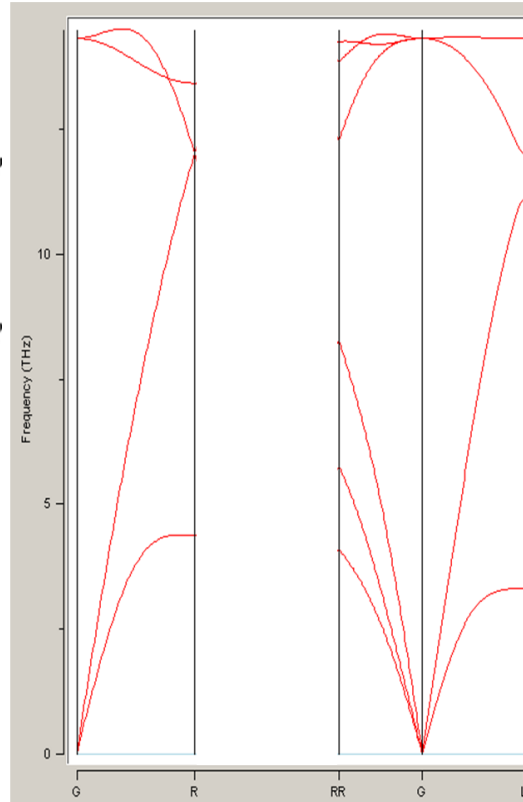
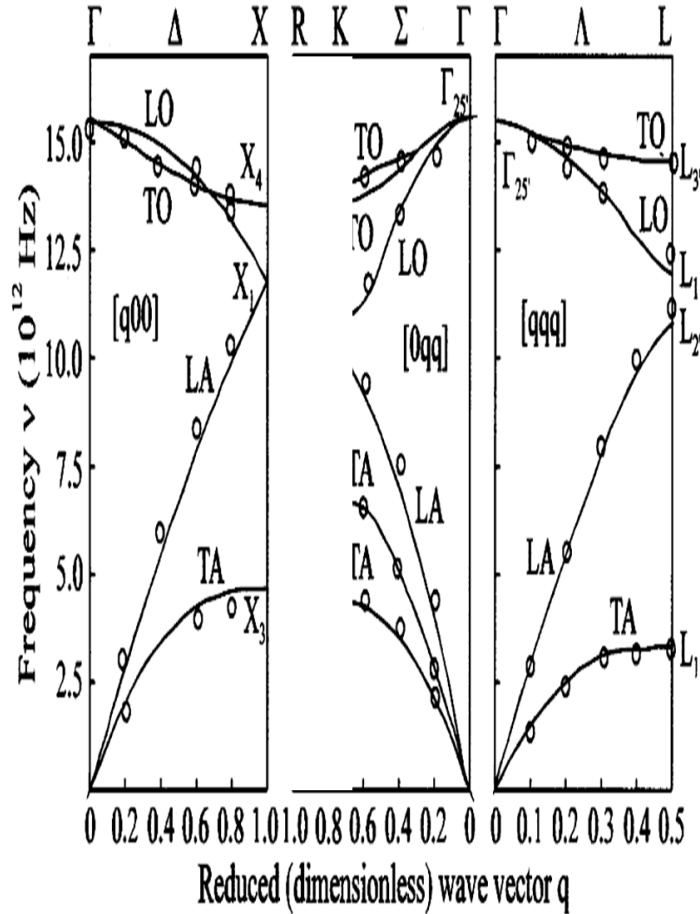
Available Output Files

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 $\langle U^2 \rangle$ as a function of temperature. One column format.
*.d32	thermal displacements $\langle U^2 \rangle$: XX, XY, XZ, YX, YY, YZ, ZX, ZY, ZZ as a function of temperature. Six columns format. Input.
*.d33	thermal displacements $\langle U^2 \rangle$: 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.

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:

- C_v : vibrational heat capacity at constant volume
- $E_{\text{vib}}(T) = E(T) - E(0)$: the change in vibrational internal energy from 0 K, where $E(0) = E_{\text{elec}} + \text{ZPE}$ 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 $E_{\text{elec}} + \text{ZPE} + E_{\text{vib}}(T)$
- $A(T)$: the electronic plus vibrational Helmholtz free energy, $E(T) - T.S(T)$

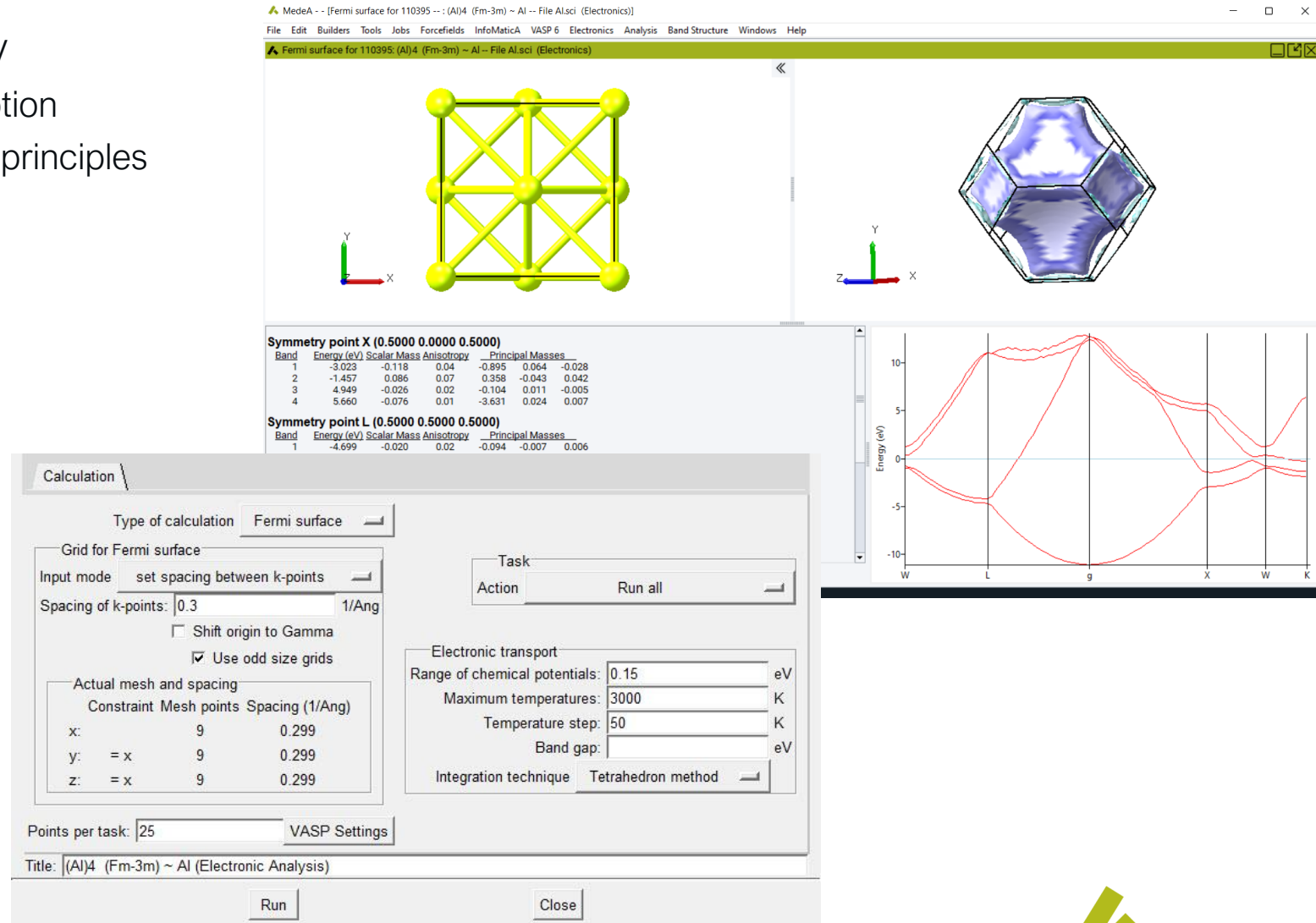
Note that the electronic energy, which is part of the enthalpy and free energies, is set to zero because the reference energies of the elements in their standard state are unavailable.

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	C_v 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	31.4170	2.9527	20.6527	1.4692	16.4700	12.0481

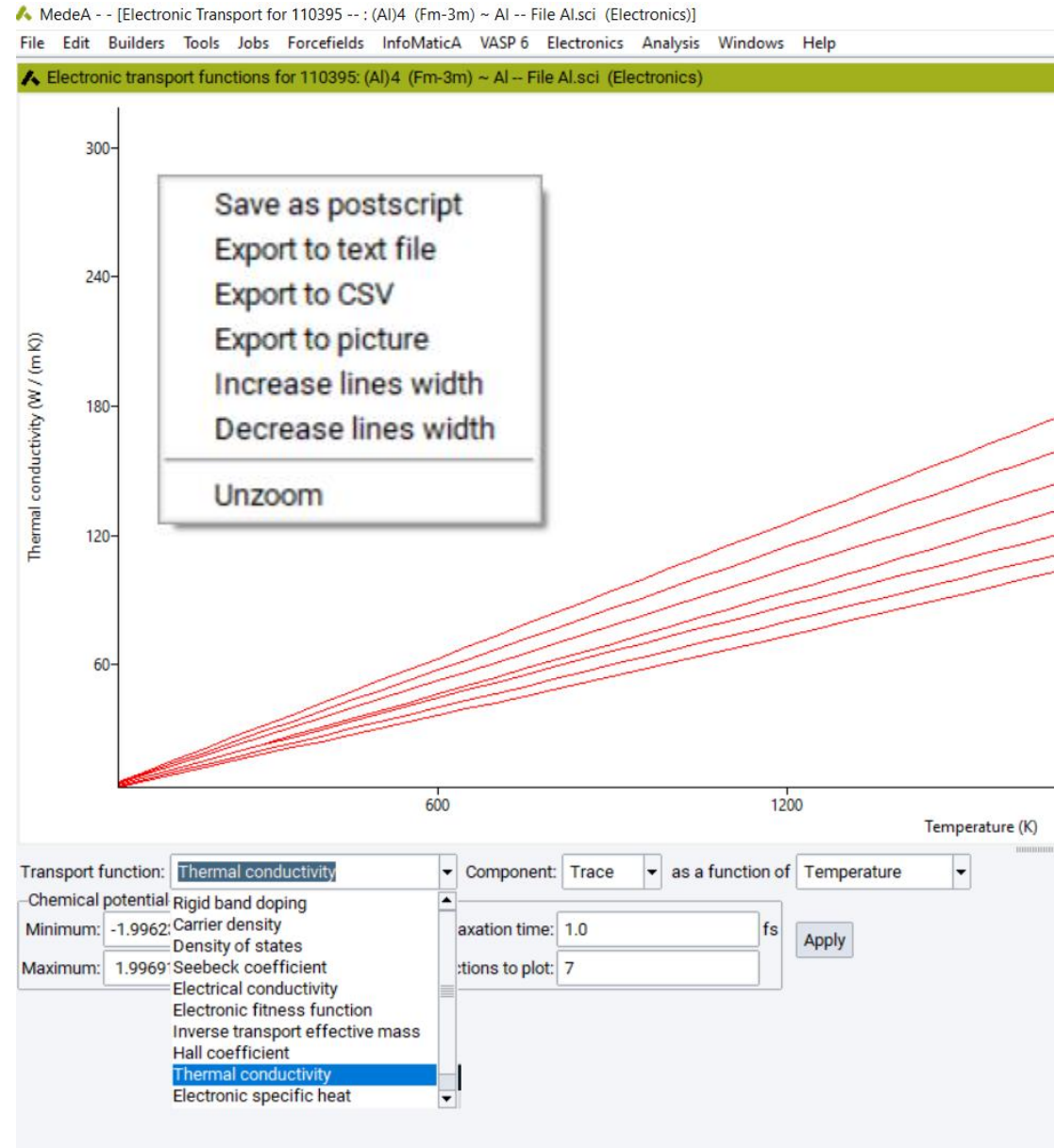
Electronics module

- 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



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](https://doi.org/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

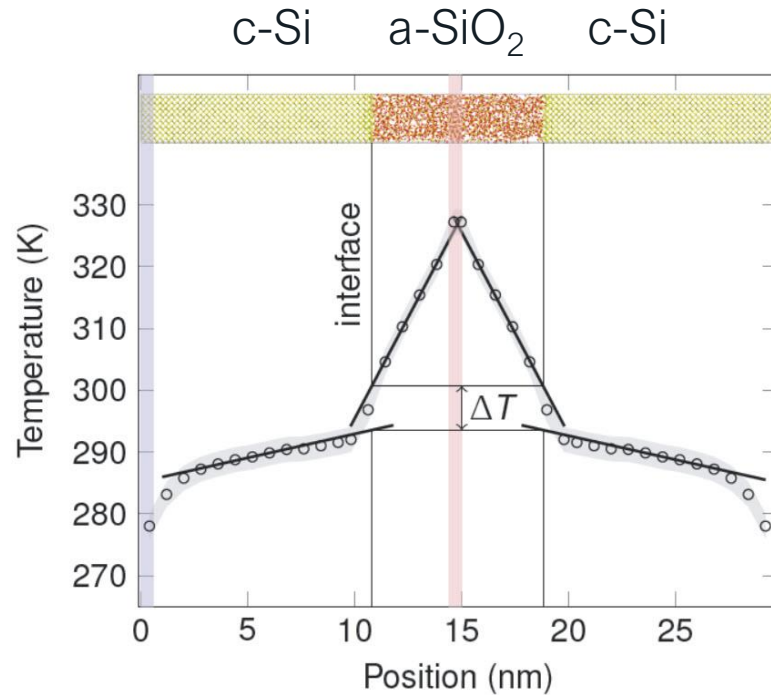
Yu Li ^a  , Kuan Ma ^a, Xing Fan ^{a, b}, Fusheng Liu ^a, Junqin Li ^a  , Heping Xie ^a



Thermal Conductivity

Reverse non-equilibrium molecular dynamics

Sharp interface between crystalline Si and amorphous SiO₂



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⁻¹K⁻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>

Example

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

***Ab initio* parameterization of a charge optimized many-body forcefield for Si–SiO₂: Validation and thermal transport in nanostructures**

Arthur France-Lanord,^{1,2,a)} Patrick Soukiassian,² Christian Glattli,² and Erich Wimmer¹

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*

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** Machine Learning Potential Generator

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**

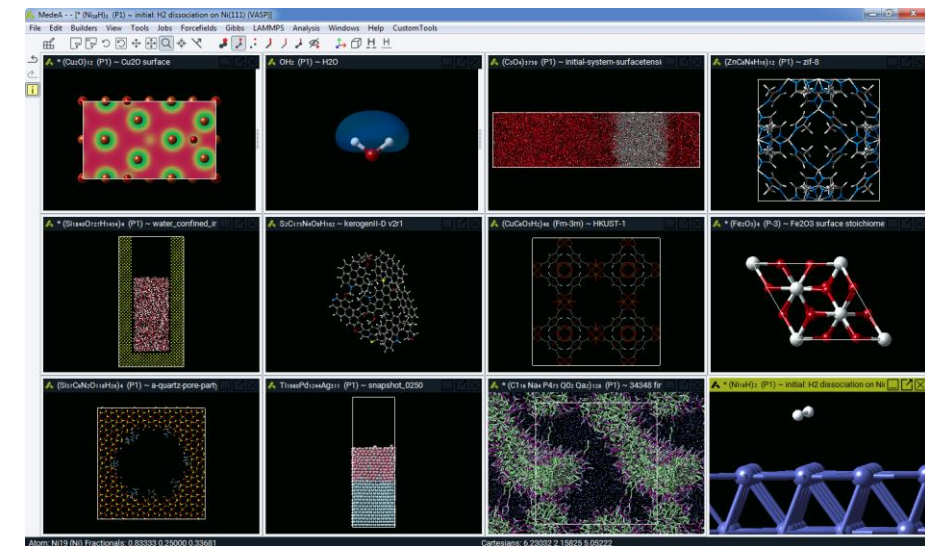
Analysis Tools

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

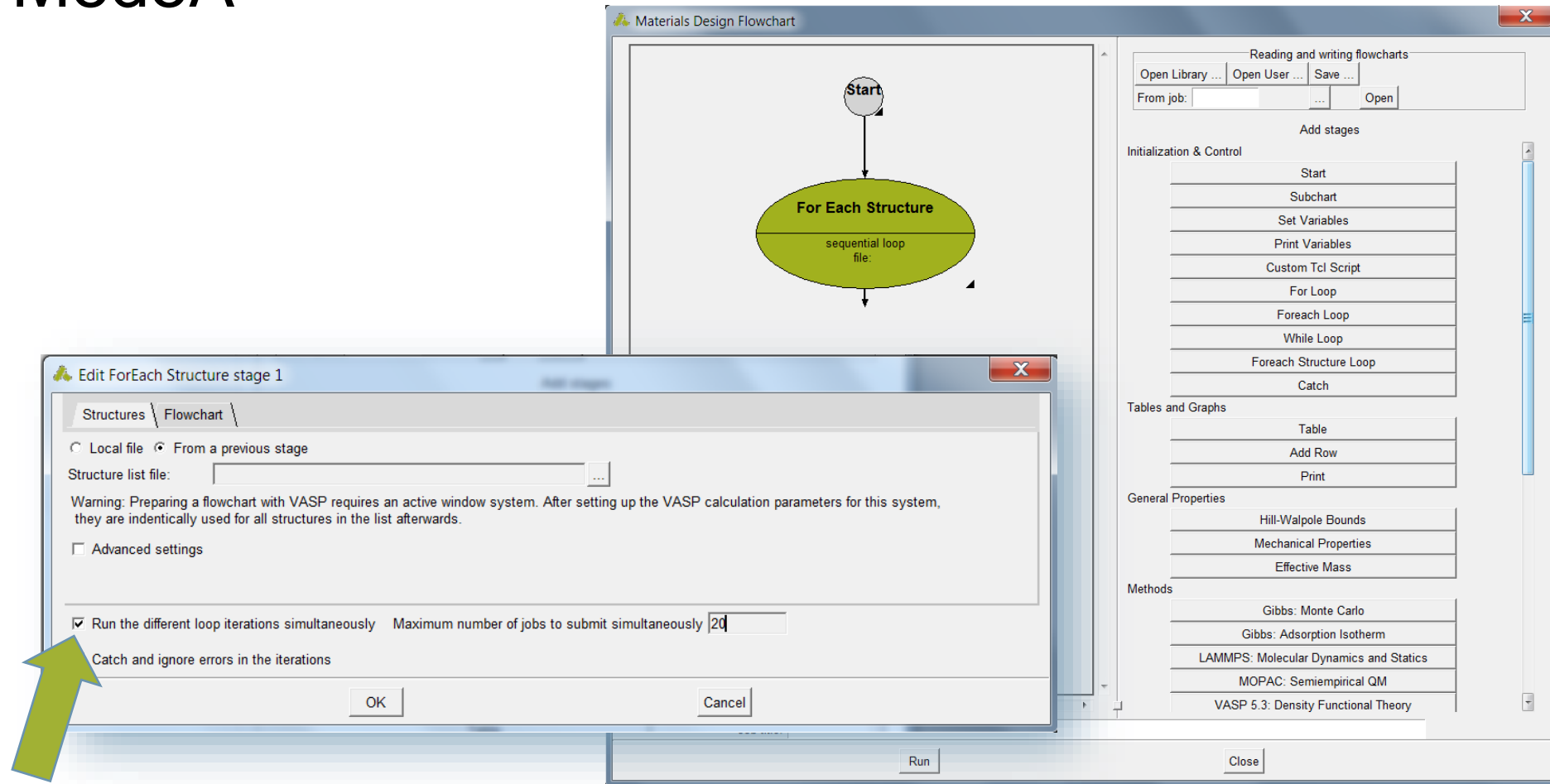
JobServer & TaskServer

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

MedeA environment



HT in MedeA



- Value: Highly efficient screening of large number of compounds

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** Machine Learning Potential Generator

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**

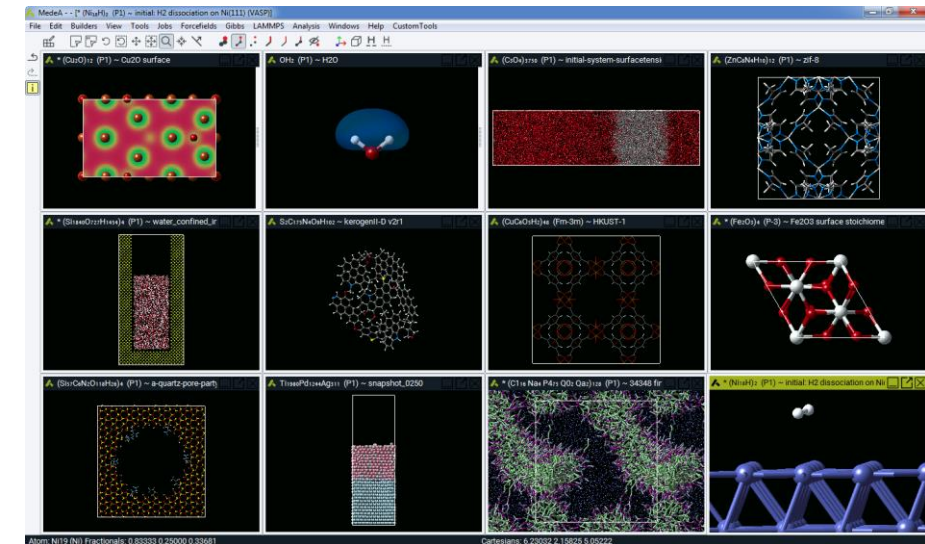
Analysis Tools

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



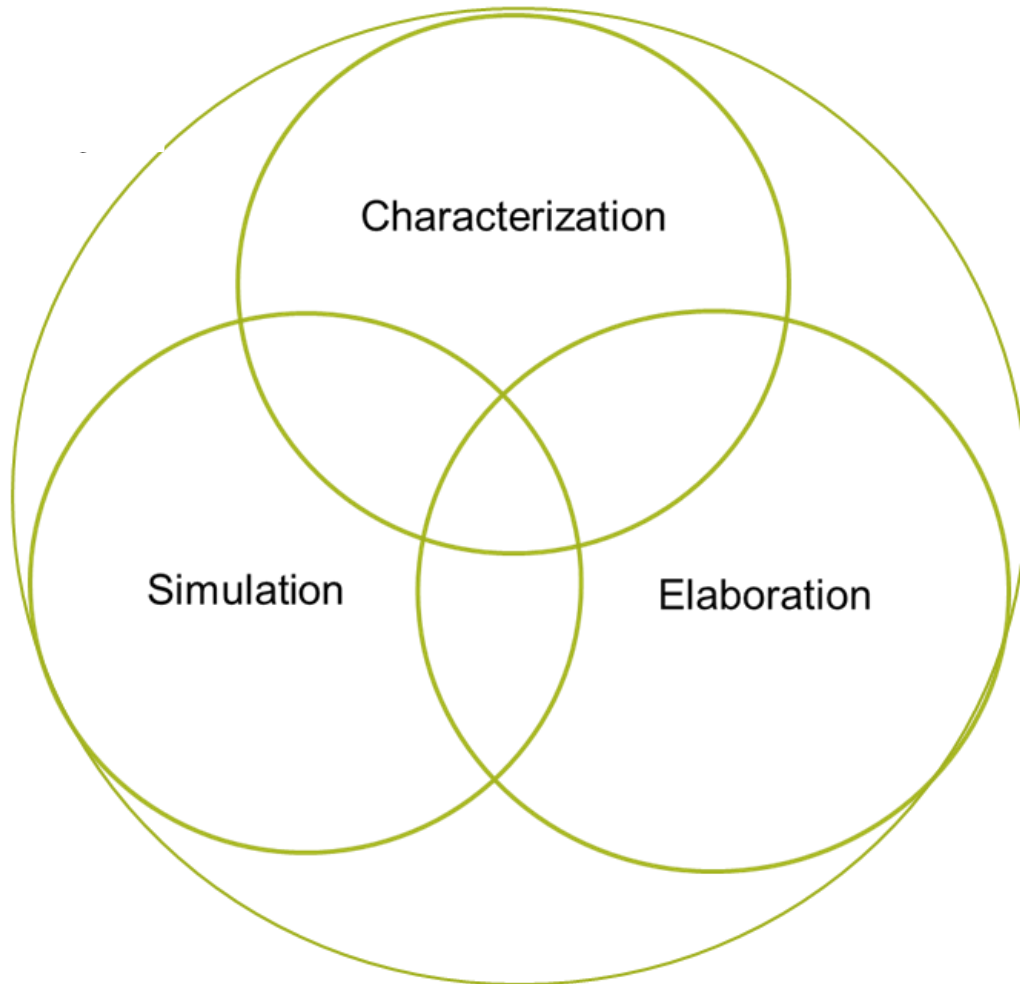
MedeA's 3-Tier Architecture

- 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.

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.**"*

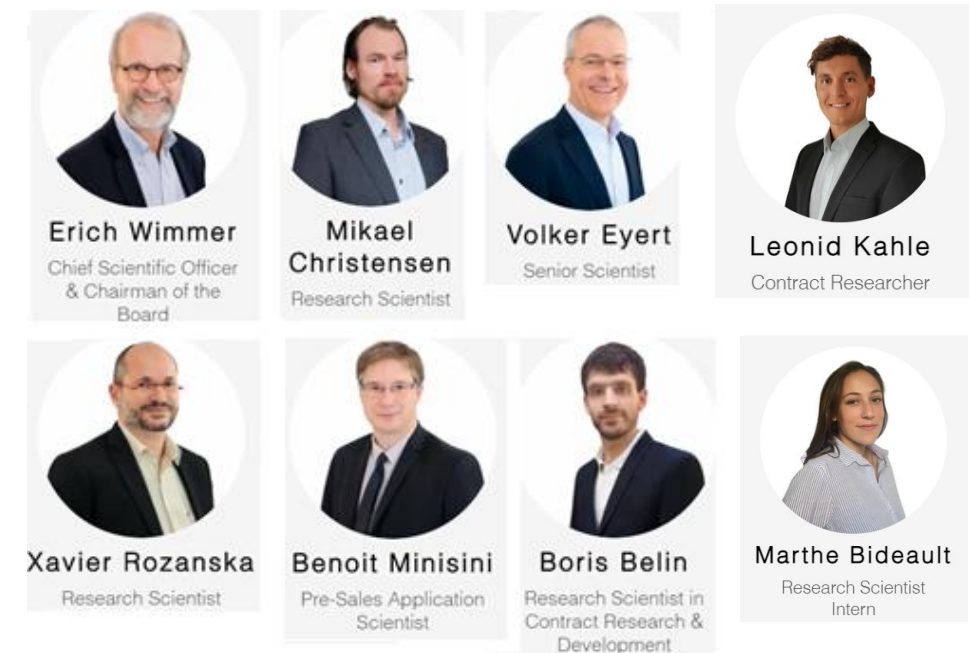
-Michael L. Zerkle, Ph.D.
Senior Advisor, Reactor Physics Methods Development,
Naval Nuclear Laboratory

Materials Design: Technical Teams

Development Team



Research Team



Support Team

