MedeA Flowcharts: Design and Automate Simulation Workflows

Contents

The *MedeA* environment provides graphical flowcharts to support the efficient construction of complex computational protocols. These flowcharts can be easily created to describe and control the flow of calculations, allowing simple and straightforward access to the various computation engines of *MedeA*, such as *LAMMPS*, *GIBBS*, *VASP*, *MOPAC* and *Gaussian*. These different engines may be combined within a single flowchart, so that a VASP optimization of a unit cell, for example, may be employed as a prelude to a larger scale LAMMPS simulation using an embedded atom method (EAM) forcefield. In addition, the structure can be modified within the flowchart using the provided building and editing capabilities.

The backbone of the flowchart infrastructure is the Tcl language (see https://www.tcl.tk/) which can be directly accessed within custom-scripting stages. Once created the flowcharts can be saved as ASCII files allowing them to be reused and distributed.

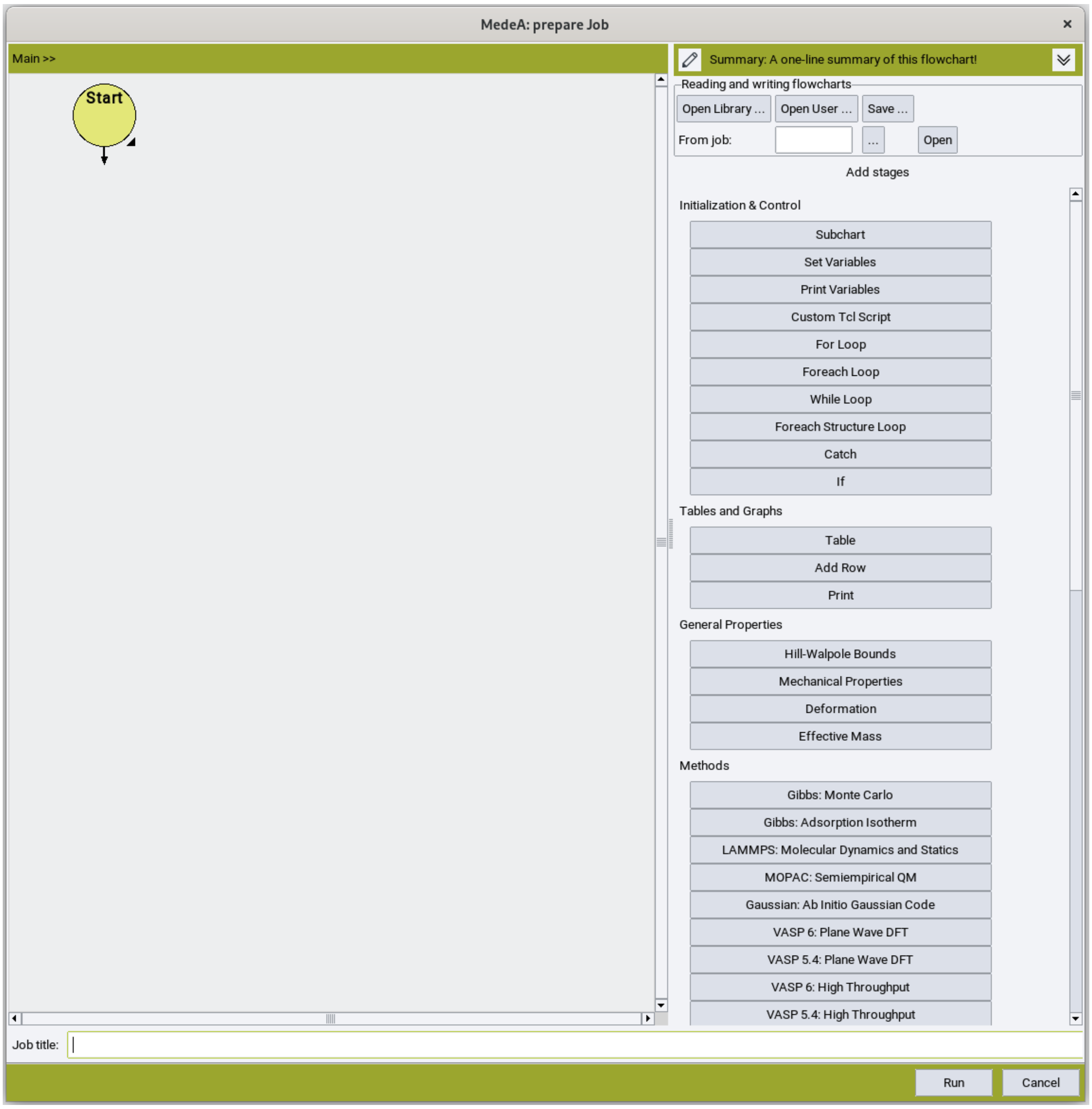
Although flowcharts are customizable and flexible their use is straightforward. In this section the basic concepts are summarized, allowing for the construction of both simple and complex flowcharts. Additional details for specific tools are provided elsewhere within the *MedeA* User's Guide.

1 Flowcharts Overview

Flowcharts are accessed via the Jobs >> New Job... menu item. This command yields the main flowchart user interface, where flowcharts are constructed, read from disk or previous calculations or saved to the disk.

Flowcharts provide a variety of control capabilities, such as a While Loop, For Loop, Foreach Structure Loop, If and Foreach Loop. This allows for considerable flexibility in the automation of simulations. For example, a scan of possible system temperatures and pressures for molecular dynamics calculations may be achieved with nested Foreach loops.

Additionally, custom Tcl scripting may be included in a flowchart. Key results from simulation stages are available as variables, which can be operated on, tabulated, and also used to control subsequent stages, allowing the convenient construction of highly automated procedures for selected applications. If more complex manipulation of the results are required, a custom Tcl stage can be used to process the outputs of the current and any previous stages.



Materials Design flowcharts begin with the `Start` command which is automatically placed on the left-hand panel of the flowchart dialog. Typically after the `Start` stage, several variables will be set using a `Set Variables` stage. The stage is added to the flowchart by clicking the `Set Variables` button on the right-hand panel.

In general, stages are added to a flowchart by clicking the appropriate element on the right-hand pane of the flowchart dialog or user interface. Once added to a flowchart, most stages may be edited by either right-clicking that element and selecting `Edit`, or double-clicking on that stage.

A summary of the functionality and use of specific flowchart elements is provided below.

2 Initialization and Control

This section of the flowchart interface provides the following stages: Subchart, Set Variables, Print Variables, Custom Tcl Script, and loop related commands: For Loop, Foreach Loop, While Loop, Foreach Structure Loop, Catch and If.

As discussed above, every flowchart begins with a Start stage, this is employed as the starting point of execution for the flowchart and is automatically included in the flowchart. The Subchart stage is simply a container that can hold other flowcharts. This provides a convenient way to break up a large more complicated flowchart into simpler parts and provides a simple way to include a previous flowchart as a building block into a more complicated protocol.

The Set Variables stage allows the user to set the value and units of specific variables that will be employed in later stages in the flowchart. For example, the Set Variables stage can be used to set:

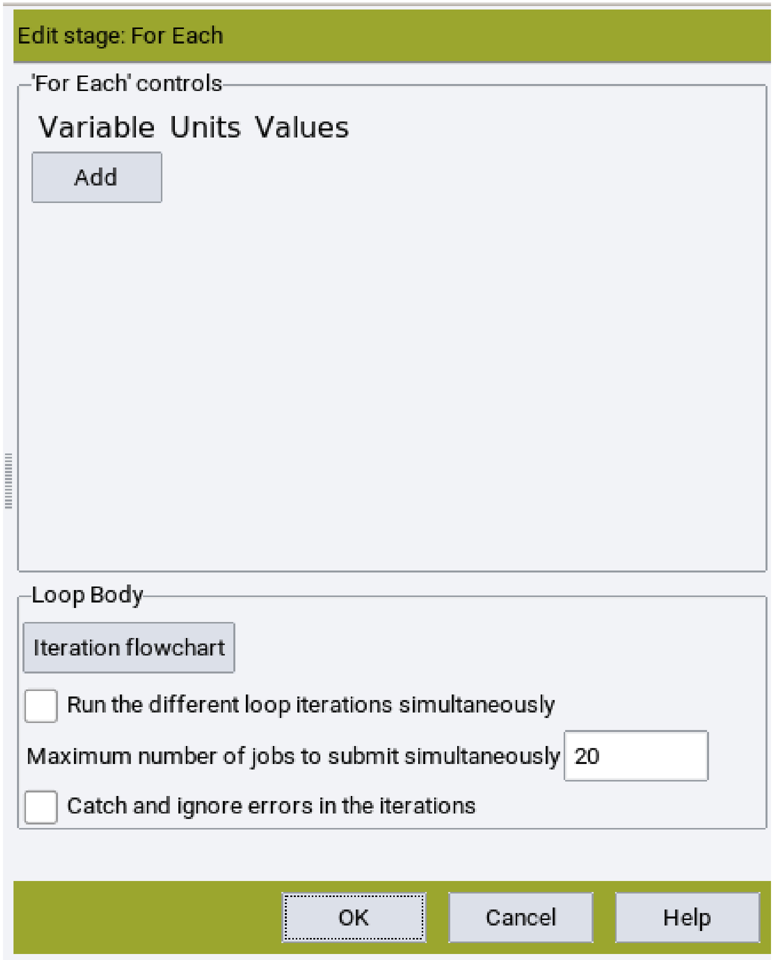
Variable	Value	Unit
T	300	K
tstep	1	fs
P	1	atm

These variables will then be used throughout subsequent stages in LAMMPS calculations, which employ `T`, `tstep`, and `P` as default variables for temperature, timestep, and pressure, respectively. This centralization of the variable setting is convenient in exploring the effect of the system variables on simulated properties. Once declared variables can be accessed, following the Tcl paradigm, by adding a `$` sign in front of the variable name, for example, the variable `tstep` can be accessed with `$tstep`.

The Print Variables reports (calculated) variables matching a specific name, including variables created and made accessible by any previous stage. These variables can be printed to tables or added to structure lists.

The Custom Tcl Script allows you to enter, or retrieve from a file Tcl commands (see https://www.tcl.tk/) which may be used to carry out specific actions during the execution of a flowchart. This can be useful in preparing result summaries or in determining whether specific simulation conditions have been met.

The For Loop includes a flowchart executed repeatedly as defined by the control variables and test conditions.



The Foreach Loop and While Loop stages allow for the introduction of control structures within a flowchart. In each case, allowing for the introduction of a complete flowchart to be executed repeatedly until the foreach vector (like {`T, P`}) of variables is exhausted, or the while condition is no longer true.

The Foreach Structure Loop takes structures contained in a Structures List or a previous Trajectory and performs on each of these structures the same calculation protocol as defined in the Foreach Structure Loop flowchart. This stage is part of the *MedeA HT-Launchpad* module.

Stages within the loops are executed either sequentially, meaning that each iteration is completed before the next is started, or simultaneously, where multiple iterations run in parallel. The **simultaneous** operation mode can be switched on by checking Run the different loop iterations simultaneously, specifying the degree of parallel operation by the parameter Maximum number of jobs to submit simultaneously. All looping structures have an option to Catch and ignore errors in the iterations.

The Catch stage allows for more elaborate error handling, that is in case the flowchart runs into an error, it is caught and another flowchart is executed.

The If stage allows execution of a flowchart if a condition is true (then), or an alternative flowchart (else).

3 Tables and Graphs

This section allows defining a Table, insert results as soon as they occur with Add Row, and finally Print the entire table. The flowchart below is just an illustration, leaving out all looping and calculation.

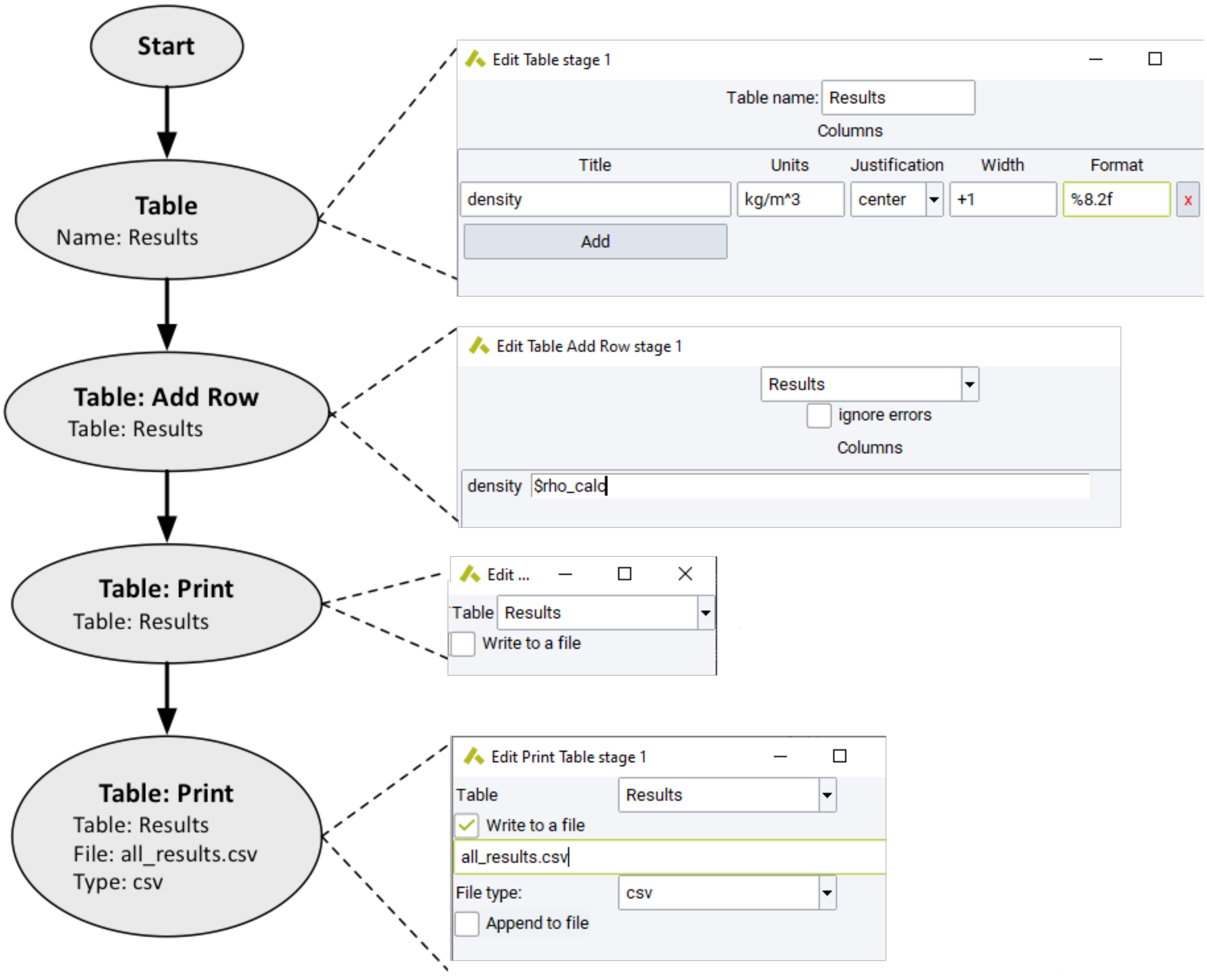


Table name: Results

density | kg/m^3 | center | +1 | %8.2f

Results

☐ ignore errors

density $rho_calc

Table Results

☐ Write to a file

Table Results

☑ Write to a file

all_results.csv

File type: csv

☐ Append to file

With Table you define a Table by giving it a name and adding columns. Each column has a

- `Title:` Name of the column
- `Units`: Results are converted into units chosen. If no unit is specified, the default unit is used.
- `Justification`: Left, right, or center
- `Width`: How much "space" on the left and right
- `Format`: Can be provided in the printf format. For example; `%#d` or `%#i` for integer values, `%#.#f` for float/double values, `%#c` for characters, `%#s` for strings, and `%#x` for hexadecimal values.

> **Hint:** The maximum number of characters/digits that can be used to print a given variable can be defined by an integer value `#` between the `%` sign and the character. In the case of a float value two numbers, separated by a comma, can be used. In this case, the second number defines the number of digits after the comma used to print the value. For example, `%8.2f` displays a floating-point variable with up to 8 characters in total and two digits after the comma.

Table: Add Row adds a line of results to a specified table. Variables can be added, following the Tcl paradigm, by adding a `$` sign in front of the variables name, e.g., the variable `Etotal_calc` can be printed with `$Etotal_calc` into a table. See *Available Variables* for a list of available variables that can be added.

Table: Print the selected Table. You can also save or append the result to a file as formatted text, comma separated values (csv), tab-delimited , or delimited by a different Separator like `;`.

4 General Properties

`Hill-Walpole bounds`: applies Hill-Walpole statistics on top of Mechanical Properties (see the section on Hill-Walpole bounds for amorphous systems).

`Mechanical Properties` determines the mechanical properties with LAMMPS or VASP based on given `Strains`. For more information refer to the chapter on the Theory of elasticity.

`Deformation` performs deformation simulations beyond the elastic regime with LAMMPS or VASP. For more information refer to the MedeA Deformation section.

`Effective Mass`: uses VASP to determine the effective mass for a specified k-point. For a more detailed description of the use of this stage see the section on Accurate Effective Mass calculations.

5 Methods

The Methods section of the flowchart interface provides access to a computational engine such as GIBBS, LAMMPS, MOPAC, GAUSSIAN or VASP (VASP flowcharts or a stage accessing the VASP GUI otherwise accessible from the Tools menu). In each case, the interface provided allows you to start a new flowchart and execute relevant specific commands within this new flowchart.

In addition, there are methods available making use of the computational engines above to calculate vibrational properties, phonon dispersion, and phonon density of states (Phonon), to optimize cluster expansions for alloys and other disordered systems and perform Monte Carlo simulations for larger ensembles (UNCLE), to predict properties of polymers using correlations (P3C) or group contributions (QSPR), and to optimize force field parameters by fitting to *ab initio* data (Forcefield Optimizer and MLP Generator).

Additional information on each of the Methods available in this section of the flowchart interface is available in the section of the **User's Guide** dealing with each method.

6 Building and Editing

Flowchart building commands allow for the construction and adjustment of atomic models.

6.1 Set Cell

The `Set Cell` stage permits the adjustment of unit cell dimensions for periodic systems. Here a variety of options are supported, the density or volume may be specified, or an expansion factor applied to the current system, or specific unit cell dimensions set. This stage may be combined with an appropriate `Foreach Loop` to explore the volumetric or density-specific behavior of a given system property.

6.2 Change periodicity

A stage to turn on or remove periodic boundary conditions. In this stage the specify a gap to leave between the periodic building blocks. This stage may be used to combine a non-periodic calculation, for example with MOPAC, with a periodic VASP calculation.

6.3 Supercell

The `Supercell` command may be applied to increase the size of a given model. As this building process is executed on the JobServer this is an efficient mechanism to create large systems.

6.4 Amorphous builder

The `Amorphous Builder` stage can be used to create amorphous models. *System composition source* can be set to the `current system`, where the current structure is split into molecules and recombined, to `composition files` saved on the local machine, and to a composition used in a previous job with `jobserver`. The *system geometry* of the amorphous material can be either `bulk cell` or `layer` and is build according to the set `Temperature` and cell dimensions. The latter is set with *specify cell* and can be a mixture of the specific cell dimensions a, b, and c in combination with density. Accordingly, additional options become available. The number of mols of the defined composition is set with *Nmols*. As this is a stochastic process the *number of configurations* that is to be created can be set. Multiple amorphous structures can be used to determine the average property of a given model. See the section on Amorphous Materials Builder for more information.

6.5 Thermoset Builder

The `Thermoset Builder` creates a single configuration of a densely crosslinked thermoset structure from an equilibrated bulk amorphous system. See the section on Thermoset Builder for more information.

6.6 Translate Atoms

The `Translate Atoms` command can be used to adjust the position of atoms within the current system. Thereby it is possible to `explicitly` select atoms of the active structure or to select a `subset`. Atoms can be translated `by a translation` vector or `to a point`. The displacement can be in `fractional` or `cartesian` coordinates.

6.7 Docking

The `Docking` stage combines two structures. The host structure is the 'stream' structure upon which the Flowchart is operating. The `Guest from Job` is specified as the final.sci of the specified job on the current Job Server, the Host is specified as the input structure submitted with the flowchart. `Number of guests` defines how many guest molecules are put into the host, for each guest this process is repeated for `Maximum iterations`. The `Maximum displacement` (Ang) should be larger than the diameter of any ring to avoid the interlocking of molecules. `Scale rotations by` and `Temperature` (K), as well as the underlying theory, is explained in the section on Docking.

6.8 Randomly Substitute Atoms

Replaces a defined number of atoms, accounting for the symmetry of the structure, of *element A* with either *vacancies* or atoms of *element B*. For more information refer to the section on Random Substitution.

6.9 Simple Dynamics & Minimization

This stage uses the same simple dynamics and minimization algorithm that is also accessible from the MedeA GUI. The `Number of dynamics steps` and the `Number of minimization steps` can be set separately. Use this stage to pre-optimize a structure before applying a computationally more demanding algorithm to it.

6.10 Subset Manager

Manipulate existing subsets in a structure.

7 Structures Lists

These are a collection of commands to handle Structures Lists:

New List creates a new structure list that is accessible by the current flowchart. The List name and the File name of the structure lists can be defined. If no subfolder is specified the list will be placed in the job folder. The list can be initialized from an initial list that is saved locally on the machine running the MedeA GUI. Note, that multiple structure lists can be active at the same time.

Save to List adds the current structure to any of the active structure lists. In addition, the structure can be saved with multiple properties.

Extract from List will extract a structure, specified by Structure index and Configuration index, from any of the active lists.

Sort List will sort any of the active structure lists according to a specific property.

Remove Duplicates from List remove all duplicates from a given list. Duplicates are identified by making use of symmetry.

Compute Descriptors on a list define and compute descriptors on a list.

Apply QSAR model on a List by loading the equation from an XML QSAR model file.

For more details, please see the MedeA High-Throughput section.

Documentation_HT

8 Forcefield

Set Forcefield allows you to specify a forcefield.

Assign Atom Types and Charges allows you to readjust or set atomic forcefield parameters. This requires a forcefield with auto-typing.

9 Analysis

Orientation determines the orientation of a subset to a given reference vector:(x , y , or z).

10 Available Variables

Properties listed below are made available in the flowchart after a specified stage as **variables**. To access the value of any of these variables use a `$` sign in front of the property name. For example, the value of the variable `Etotal_calc` can be accessed with `$Etotal_calc`.

10.1 Structure-Specific Properties

Different properties of structures (systems) are available through variables without performing any calculation. The name of the active system can be accessed with `$system_name`.

Table1: System-specific variables

Property	Unit	Description
system_name	none	name of the active system

Values of the properties listed in the below table can change after calculations, i.e. can be different prior and after calculations are performed. The syntax to access the value of any of the properties is `[$system get property]`, whereby `[` and `]` is the Tcl syntax to declare a string in command (see https://www.tcl.tk/), and `Property` should be replaced by one of the properties in the below table. For example, the Tcl command `[$system get density]` returns the value `1.2345 kg/m^3`, i.e. a number together with a unit. The Tcl command `[$system get cell.a]` returns only a single value without a unit but the value is in the unit of Å.

Table2: System-specific variables obtainable with get

Property	Unit	Description	Remark
density	kg/m^3	mass density	only available for structures with simulation/crystal cells and periodic boundary conditions
volume	m^3	volume of conventional simulation/crystal cell	only available for structures with simulation/crystal cells and periodic boundary conditions
primitiveCellVolume	m^3	volume of primitive simulation/crystal cell with the space group P1	only available for structures with simulation/crystal cells and periodic boundary conditions
mass	kg	sum of molar atomic masses	available for all structures
forcefield_mass	none	sum of atomic masses that are determined by the assigned forcefield parameters	only available for structures with simulation/crystal cells and periodic boundary conditions after forcefield parameters were assigned
nAtoms	none	number of constituting atoms	available for all structures
nPrimitiveAtoms	none	number of atoms in the primitive cell	only available for structures with simulation/crystal cells and periodic boundary conditions
celldata	none	returns a list of the cell parameters in the sequence a, b, c, α, β, γ whereby cell lengths are in Å and angles in degrees.	only available for structures with simulation/crystal cells and periodic boundary conditions
formula	none	returns the total composition of a structure	available for all structures
empiricalFormula	none	returns the composition of the basic formula unit (stoichiometric unit) of a structure	available for all structures
empiricalRatio	none	returns the number of formula units in a structure that is determined by the ratio of the values of the variables formula and empiricalFormula	available for all structures
cell.a	none	returns the value (in Å) of the length a of the simulation cell (crystal structure)	only available for structures with simulation/crystal cells and periodic boundary conditions
cell.b	none	returns the value (in Å) of the length b of the simulation cell (crystal structure)	only available for structures with simulation/crystal cells and periodic boundary conditions
cell.c	none	returns the value (in Å) of the length c of the simulation cell (crystal structure)	only available for structures with simulation/crystal cells and periodic boundary conditions
cell.alpha	none	returns the value (in degree) of the cell angle α of the simulation cell (crystal structure)	only available for structures with simulation/crystal cells and periodic boundary conditions
cell.beta	none	returns the value (in degree) of the cell angle β of the simulation cell (crystal structure)	only available for structures with simulation/crystal cells and periodic boundary conditions
cell.gamma	none	returns the value (in degree) of the cell angle γ of the simulation cell (crystal structure)	only available for structures with simulation/crystal cells and periodic boundary conditions
charge	none	returns the total charge (number of excess electrons) of a molecular (non-periodic) structure	only available for molecular (non-periodic) structures
spinMultiplicity	none	returns the total electronic spin multiplicity of a molecular (non-periodic) structure	only available for molecular (non-periodic) structures
beadFamily	none	returns the name of mesoscale forcefield to which the beads of the mesoscale structure belong	available for all mesoscale structures (periodic and non-periodic)

10.2 Structure Lists

Values saved with structures in a structure list can be accessed for each entry in that list using the `For Each Structure` stage. Within that loop variables are accessed for the active structure with `$system_properties(NAME)` where `NAME` defines the name of the desired and available property. So, if the variable `T` has been saved with the structure then its value can be fetched with `$system_properties(T)`.

10.3 *MedeA* LAMMPS

Table3: Output from Single Point Energy and Single Point Forces stage

Property	Unit	Description
Epot_singlepoint_calc	kJ/mol	calculated potential energy
Evdwl_singlepoint_calc	kJ/mol	van der Waals pairwise energy including long-range tail correction, Coulomb interactions and interactions between bonded particles are not included
Etail_singlepoint_calc	kJ/mol	van der Waals energy long-range tail correction
Eangle_singlepoint_calc	kJ/mol	calculated energy due to angular interactions between three particles that are connected through two bonds
Ebond_singlepoint_calc	kJ/mol	calculated energy due interactions between two bonded particles
Ecoul_singlepoint_calc	kJ/mol	calculated Coulomb energy due to interactions between charged, non-bonded particles; it is the sum of the short-range Coulomb interaction calculated in real space and long-range Coulomb interaction that is calculated in reciprocal space
Edihed_singlepoint_calc	kJ/mol	calculated energy due to torsional (dihedral) interactions between four particles in a row that connected through three bonds
Eimpro_singlepoint_calc	kJ/mol	calculated energy due to out-of-plane angles interactions between 4 particles that are connected by three bonds, whereby one particle is bonded to all the other three particles
Elong_singlepoint_calc	kJ/mol	long-range k-space energy

When performing a molecular dynamics simulation the mean value of a property is returned with `{property}_calc` and its uncertainty with `{property}_uncertainty_calc`. The value of the uncertainty is given in the same unit as the calculated property. In addition, `{property}_converged_calc` is returned with the value of `1` if the calculated property has converged during the simulation otherwise it is returned with the value of `0`.

Table4: Optimization and Molecular Dynamics Simulations (last structure)

Property	Unit	Averaged	Description
t_calc	fs	no	total simulation time
T_calc	K	yes	calculated mean temperature
P_calc	atm	yes	calculated mean pressure
V_calc	$\mathring{A}^3$	yes	calculated mean cell volume
rho_calc	g/mL	yes	calculated mean mass density
Etotal_calc	kJ/mol	yes	calculated mean total energy, i.e. the sum of potential energy and kinetic energy
Epot_calc	kJ/mol	yes	calculated mean potential energy

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Table 4 – continued from previous page

Property	Unit	Averaged	Description
Ekin_calc	kJ/mol	yes	calculated mean kinetic energy
Evdw_calc	kJ/mol	yes	calculated mean energy that includes **all** of the charge-independent energy terms for interactions between particles that are not bonded, such as 3-body interactions of a Tersoff potential and a Stillinger-Weber potential, all charge-independent terms of a COMB3 potential and ReaxFF potential, all contributions of a SNAP forcefield, etc; anything related to Coulomb interactions and interactions between bonded particles are not included
Ecoul_calc	kJ/mol	yes	calculated mean Coulomb energy due to interactions between charged, non-bonded particles; it is the sum of the short-range Coulomb interaction calculated in real space and long-range Coulomb interaction that is calculated in reciprocal space
Enonbond_calc	kJ/mol	yes	calculated mean energy due to interactions between non-bonded particles, i.e. the sum of the values of Ecoul_calc and Evdw_calc
Ebond_calc	kJ/mol	yes	calculated mean energy due interactions between two bonded particles
Eangle_calc	kJ/mol	yes	calculated mean energy due to angular interactions between three particles that are connected through two bonds
Edihed_calc	kJ/mol	yes	calculated mean energy due to torsional (dihedral) interactions between four particles in a row that connected through three bonds
Eimp_calc	kJ/mol	yes	calculated mean energy due to out-of-plane angles interactions between 4 particles that are connected by three bonds, whereby one particle is bonded to all the other three particles
Eint_calc	kJ/mol	yes	calculated mean energy due to all interactions between bonded particles, i.e. the sum of Eebond_calc, Eangle_calc, Edihed_calc, and Eimp_calc.
a_calc	Å	yes	calculated mean lattice parameter a
b_calc	Å	yes	calculated mean lattice parameter b
c_calc	Å	yes	calculated mean lattice parameter c
alpha_calc	^{0}	yes	calculated mean lattice parameter α
beta_calc	^{0}	yes	calculated mean lattice parameter β
gamma_calc	^{0}	yes	calculated mean lattice parameter γ
Sxx_calc	atm	yes	calculated mean tensile/compressive stress in x direction
Syy_calc	atm	yes	calculated mean tensile/compressive stress in y direction
Szz_calc	atm	yes	calculated mean tensile/compressive stress in z direction
Syz_calc	atm	yes	calculated mean shear stress in y-z-plane
Sxz_calc	atm	yes	calculated mean shear stress in x-z-plane
Sxy_calc	atm	yes	calculated mean shear stress in x-y-plane
nSteps_calc	none	no	total number of the MD steps
Fmax_calc	kJ/mol/Å	no	calculated maximum remaining particle force after structure minimization
Frms_calc	kJ/mol/Å	no	calculated root mean square (RMS) of all particle forces after structure minimization

Additional properties available when using *LAMMPS* property modules.

Table5: Cohesive Energy Density

Property	Unit	Averaged	Description
CED_calc	J/cm^3	yes	calculated mean cohesive energy density
CEDvdw_calc	J/cm^3	yes	calculated mean contribution of all non-Coulomb, non-bond interactions to the cohesive energy density
CEDcoul_calc	J/cm^3	yes	calculated mean contribution of the Coulomb interactions to the cohesive energy density
dHvap (ideal)_calc	kJ/mol	yes	calculated mean enthalpy of vaporization (ΔH_{vap})

Table6: Thermal Conductivity

Property	Unit	Averaged	Description
deltaQ_calc	kJ/mol	no	total amount of heat that is transferred during a reverse non-equilibrium molecular dynamics (RNEMD) simulation that employs the Müller-Plathe approach to calculate the thermal conductivity
dQ/dt_calc	kJ/mol/fs	yes	mean heat transfer rate that is computed in a reverse non-equilibrium molecular dynamics (RNEMD) simulation that employs the Müller-Plathe approach to calculate thermal conductivity

Table7: Viscosity

Property	Unit	Averaged	Description
deltapx_calc	Å/fs*g/mol	no	total momentum that is transferred during a reverse non-equilibrium molecular dynamics (RNEMD) simulation that employs the Müller-Plathe approach to calculate shear viscosity
dpx/dt_calc	Å/fs*g/mol/fs	yes	mean momentum transfer rate that is computed in a reverse non-equilibrium molecular dynamics (RNEMD) simulation that employs the Müller-Plathe approach to calculate shear viscosity

Table8: Diffusion

Property	Unit	Averaged	Description
D_calc	cm^2/s	yes	norm of the calculated self-diffusion coefficient of all atoms
D_calc_subset	cm^2/s	yes	norm of the calculated self-diffusion coefficient for the atoms of subset “subset”
Dx_calc	cm^2/s	yes	calculated self-diffusion coefficient along the x-axis of all atoms
Dx_calc_subset	cm^2/s	yes	calculated self-diffusion coefficient along the x-axis for the atoms of subset “subset”
Dy_calc	cm^2/s	yes	calculated self-diffusion coefficient along the y-axis of all atoms
Dy_calc_subset	cm^2/s	yes	calculated self-diffusion coefficient along the y-axis for the atoms of subset “subset”
Dz_calc	cm^2/s	yes	calculated self-diffusion coefficient along the z-axis of all atoms
Dz_calc_subset	cm^2/s	yes	calculated self-diffusion coefficient along the z-axis for the atoms of subset “subset”

Table9: Surface Tension

Property	Unit	Averaged	Description
Surface_Tension_calc	mN/m	yes	calculated surface tension

Table10: MD Phonon

Property	Unit	Description
Evib_calc	kJ/mol	total vibrational internal energy (classical and quantum contributions)
Evib_QC_calc	kJ/mol	quantum contributions to total vibrational internal energy
Epot_total	kJ/mol	sum of MD potential energy Epot, and the vibrational quantum contributions Evib_QC
Avib_calc	kJ/mol	total vibrational Helmholtz free energy (classical and quantum contributions)
ZPE_calc	kJ/mol	total vibrational zero point energy
SvibT_calc	kJ/mol	total vibrational entropy times temperature
Svib_calc	J/K/mol	total vibrational entropy (classical and quantum contributions)
Cv_calc	J/K/mol	heat capacity at constant volume

10.4 *MedeA VASP*

Different properties are calculated depending on the type of VASP calculation configured within the VASP stage. Properties listed in the first table are always available after a successful VASP calculation.

Table11: All calculation types (last structure)

Property	Unit	Description
Eelectronic_calc	eV	VASP energy (for primitive cell)
Eelectronic_conventionalCell_calc	eV	VASP energy (for conventional cell)
Eelectronic_empiricalFormula_calc	eV	VASP energy (for empirical formula)
Eelectronic_sigma0_calc	eV	VASP energy extrapolated to zero smearing (for primitive cell)
Enon-dispersive_calc	eV	VASP energy without van der Waals contribution, if van der Waals forcefield is applied *(for primitive cell)*
EVanderWaals_calc	eV	VASP energy, van der Waals contribution, if van der Waals forcefield is applied (for primitive cell)
Forces_calc	eV/Ang	List of atomic forces in Cartesian coordinates
Force_max_calc	eV/Ang	Maximum absolute atomic force value
FormulaPrimitiveCell_calc		Formula of the primitive cell
FormulaConventionalCell_calc		Formula of the conventional cell
FormulaEmpirical_calc		Empirical formula
FactorEmpiricalToPrimitive_calc		Factor to convert empirical formula to primitive cell formula
FactorEmpiricalToConventional_calc		Factor to convert empirical formula to conventional cell formula
Efermi_calc	eV	Fermi energy
a_calc	Å	Lattice parameter a
b_calc	Å	Lattice parameter b
c_calc	Å	Lattice parameter c
alpha_calc	degree	Lattice parameter
beta_calc	degree	Lattice parameter
gamma_calc	degree	Lattice parameter
Vprim_calc	Å^3	Volume (primitive cell)
rho_calc	Mg/m^3	Density
mu_calc	μ_B	Total magnetic moment (spin-polarized)

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Table 11 – continued from previous page

Property	Unit	Description
mux_calc	μ_B	Total magnetic moment in x direction (spin-orbit or non-collinear magnetic)
muy_calc	μ_B	Total magnetic moment in y direction (spin-orbit or non-collinear magnetic)
muz_calc	μ_B	Total magnetic moment in z-direction (spin-orbit or non-collinear magnetic)
approximateMaterial_calc		Type of material: metal, semiconductor or insulator
approximateGap_calc	eV	Band gap width
approximateGapType_calc		Type of band gap: direct, indirect, no
approximateVBMaxPosition_calc		Approximate position of the valence band maximum in the Brillouin zone (fractional coordinates of a vector in k-space)
approximateCBMinPosition_calc		Approximate position of the conduction band minimum in the Brillouin zone (fractional coordinates of a vector in k-space)
return_status_calc		Return status: finished, warnings, error
planewaveCutoff_calc	eV	Plane wave cutoff
nKPoints_calc		Number of k-points in the Brillouin zone
FFTGridX_calc		Coarse Fast-Fourier grid in x direction
FFTGridY_calc		Coarse Fast-Fourier grid in y direction
FFTGridZ_calc		Coarse Fast-Fourier grid in z direction
FFTFineGridX_calc		Fine Fast-Fourier grid in x direction
FFTFineGridY_calc		Fine Fast-Fourier grid in y direction
FFTFineGridZ_calc		Fine Fast-Fourier grid in z direction
FFTAddedGridX_calc		Extrafine Fast-Fourier grid in x direction added for evaluation of augmentation charges and accurate forces
FFTAddedGridY_calc		Extrafine Fast-Fourier grid in y direction added for evaluation of augmentation charges and accurate forces
FFTAddedGridZ_calc		Extrafine Fast-Fourier grid in z direction added for evaluation of augmentation charges and accurate forces
FFTCompleteGridX_calc		Minimum Fast-Fourier grid in x direction to avoid aliasing errors
FFTCompleteGridY_calc		Minimum Fast-Fourier grid in y direction to avoid aliasing errors
FFTCompleteGridZ_calc		Minimum Fast-Fourier grid in z direction to avoid aliasing errors

Table12: Single Point and Structure Optimization (optimized structure)

Property	Unit	Description
V_calc	$\AA^3$	Volume (conventional cell)
P_calc	GPa	Pressure
Sxx_calc	GPa	Stress tensor component xx
Syy_calc	GPa	Stress tensor component yy
Szz_calc	GPa	Stress tensor component zz
Syz_calc	GPa	Stress tensor component yz
Sxz_calc	GPa	Stress tensor component xz
Sxy_calc	GPa	Stress tensor component xy

Table13: Ab initio Molecular Dynamics

Property	Unit	Description
Etotal_calc	kJ/mol	Total energy (average)
Etotal_uncertainty_calc	kJ/mol	Total energy (standard deviation)
Ekin_calc	kJ/mol	Kinetic energy (average)
Ekin_uncertainty_cal	kJ/mol	Kinetic energy (standard deviation)
Epot_calc	kJ/mol	Potential energy (average)
Epot_uncertainty_calc	kJ/mol	Potential energy (standard deviation)
V_calc	Å^3	Volume (average)
V_uncertainty_calc	Å^3	Volume (standard deviation)
P_calc	GPa	Pressure (average)
P_uncertainty_calc	GPa	Pressure (standard deviation)
T_calc	K	Temperature (average)
T_uncertainty_cal	K	Temperature (standard deviation)
Sxx_calc	GPa	Stress tensor component xx (average)
Sxx_uncertainty_calc	GPa	Stress tensor component xx (standard deviation)
Syy_calc	GPa	Stress tensor component yy (average)
Syy_uncertainty_calc	GPa	Stress tensor component yy (standard deviation)
Szz_calc	GPa	Stress tensor component zz (average)
Szz_uncertainty_calc	GPa	Stress tensor component zz (standard deviation)
Syz_calc	GPa	Stress tensor component yz (average)
Syz_uncertainty_calc	GPa	Stress tensor component yz (standard deviation)
Sxz_calc	GPa	Stress tensor component xz (average)
Sxz_uncertainty_calc	GPa	Stress tensor component xz (standard deviation)
Sxy_calc	GPa	Stress tensor component xy (average)
Sxy_uncertainty_calc	GPa	Stress tensor component xy (standard deviation)

Table14: (Total, valence) charge density, Bader analysis

Property	Unit	Description
BaderCharges_calc		electron charge. Bader charge per atom for each site
BaderChargeTransfers_calc		electron charge. Charge transfer per atom for each site
BaderVolumes_calc	Å^3	Bader volume per atom for each site
BaderDistances_calc	Å	Bader distance for each site
BaderVacuumCharge_calc		electron charge. Bader charge of the vacuum region
BaderVacuumVolume_calc	Å^3	Bader volume of the vacuum region
BaderTotalVolume_calc	Å^3	Total Bader volume

Table15: Density of states and Optical spectra

Property	Unit	Description
DOS_approximateMaterial_calc		Type of material: metal, semiconductor or insulator
DOS_approximateGap_calc	eV	Band gap width
DOS_approximateGapType_calc		Type of band gap: direct, indirect, no
DOS_approximateVBMaxPosition_calc		Approximate position of the valence band maximum in the Brillouin zone (fractional coordinates of a vector in k-space)
DOS_approximateCBMinPosition_calc		Approximate position of the conduction band minimum in the Brillouin zone (fractional coordinates of a vector in k-space)
DOS_Efermi_calc	eV	Fermi energy
DOS_nKPoints_calc		Number of k-points in the Brillouin zone

Table16: Optical spectra

Property	Unit	Description
OpticalSpectraComponents_calc		A list of components applicable for all optical functions, depending on the symmetry of the system. For isotropic materials only component x occurs, for anisotropic materials also components y, z, xy, yz, and zx may occur in the list. Off-diagonal elements xy, yz, and zx are only available for the dielectric function and optical conductivity. Diagonal elements x, y, and z apply to all optical functions.
OpticalSpectraEnergyGrid_calc	eV	Energy grid for which all optical functions are given
DielectricFunction_Imx_calc		Imaginary part of the dielectric function, x component
DielectricFunction_Imy_calc		Imaginary part of the dielectric function, y component
DielectricFunction_Imz_calc		Imaginary part of the dielectric function, z component
DielectricFunction_Imxy_calc		Imaginary part of the dielectric function, xy component
DielectricFunction_Imyz_calc		Imaginary part of the dielectric function, yz component
DielectricFunction_Imzx_calc		Imaginary part of the dielectric function, zx component
DielectricFunction_Rex_calc		Real part of the dielectric function, x component
DielectricFunction_Rey_calc		Real part of the dielectric function, y component
DielectricFunction_Rez_calc		Real part of the dielectric function, z component
DielectricFunction_Rexy_calc		Real part of the dielectric function, xy component
DielectricFunction_Reyz_calc		Real part of the dielectric function, yz component
DielectricFunction_Rezx_calc		Real part of the dielectric function, zx component
OpticalConductivity_Imx_calc	eV	Imaginary part of the optical conductivity, x component
OpticalConductivity_Imy_calc	eV	Imaginary part of the optical conductivity, y component
OpticalConductivity_Imz_calc	eV	Imaginary part of the optical conductivity, z component
OpticalConductivity_Imxy_calc	eV	Imaginary part of the optical conductivity, xy component
OpticalConductivity_Imyz_calc	eV	Imaginary part of the optical conductivity, yz component
OpticalConductivity_Imzx_calc	eV	Imaginary part of the optical conductivity, zx component
OpticalConductivity_Rex_calc	eV	Real part of the optical conductivity, x component
OpticalConductivity_Rey_calc	eV	Real part of the optical conductivity, y component
OpticalConductivity_Rez_calc	eV	Real part of the optical conductivity, z component
OpticalConductivity_Rexy_calc	eV	Real part of the optical conductivity, xy component
OpticalConductivity_Reyz_calc	eV	Real part of the optical conductivity, yz component
OpticalConductivity_Rezx_calc	eV	Real part of the optical conductivity, zx component
TransmissionCoefficient_x_calc		Transmission coefficient, x component
TransmissionCoefficient_y_calc		Transmission coefficient, y component
TransmissionCoefficient_z_calc		Transmission coefficient, z component
AttenuationCoefficient_x_calc		Attenuation coefficient, x component
AttenuationCoefficient_y_calc		Attenuation coefficient, y component
AttenuationCoefficient_z_calc		Attenuation coefficient, z component
AbsorptionCoefficient_x_calc		Absorption coefficient, x component
AbsorptionCoefficient_y_calc		Absorption coefficient, y component
AbsorptionCoefficient_z_calc		Absorption coefficient, z component
RefractiveIndex_x_calc		Refractive index, x component
RefractiveIndex_y_calc		Refractive index, y component
RefractiveIndex_z_calc		Refractive index, z component

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Table 16 – continued from previous page

Property	Unit	Description
ExtinctionCoefficient_x_calc		Extinction coefficient, x component
ExtinctionCoefficient_y_calc		Extinction coefficient, y component
ExtinctionCoefficient_z_calc		Extinction coefficient, z component
Reflectivity_x_calc		Reflectivity, x component
Reflectivity_y_calc		Reflectivity, y component
Reflectivity_z_calc		Reflectivity, z component
SpectralEmissivity_x_calc		Spectral emissivity, x component
SpectralEmissivity_y_calc		Spectral emissivity, y component
SpectralEmissivity_z_calc		Spectral emissivity, z component

Table17: Zone center phonons

Property	Unit	Description
PhononFrequencyGamma_calc	THz	Phonon frequencies at the Γ-point from finite differences

Table18: Response tensors

Property	Unit	Description
eps_0xx_calc		Dielectric constant e_0, xx component
eps_0yy_calc		Dielectric constant e_0, yy component
eps_0zz_calc		Dielectric constant e_0, zz component
eps_0yz_calc		Dielectric constant e_0, yz component
eps_0xz_calc		Dielectric constant e_0, xz component
eps_0xy_calc		Dielectric constant e_0, xy component
eps_infxx_calc		Dielectric constant e_{infinity}, xx component
eps_infyy_calc		Dielectric constant e_{infinity}, yy component
eps_infzz_calc		Dielectric constant e_{infinity}, zz component
eps_infyz_calc		Dielectric constant e_{infinity}, yz component
eps_infxz_calc		Dielectric constant e_{infinity}, xz component
eps_infxy_calc		Dielectric constant e_{infinity}, xy component
BornEffectiveCharges_calc		electron charge. 3x3 Born effective charges matrices for each atom position
PhononFrequencyGammaResponse_calc	THz	Phonon frequencies at the Γ-point from linear response
piezo_clampedion11_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 11
piezo_clampedion12_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 12
piezo_clampedion13_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 13
piezo_clampedion14_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 14
piezo_clampedion15_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 15
piezo_clampedion16_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 16
piezo_clampedion21_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 21
piezo_clampedion22_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 22
piezo_clampedion23_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 23
piezo_clampedion24_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 24
piezo_clampedion25_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 25
piezo_clampedion26_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 26
piezo_clampedion31_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 31
piezo_clampedion32_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 32
piezo_clampedion33_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 33
piezo_clampedion34_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 34
piezo_clampedion35_cal	C/m^2	Piezoelectric tensor (clamped ion) comp. 35
piezo_clampedion36_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 36

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Table 18 – continued from previous page

Property	Unit	Description
piezo_relaxedion11_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 11
piezo_relaxedion12_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 12
piezo_relaxedion13_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 13
piezo_relaxedion14_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 14
piezo_relaxedion15_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 15
piezo_relaxedion16_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 16
piezo_relaxedion21_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 21
piezo_relaxedion22_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 22
piezo_relaxedion23_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 23
piezo_relaxedion24_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 24
piezo_relaxedion25_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 25
piezo_relaxedion26_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 26
piezo_relaxedion31_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 31
piezo_relaxedion32_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 32
piezo_relaxedion33_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 33
piezo_relaxedion34_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 34
piezo_relaxedion35_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 35
piezo_relaxedion36_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 36

Table19: NMR chemical shifts

Property	Unit	Description
ChemicalShiftTensorsSym_calc	ppm	Absolute symmetrized chemical shift tensor for each atom, excluding core contributions
ChemicalShiftTensorG0_calc	ppm	Chemical shift tensor arising solely from the G=0 component of the induced field
MagneticSusceptibilityG0_calc	$10^{-6}*$ cm^3/mol	Approximate magnetic susceptibility
ChemicalShiftsCore_calc	ppm	Core contribution to the chemical shift
MagneticSusceptibilityCore_calc	$10^{-6}*$ cm^3/mol	Core contribution to the magnetic susceptibility
CSA_IsoShifts_val_calc	ppm	Chemical shift anisotropy (CSA), isotropic shift, excluding G=0, valence contribution only
CSA_Spans_val_calc	ppm	Chemical shift anisotropy (CSA), span, excluding G=0, valence contribution only
CSA_Skews_val_calc		Chemical shift anisotropy (CSA), skew, excluding G=0, valence contribution only
CSA_IsoShiftG0s_val_calc	ppm	Chemical shift anisotropy (CSA), isotropic shift, including G=0, valence
CSA_SpanG0s_val_calc	ppm	Chemical shift anisotropy (CSA), span, including G=0, valence contribution only
CSA_SkewG0s_val_calc		Chemical shift anisotropy (CSA), skew, including G=0, valence contribution only
CSA_IsoShifts_calc	ppm	Chemical shift anisotropy (CSA), isotropic shift, excluding G=0, valence and core contribution
CSA_Spans_calc	ppm	Chemical shift anisotropy (CSA), span, excluding G=0, valence and core contribution
CSA_Skews_calc		Chemical shift anisotropy (CSA), skew, excluding G=0, valence and core contribution
CSA_IsoShiftG0s_calc	ppm	Chemical shift anisotropy (CSA), isotropic shift, including G=0, valence and core contribution
CSA_SpanG0s_calc	ppm	Chemical shift anisotropy (CSA), span, including G=0, valence and core contribution
CSA_SkewG0s_calc		Chemical shift anisotropy (CSA), skew, including G=0, valence and core contribution

Table20: NMR chemical shifts

Property	Unit	Description
ChemicalShiftTensorsSym_calc	ppm	Absolute symmetrized chemical shift tensor for each atom, excluding core contributions
ChemicalShiftTensorG0_calc	ppm	Chemical shift tensor arising solely from the G=0 component of the induced field
MagneticSusceptibilityG0_calc	$10^{-6} \times cm^3/mol$	Approximate magnetic susceptibility
ChemicalShiftsCore_calc	ppm	Core contribution to the chemical shift
MagneticSusceptibilityCore_calc	$10^{-6} \times cm^3/mol$	Core contribution to the magnetic susceptibility
CSA_IsoShifts_val_calc	ppm	Chemical shift anisotropy (CSA), isotropic shift, excluding G=0, valence contribution only
CSA_Spans_val_calc	ppm	Chemical shift anisotropy (CSA), span, excluding G=0, valence contribution only
CSA_Skews_val_calc		Chemical shift anisotropy (CSA), skew, excluding G=0, valence contribution only
CSA_IsoShiftG0s_val_calc	ppm	Chemical shift anisotropy (CSA), isotropic shift, including G=0, valence
CSA_SpanG0s_val_calc	ppm	Chemical shift anisotropy (CSA), span, including G=0, valence contribution only
CSA_SkewG0s_val_calc		Chemical shift anisotropy (CSA), skew, including G=0, valence contribution only
CSA_IsoShifts_calc	ppm	Chemical shift anisotropy (CSA), isotropic shift, excluding G=0, valence and core contribution
CSA_Spans_calc	ppm	Chemical shift anisotropy (CSA), span, excluding G=0, valence and core contribution
CSA_Skews_calc		Chemical shift anisotropy (CSA), skew, excluding G=0, valence and core contribution
CSA_IsoShiftG0s_calc	ppm	Chemical shift anisotropy (CSA), isotropic shift, including G=0, valence and core contribution
CSA_SpanG0s_calc	ppm	Chemical shift anisotropy (CSA), span, including G=0, valence and core contribution
CSA_SkewG0s_calc		Chemical shift anisotropy (CSA), skew, including G=0, valence and core contribution

Table21: Electric field gradients

Property	Unit	Description
EFGs_Vxx_calc	V/Å^2	Electric field gradient for each atom, component xx
EFGs_Vyy_calc	V/Å^2	Electric field gradient for each atom, component yy
EFGs_Vzz_calc	V/Å^2	Electric field gradient for each atom, component zz
EFGs_Vyz_calc	V/Å^2	Electric field gradient for each atom, component yz
EFGs_Vxz_calc	V/Å^2	Electric field gradient for each atom, component xz
EFGs_Vxy_calc	V/Å^2	Electric field gradient for each atom, component xy
EFGs_diagonalized_Vxx_calc	V/Å^2	Electric field gradient diagonalized for each atom, component xx
EFGs_diagonalized_Vyy_calc	V/Å^2	Electric field gradient diagonalized for each atom, component yy
EFGs_diagonalized_Vzz_calc	V/Å^2	Electric field gradient diagonalized for each atom, component zz
EFGs_asymmetry_calc		Electric field gradient asymmetry parameter
EFGs_EigenVectors		Electric field gradient eigen vectors
NMRQuadrupolarParameters_calc		Nuclear quadrupolar parameter of each atom
NucElecQuadrupoleMoments_calc		Nuclear electric quadrupole moment of each atom

Table22: Hyperfine parameters

Property	Unit	Description
HyperfineTotal_Axx_calc	MHz	Total hyperfine coupling parameter diagonalized for each atom, component xx
HyperfineTotal_Ayy_calc	MHz	Total hyperfine coupling parameter diagonalized for each atom, component yy
HyperfineTotal_Azz_calc	MHz	Total hyperfine coupling parameter diagonalized for each atom, component zz
HyperfineFermiContact_calc	MHz	Fermi contact (isotropic) hyperfine coupling parameter for each atom
HyperfineDipolar_Axx_calc	MHz	Dipolar hyperfine coupling parameters for each atom, component xx
HyperfineDipolar_Ayy_cal	MHz	Dipolar hyperfine coupling parameters for each atom, component yy
HyperfineDipolar_Azz_calc	MHz	Dipolar hyperfine coupling parameters for each atom, component zz
HyperfineDipolar_Ayz_calc	MHz	Dipolar hyperfine coupling parameters for each atom, component yz
HyperfineDipolar_Axz_calc	MHz	Dipolar hyperfine coupling parameters for each atom, component xz
HyperfineDipolar_Axy_calc	MHz	Dipolar hyperfine coupling parameters for each atom, component xy
HyperfineAsymmetry_calc	MHz	Hyperfine coupling asymmetry parameter

Table23: Work function (surfaces only)

Property	Unit	Description
WorkFunction_calc	eV	Work function for identical terminations
WorkFunction_left_calc	eV	Work function for different terminations
WorkFunction_right_calc	eV	Work function for different terminations

Table24: Work function (surfaces only) - additional properties resulting from dipole correction

Property	Unit	Description
DipoleMoment_calc	e Å	Dipole moment of the slab (vector)
TraceQuadrupoleMoment_calc		Trace of the quadrupole moment tensor
EcorrDipoleQuadrupole_calc	eV	Dipol+quadrupol energy correction
EcorrCharge_calc	eV	Energy correction for charged systems

Table25: Energy of formation

Property	Unit	Description
Eformation_calc	kJ/mol	Formation energy
Hformation_calc	kJ/mol	Heat of formation (including the pV term)

10.5 *MedeA* Mechanical Properties / MT - Elastic Constants.

This applies to the Mechanical Properties stage and the MT - Elastic constants type of calculation in the VASP 5.4 and VASP 6 stage

Property	Unit	Description
Cij_calc(Cij)	GPa	Elastic constants C_{ij} ($1 \leq i,j \leq 6$)

Continued on next page

Table 26 – continued from previous page

Property	Unit	Description
Cij_uncertainty_calc(Cij)	GPa	Standard deviation for elastic constants C_{ij}
CijMatrix_calc	GPa	Elastic constants matrix (full 6x6 matrix)
SijMatrix_calc	1/GPa	Compliance tensor (full 6x6 matrix)
LeastSquaresResidual_calc		Residual % to which the least squares converged
ResidualStrain_calc(lat)		Residual strain (lat = a, b, c, alpha, beta, gamma)
PredictedCellParameter_calc(lat)	Å	Cell parameters predicted from the least squares fit (lat = a, b, c, alpha, beta, gamma)
MechanicalStabilityEigenValues_calc		Eigenvalues of the elastic constant matrix
MechanicalStabilityEigenVectors_calc		Eigenvectors of the elastic constant matrix
IsMechanicallyStable_calc		Whether mechanically stable (1) or not (0)
VoigtBulkModulus_calc	GPa	Bulk modulus from Voigt's average
ReussBulkModulus_calc	GPa	Bulk modulus from Reuss' average
HillBulkModulus_calc	GPa	Bulk modulus from Hill's average
VoigtShearModulus_calc	GPa	Shear modulus from Voigt's average
ReussShearModulus_calc	GPa	Shear modulus from Reuss' average
HillShearModulus_calc	GPa	Shear modulus from Hill's average
VoigtYoungsModulus_calc	GPa	Young's modulus from Voigt's average
ReussYoungsModulus_calc	GPa	Young's modulus from Reuss' average
HillYoungsModulus_calc	GPa	Young's modulus from Hill's average
VoigtLongitudinalModulus_calc	GPa	Longitudinal modulus from Voigt's average
ReussLongitudinalModulus_calc	GPa	Longitudinal modulus from Reuss' average
HillLongitudinalModulus_calc	GPa	Longitudinal modulus from Hill's average
VoigtPoissonRatio_calc		Poisson's ratio from Voigt's average
ReussPoissonRatio_calc		Poisson's ratio from Reuss' average
HillPoissonRatio_calc		Poisson's ratio from Hill's average
VoigtPughsRatio_calc		Pugh's ratio from Voigt's average
ReussPughsRatio_calc		Pugh's ratio from Reuss' average
HillPughsRatio_calc		Pugh's ratio from Hill's average
VoigtChenVickersHardness_calc	GPa	Vickers hardness according to Chen's model from Voigt's average
ReussChenVickersHardness_calc	GPa	Vickers hardness according to Chen's model from Reuss' average
HillChenVickersHardness_calc	GPa	Vickers hardness according to Chen's model from Hill's average
VoigtTianVickersHardness_calc	GPa	Vickers hardness according to Tian's model from Voigt's average
ReussTianVickersHardness_calc	GPa	Vickers hardness according to Tian's model from Reuss' average
HillTianVickersHardness_calc	GPa	Vickers hardness according to Tian's model from Hill's average
TransverseSpeedOfSound_calc	m/s	Speed of sound of transverse waves
LongitudinalSpeedOfSound_calc	m/s	Speed of sound of longitudinal waves
SpeedOfSound_calc	m/s	Mean speed of sound
HaveSpeedOfSound_calc		Whether or not speed of sound is available (1/0)
DebyeTemperature_calc	K	Debye temperature (Hill's average)
MeltingTemperatureLindemann_calc	K	Melting temperature estimated from Lindemann's expression (Hill's average)
GrueneisenParameter_calc		Grüneisen parameter (Hill's average)
E0_calc	kJ/mol	Energy at 0K = electronic energy + zero-point energy
Epv_calc	kJ/mol	Energy contribution of the PV term
Ezp_calc	kJ/mol	Zero-point energy
H0_calc	kJ/mol	Enthalpy at 0 K = E0_calc + Epv_calc
Thermodynamic_calc(T)	K	Temperature grid for thermodynamic functions

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Property	Unit	Description
Thermodynamic_calc(Cv)	J/K/mol	Constant volume heat capacity
Thermodynamic_calc(dH)	kJ/mol	Enthalpy, temperature dependent part
Thermodynamic_calc(dG)	kJ/mol	Gibbs free energy, temperature dependent part
Thermodynamic_calc(E)	kJ/mol	Internal energy including E0_calc
Thermodynamic_calc(H)	kJ/mol	Enthalpy including H0_calc
Thermodynamic_calc(G)	kJ/mol	Gibbs free energy
Thermodynamic_calc(A)	kJ/mol	Helmholtz free energy
Thermodynamic_calc(S)	J/K/mol	Entropy
Thermodynamic_calc(alpha)		Coefficient of thermal expansion

10.6 *MedeA* Phonon (Flowchart)

This applies to the Phonon stage, but not to the Phonon GUI (from the Tools menu), which cannot be integrated into a Flowchart

Property	Unit	Description
E0_calc	kJ/mol	Energy at 0K = electronic energy + zero-point energy
Epv_calc	kJ/mol	Energy contribution of the PV term
Ezp_calc	kJ/mol	Zero-point energy
H0_calc	kJ/mol	Enthalpy at 0 K = E0_calc + Epv_calc
Thermodynamic_calc(T)	K	Temperature grid for thermodynamic functions
Thermodynamic_calc(Cv)	J/K/mol	Constant volume heat capacity
Thermodynamic_calc(dH)	kJ/mol	Enthalpy, temperature dependent part
Thermodynamic_calc(dG)	kJ/mol	Gibbs free energy, temperature dependent part
Thermodynamic_calc(E)	kJ/mol	Internal energy including *E0_calc*
Thermodynamic_calc(H)	kJ/mol	Enthalpy including *H0_calc*
Thermodynamic_calc(G)	kJ/mol	Gibbs free energy
Thermodynamic_calc(A)	kJ/mol	Helmholtz free energy
Thermodynamic_calc(S)	J/K/mol	Entropy

10.7 *MedeA* GIBBS

Table27: All calculation types

Property	Unit	Description
Pvirial_calc_<phase>_<run>	MPa	Virial Pressure (NVT, NPT & only fluid in GCMC)
alphaT_calc_<phase>_<run>	1/Pa	Isothermal Compressibility (NPT)
cp_calc_<species>_<phase>_<run>	kJ/mol	Chemical Potential

Table28: NVT & NPT with test insertions, GEMC, GCMC

Property	Unit	Description
Utot_calc_<species>_<phase>_<run>	kJ/mol	Average total potential energy (per mol of system)
ThermE_calc_<phase>_<run>	1/K	Thermal Expansivity (NPT)
Cpres_calc_<phase>_<run>	J/mol/K	Residual Heat Capacity (NPT constant Pressure)
U_el_calc_<phase>_<run>	kJ/mol	Average Electrostatic Energy (per mol of system)
N_calc_<phase>_<run>		Average total number of molecules
MVol_calc_<phase>_<run>	L/mol	Average molar volume
rho_calc_<phase>_<run>	Mg/m^3	Average phase density
vol_calc_<phase>_<run>	Å^3	Average phase volume
fug_calc_<species>_<phase>_<run>	Pa	Fugacity (NVT & NPT with test insertions, GEMC, GCMC)
U_el_grid_calc_<phase>_<run>	Pa	Average grid electrostatic energy (GCMC)
CompF_calc_<phase>_<run>		Isentropic compressibility coefficient Cp/Cv (NPT)
U_ext_calc_<phase>_<run>	kJ/mol	Average external energy (intermolecular energy)
DHvap_calc_<run>	kJ/mol	Vaporization Enthalpy

Table29: GEMC constant V, pure compounds

Property	Unit	Description
x_calc_<species>_<phase>_<run>		Molar Fraction
JT_calc_<phase>_<run>	K/MPa	Joule-Thomson coefficient (NPT, Value for ideal heat capacity defined in flowchart)
vs_calc_<phase>_<run>	m/s	Speed of Sound (NPT, Value for ideal heat capacity defined in flowchart)

10.8 *MedeA* MOPAC

Table30: Structure and Energy, available after any MOPAC calculation

Property	Unit	Description
Acosmo_calc	Å^2	Molecule area
DipoleMoment_calc	Debye	Dipole moment
Ef_calc	kJ/mol	Standard heat of formation, at 298 K
Ehomo_calc	eV	HOMO energy
Elumo_calc	eV	LUMO energy
Emopac_calc	eV	Total electronic energy
EmpiricalFormula_calc		Chemical empirical formula
IP_calc	eV	Ionic potential
PointGroup_calc		Symmetry point group
Vcosmo_calc	Å^3	Molecule volume

Table31: Property accessible after a Thermodynamics calculation

Property	Unit	Description
{Cp,rotational_calc}	J/mol/K	A list of rotational heat capacities at constant pressure
{Cp,translational_calc}	J/mol/K	A list of translational heat capacities at constant pressure
{Cp,vibrational_calc}	J/mol/K	A list of vibrational heat capacities at constant pressure
{Cp298,rotational_calc}	J/mol/K	Rotational constant pressure heat capacity at 298 K
{Cp298,translational_calc}	J/mol/K	Translational constant pressure heat capacity at 298 K
{Cp298,vibrational_calc}	J/mol/K	Vibrational constant pressure heat capacity at 298 K
Cp298_calc	J/mol/K	Constant pressure heat capacity at 298 K
Cp_calc	J/mol/K	A list of constant pressure heat capacities
{H,rotational_calc}	kJ/mol	A list of rotational enthalpies
{H,translational_calc}	kJ/mol	A list of translational enthalpies
{H,vibrational_calc}	kJ/mol	A list of vibrational enthalpies
{H298,rotational_calc}	kJ/mol	Rotational enthalpy at 298 K
{H298,translational_calc}	kJ/mol	Translational enthalpy at 298 K
{H298,vibrational_calc}	kJ/mol	Vibrational enthalpy at 298 K
H298_calc	kJ/mol	Enthalpy at 298 K
H_calc	kJ/mol	A list of enthalpies
Hf298_calc	kJ/mol	Heat of formation at 298 K
Hf_calc	kJ/mol	A list of heats of formation
{S,rotational_calc}	J/mol/K	A list of rotational entropies
{S,translational_calc}	J/mol/K	A list of translational entropies
{S,vibrational_calc}	J/mol/K	A list of vibrational entropies
{S298,rotational_calc}	J/mol/K	Rotational entropy at 298 K
{S298,translational_calc}	J/mol/K	Translational entropy at 298 K
{S298,vibrational_calc}	J/mol/K	Vibrational entropy at 298 K
S298_calc	J/mol/K	Entropy at 298 K
S_calc	J/mol/K	A list of entropies
Ts_calc	K	The list of temperatures at which the temperature dependent properties given as a list have been calculated

10.9 *MedeA* Gaussian

Property	Unit	Description
Pvirial_calc_<phase>_<run>	MPa	Virial Pressure (NVT, NPT & only fluid in GCMC)
alphaT_calc_<phase>_<run>	1/Pa	Isothermal Compressibility (NPT)

Table32: Single point energy and geometry optimization

Property	Unit	Description
energy_total_calc	Ha	The total energy of the system
charge_calc	e	The total charge of the system
spin_multiplicity_calc		The spin multiplicity of the system
basis_calc		The basis set used
calculation_type_calc		Gaussian's representation of the calculation type
method_calc		Gaussian's representation of the calculation method
route_calc		The route section of the input file
mulliken_charges_calc(%ATOMID%)	e	The Mulliken charge of atom %ATOMID%

If the calculation uses a post-Hartree-Fock method then an appropriate subset of the following total energies and corrections will also be available, where a correction indicates the contribution to the total energy from the specified level of theory only. All energies have units of Hartree.

Table33: Energies

energy_scf_calc	energy_mp2_calc	energy_mp3_calc
energy_mp4dq_calc	energy_mp4sdq_calc	energy_mp4sdtq_calc
energy_ccsd_calc	energy_ccsdt_calc	energy_ccsdt_e4t_calc
energy_mp2_correction_calc	energy_mp3_correction_calc	energy_mp4dq_correction_calc
energy_mp4sdq_correction_calc	energy_mp4sdtq_correction_calc	energy_ccsd_correction_calc
energy_ccsdt_correction_calc	energy_ccsdt_e4t_correction_calc	

If the calculation uses either Hartree-Fock or density functional theory then the dipole and quadrupole moments are also available. The dipole moment has units of e*a0 and the quadrupole moment has units of e*a0^2.

Table34: Dipole moments

dipole_moment_au_calc(x)	dipole_moment_au_calc(y)	dipole_moment_au_calc(z)
dipole_moment_magnitude_calc	quadrupole_moment_au_calc(xx)	quadrupole_moment_au_calc(xy)
quadrupole_moment_au_calc(xz)	quadrupole_moment_au_calc(yy)	quadrupole_moment_au_calc(yz)
quadrupole_moment_au_calc(zz)		

Table35: Frequencies (available after a frequencies calculation)

Property	Unit	Description
mode_numbers_calc		A list of the included mode numbers
mode_symmetries_calc		A list of the included mode symmetries
mode_frequencies_calc	1/cm	A list of mode frequencies
mode_IR_intensities_calc	km/mol	A list of IR intensities
mode_reduced_masses_calc	u	A list of the reduced masses
force_constants_calc	mDyne/Ang	A list of the force constants
low_frequency_modes_calc	1/cm	The lowest frequencies in the system, corresponding to translations and rotations
enthalpy_thermal_correction_calc	Ha	The thermal correction to the enthalpy
gibbs_free_energy_thermal_correction_calc	Ha	The thermal correction to the Gibbs free energy
zero_point_energy_calc	Ha	The zero point energy
inertia_principle_axes_calc		A list of the principle axes of inertia
inertia_principle_moments_calc	me/a0^2	A list of the principle moments of inertia
rotational_constants_calc	GHz	The rotational constants
rotational_temperatures_calc	K	The rotational temperatures
pressure_calc	atm	The calculation pressure
temperature_calc	K	The calculation temperature
apt_charges_calc(%ATOMID%)	e	The APT charge of atom %ATOMID%

If the calculation method has analytic derivatives, which may not be the case for higher-order Moller-Plesset or coupled-cluster calculations, a frequencies calculation also produces a dipole and quadrupole moment. The dipole moment has units of e*a0 and the quadrupole moment has units of e*a0^2.

Table36: Dipole moments

dipole_moment_au_calc(x)	dipole_moment_au_calc(y)	dipole_moment_au_calc(x)
dipole_moment_magnitude_calc	quadrupole_moment_au_calc(xx)	quadrupole_moment_au_calc(xy)
quadrupole_moment_au_calc(xz)	quadrupole_moment_au_calc(yy)	quadrupole_moment_au_calc(yz)
quadrupole_moment_au_calc(zz)		

If the calculation method has analytic second derivatives (and hence analytic frequencies - HF, DFT, and MP2), which includes the HF, DFT and MP2 methods, a frequencies calculation also yields the polarizability and hyperpolarizability (both in atomic units) and APT charges.

Table37: Polarizabilities

polarizability_au_calc(xx)	polarizability_au_calc(xy)	polarizability_au_calc(xz)
polarizability_au_calc(yy)	polarizability_au_calc(yz)	polarizability_au_calc(zz)
hyperpolarizability_au_calc(xxx)	hyperpolarizability_au_calc(xxy)	hyperpolarizability_au_calc(xxz)
hyperpolarizability_au_calc(xzz)	hyperpolarizability_au_calc(xyy)	hyperpolarizability_au_calc(xyz)
hyperpolarizability_au_calc(yyy)	hyperpolarizability_au_calc(yyz)	hyperpolarizability_au_calc(yzz)
hyperpolarizability_au_calc(zzz)		

Polarizability

Variables available after a frequencies calculation include all of those from a commensurate single point energy calculation and the dipole moment and polarizability. The dipole moment has units of e*a0 and the polarizability is in atomic units.

Table38: Dipole moments

dipole_moment_au_calc(x)	dipole_moment_au_calc(y)	dipole_moment_au_calc(x)
dipole_moment_magnitude_calc	polarizability_au_calc(xx)	polarizability_au_calc(xy)
polarizability_au_calc(xz)	polarizability_au_calc(yy)	polarizability_au_calc(yz)
polarizability_au_calc(zz)		

If the calculation method is either Hartree-Fock or density functional theory then a polarizability calculation also produces the hyperpolarizability in atomic units.

Table39: Polarizabilities

hyperpolarizability_au_calc(xxx)	hyperpolarizability_au_calc(xxy)	hyperpolarizability_au_calc(xxz)
hyperpolarizability_au_calc(xzz)	hyperpolarizability_au_calc(xyy)	hyperpolarizability_au_calc(xyz)
hyperpolarizability_au_calc(yyy)	hyperpolarizability_au_calc(yyz)	hyperpolarizability_au_calc(yzz)
hyperpolarizability_au_calc(zzz)		

10.10 *Machine-Learned Potential Generator*

Different values are made available depending on the type of machine learning potential (MLP) set in the **MLP Generator** stage. This can be either **SNAP** or **NNP**. Properties listed in the first table are always available after the **MLP Generator** stage. The parameters and properties in the second table are available after a **SNAP** fit and those in the third table after an **NNP** fit.

Table40: Properties made available independent of the MLP type.

Property	Unit	Description
mlpg_type_calc		Can either be “SNAP” or “NNP”.
mlpg_successful_fit_calc		If successful “1” otherwise “0”.
mlpg_sli_file_calc		Structure list file containing the training set.
mlpg_frc_file_calc		Location of the frc file containing the fitted MLP.
mlpg_fit_energies_calc		“1” if energies included in the fit otherwise “0”.
mlpg_fit_forces_calc		“1” if forces included in the fit otherwise “0”.
mlpg_fit_stree_calc		“1” if stresses included in the fit otherwise “0”.
mlpg_rmse_energies_training_calc	eV/atom	RMSE error of the training set energies prediction.
mlpg_rmse_energies_validation_calc	eV/atom	RMSE error of the validation set energies prediction. Not available with SNAP.
mlpg_rmse_forces_training_calc	eV/Ang	RMSE error of the training set forces prediction.
mlpg_rmse_forces_validation_calc	eV/Ang	RMSE error of the validation set forces prediction. Not available with SNAP.
mlpg_rmse_stresses_training_calc	bar	RMSE error of the training set stresses prediction. Not available with NNP.

Table41: Additional parameters made available when using SNAP.

Property	Unit	Description
mlpg_snap_band_limit_calc		Band limit used.
mlpg_snap_radial_cutoff_calc	Ang	Global SNAP radial cutoff used.
mlpg_snap_opt_cutoff_calc		“1” if radial cutoff is optimzied otherwise “0”.
mlpg_snap_opt_radii_calc		“1” if relative element radii are optimzied otherwise “0”.
mlpg_snap_opt_weights_calc		“1” if relative element weights are optimzied otherwise “0”.

Table42: Additional properties and parameters made available when using NNP.

Property	Unit	Description
mlpg_nnp_default_SF_calc		“1” if default set of symmetry functions used otherwise “0”.
mlpg_nnp_epoch_calc		Total number of epochs.
mlpg_nnp_best_epoch_calc		Best epoch.
mlpg_nnp_number_SF_calc		Number of symmetry functions in the neural network potential.
mlpg_nnp_radial_cutoff_calc	Ang	Global cutoff radius. Only valid when using the default set of symmetry functions.
mlpg_nnp_random_seed_calc		Initial random number generator seed.

10.11 Additional Notes on Flowcharts

- The final structure obtained in the previous stage is passed to each subsequent stage. Hence, the endpoint of an NPT calculation, for example, is passed to the next stage in a simulation.
- The principal computed results are placed in local variables accessible by subsequent stages. The names of these variables are formed from the name of the property, with `_calc`, `_uncertainty_calc` and `_converged_calc` appended in the case of averages.
- The input and output files associated with each stage in a particular Job are stored on the JobServer. The directory hierarchy employed beneath each Job reflects the structure of the flowchart, which was employed in that calculation.