MedeA Analysis: Visualizing and Analyzing Simulation Results

**Contents**

1 Structure Optimization

1.1 Geometric Analysis

Click on Analysis >> Geometric Analysis to add a side panel to the active structure analyzing its geometric and structural aspects:

- General reports the symmetry information, such as space group, Pearson symbol and Wyckoff positions, as well as elementary physical properties such as cell volume and density
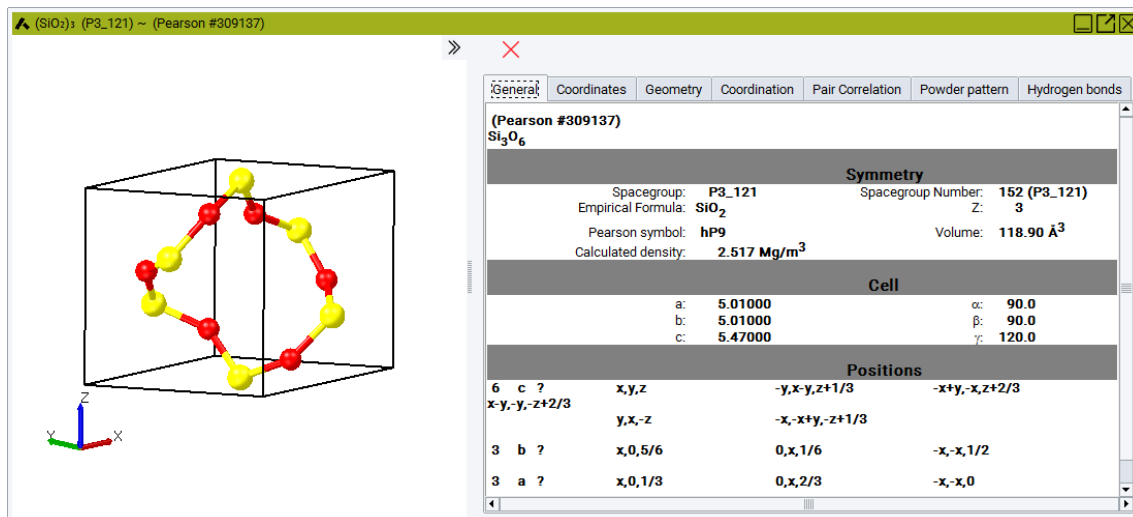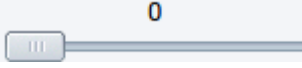
- Details about element positions are displayed in the Coordinates panel

- The Geometry panel prints distances and angles with neighboring atoms for a given reference atom

- In the Coordination panel, the number of nearest neighbors as a function of distance graph is plotted for a given reference atom

- The Pair Correlation panel graphically displays pair correlation functions for each element separately, as well as for the entire structure.

- Powder pattern shows the calculated [3] powder pattern for different X-ray sources (Co, Mo, Ag, Cr, Fe, and synchrotron) and neutron scattering. The isotropic thermal coefficient (Biso) and peak width can be varied with sliders, the wavelength for synchrotron radiation and neutrons can be entered. Use Copy lines as text to transfer the calculated angles and intensities to an external spreadsheet program.

- Hydrogen bonds searches for hydrogen bonds.

1.2 Trajectories

 Trajectories opens a dialog listing all trajectory files of completed structure optimization and molecular dynamics runs. Select one or more structures to display a trajectory of their atomic positions and lattice parameters during the simulation as a function of the simulation step. For each trajectory, additional controls appear on the animation window in *MedeA*:

[3] K Yvon, W Jeitschko, and E Parthò , "LAZY PULVERIX, a Computer Program, for Calculating X- and Neutron Diffraction Powder Patterns," *Journal of Applied Crystallography* 10, no. 1 (February 1, 1977): 73-74.

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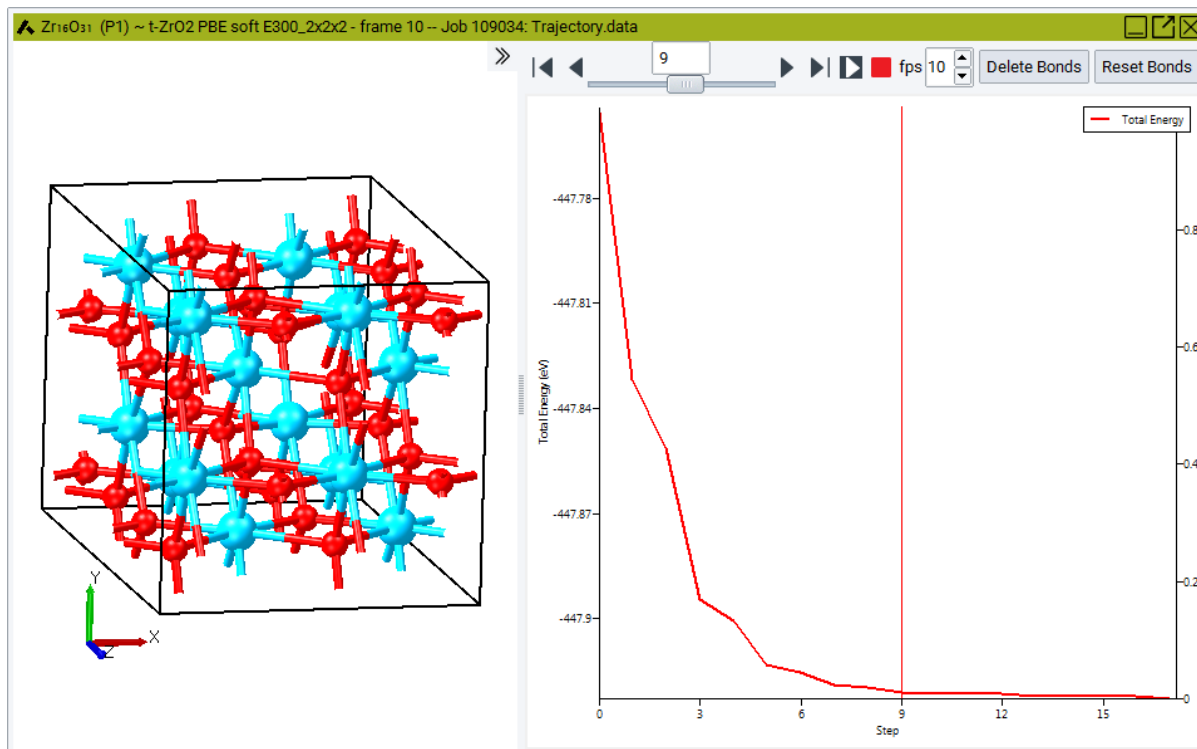
- The slider and the surrounding buttons on the left side of the animation toolbar control which frame of a trajectory to show between the initial (0) and final structures, the frame can be selected either with the slider or by entering the frame number directly in the widget above the slider

- and skip to the initial and final frame, respectively

- and move to the previous or next frame, respectively

- Start the animation to cycle from the initial structure to the final structure and back with ▷, the button changes to ❙❙ when an animation is running, pressing the button again will stop the animation

- When the record button ■ is locked, a PNG file of each frame is saved while the trajectory is animated. The PNG files are written to subfolders in ˜/MedeA/Movies, whereby "˜" denotes the home directory of the MedeA user. The directory for movie creation is customizable via File >> Preferences... .

- When the record button ■ is unlocked a dialog is shown to create a video file from the series of image files. For this purpose the external tool ffmpeg [1] needs to be installed and the path to its executable has to be provided in File >> Preferences... >> Programs .

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[1] https://ffmpeg.org/download.html
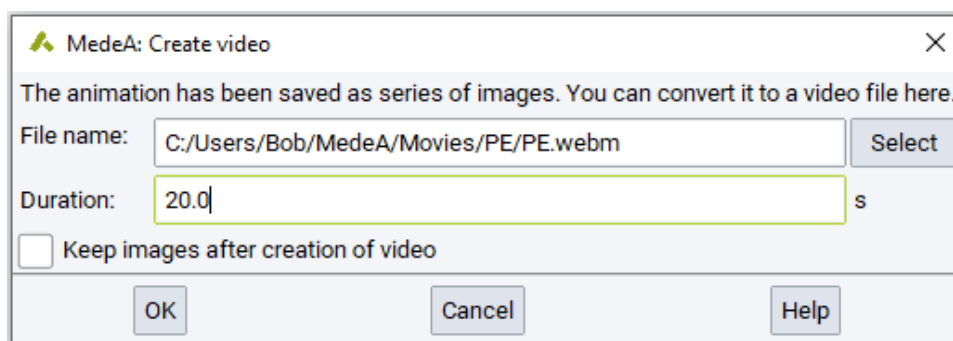
- In the dialog the path and file name of the video file can be given. In Duration it is possible to specify the desired length of the video in seconds. Some of the frames might be duplicated to accomplish the desired duration. Due to rounding effects the final length of the video might deviate by up to a second from the value asked for. Finally, when the check box Keep images after creation of video is unchecked the image files will be cleaned up after the video file has been created. A log file of the video creation will be copied to the subfolder in ˜/MedeA/Movies where the image files have been stored. A video can also be created by concatenating the PNG files with an external program, such as MovieMaker under Windows.

- The speed of the animation is controlled by the number of frames per second, set via the fps entry field or selector

- The buttons Delete bonds and Reset bonds allow to entirely remove and to restore bonds, respectively.

In the right pane, as a default for geometry optimizations, the total energy is plotted as red curve for each geometry step (see figure above). For molecular dynamics simulations, the total energy (red curve), kinetic energy (blue curve) and potential energy (black curve) are plotted as a function of the simulation time, where only the kinetic energy is referred to the axis on the right hand side.

- Zoom-in on an area of interest by left-clicking in the graph and moving the mouse while holding the button

- Right-click and use the Unzoom menu item to un-zoom or zoom back one level

A right mouse click into the right pane offers a number of menu items to save the graph, to export the data, and to customize line widths. Clicking on the last menu item Select displayed properties the graph is temporarily replaced by a control panel, an example for a trajectory of a molecular dynamics simulation is shown below.

The panel allows full customization of the graph, specifically you can

- select available properties to be displayed or hidden

- choose whether the curve should be displayed referring to the left or right axis (ordinate)

- customize the color of the curves

- change the units used in the plot

- and redefine the entire plot by changing the definition of the asbcissa.

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For each available property also the change of this property between two subsequent steps of the animation can be plotted. For instance, the change of energy between two steps can be displayed as a measure of the convergence behavior.

2 IR/Raman Spectra

Click on Analysis >> Spectra >> IR / Raman spectra to select results of calculations with computed IR and Raman spectra. Vibrational spectra are obtained from Phonon, Gaussian and MOPAC simulations.

To compare with experimental data, you Import spectra as *csv* file and display the calculated spectrum on top. Modify the Scale factor for the x-scale and apply Intensity scaling to match with experiment. Change the Line width and, under more...., line shape (Gaussian or Lorentzian) until you are created to Export... the spectrum.
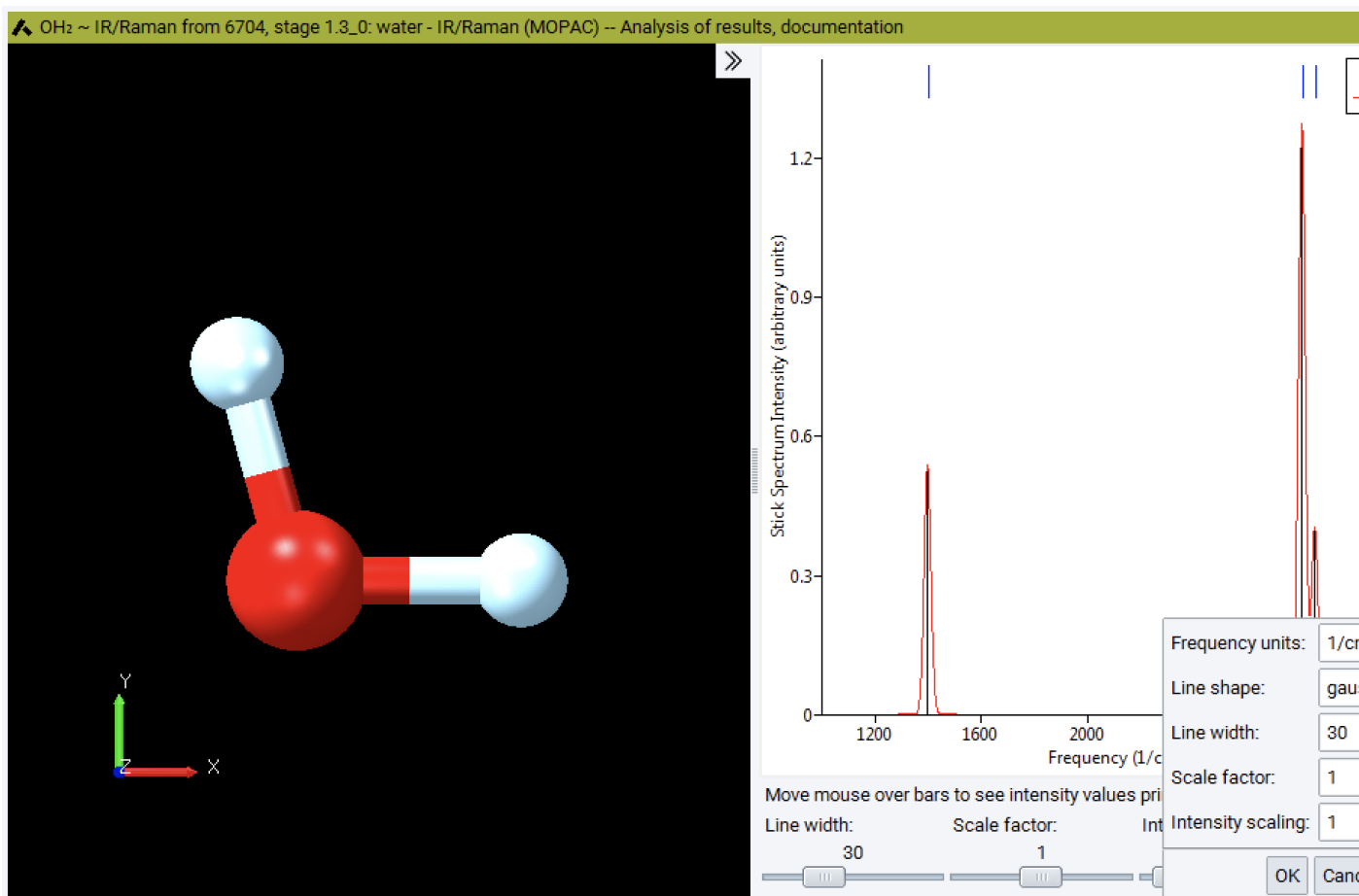
Numerical frequency data are provided at the bottom of the graph by hovering the mouse over the blue line markers above the peaks. For spectra obtained from MOPAC, the vibrational modes can be visualized by a right-click on the corresponding blue line above the peak and selecting Animate in the appearing pulldown menu. Animation of vibrational modes from Phonon calculations is not accessible directly from the IR and Raman spectra, but from the corresponding phonon dispersion curves. Handling, tuning, and recording of animated vibrational modes are identical to those discussed in the previous section on trajectory animation.

IR and Raman spectra of solid state systems from Phonon calculations can be customized in detail and recalculated to match very closely the experimental conditions applied in the measurements. To this end an additional Recalculate ... button shows up for all spectra obtained from Phonon, which brings up a control panel for specifying experimental conditions. The default parameters shown in these panels are identical to the settings applied for the underlying Phonon simulations at the JobServer. The control panels are discussed for Infrared and Raman spectra separately, below.

For Infrared spectra the Mode types to display is set to TO and LO modes , but it is also possible to restrict display to TO modes only or LO modes only . Three different kinds of absorption processes underlying the IR spectra can be chosen, namely IR absorption

- of unpolarized light by monocrystals , which is the default executed on the JobServer. Light is absorbed by TO phonon modes (orientationally independent) and by LO phonon modes (orientionally dependent). Since in monocrystal phonons propagate in all directions, the LO infrared absorption is averaged over all phonon wavevector orientations. In addition, the light polarization is averaged over all orientations of the polarization being perpendicular to the Wavevector orientation of the incoming light. Thereby, the Wavevector orientation of the incoming light is to some extent directly related to the orientation of the monocrystal, and can therefore be specified in the GUI. The orientation averaging conditions for the Average over phonon wavevectors , as well as for the Planar average over polarizations of the incoming light are specified by the Number of orientations (default 10) and two entries for the corresponding Seed . For IR absorption

- of polarized light by monocrystals the Polarization orientation of the incident light needs to be explicitly set, whereas the remaining Average over phonon wavevectors of LO modes still requires specification via Number of orientations and Seed . The direction of the incoming light has no effect on the spectrum. For IR absorption

- of unpolarized light by polycrystals the incoming light has random spherically oriented polarization due to grain orientations of the polycrystal. The orientation averaging conditions for the Average over phonon wavevectors , as well as for the Spherical average over polarizations of the incoming light are specified by the Number of orientations (default 10) and two entries for the corresponding Seed . Again, the direction of the incoming light has no impact on the spectrum.

The IR spectrum is recalculated and updated in the plot by pushing the Run button.
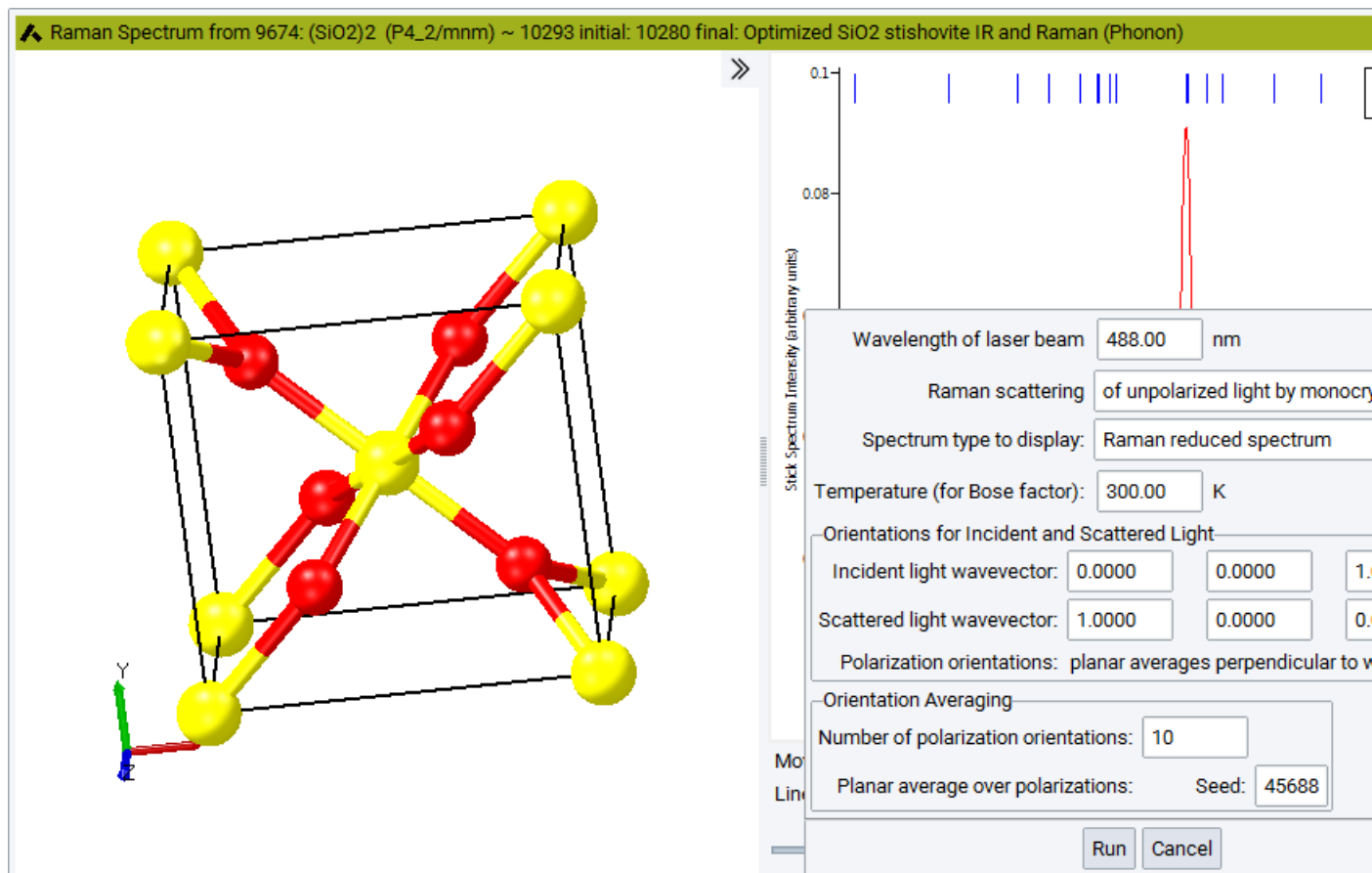
For Raman spectra the control panel for recalculation (see above) allows to characterize the incident light by entering the Wavelength of laser beam . The default of 488 nm specifies blue laser light. The Spectrum type to display offers two options, namely Raman reduced spectrum and Raman cross section . The differential cross section for Raman scattering is affected by the temperature via the Bose factor, so the Temperature (for Bose factor) can be entered. Three different kinds of scattering processes underlying the Raman spectra can be chosen, namely Raman scattering

- of unpolarized light by monocrystals , which is the default executed on the JobServer. The orientations of the Incident light wavevector and Scattered light wavevector need to be set according to the experimental setup. Since light is unpolarized the polarization vectors are averaged over random orientations, ensuring orthogonality to corresponding wavevectors. The orientation averaging conditions for the Planar average over polarizations are specified by the Number of polarization orientations (default 10) and an entry for the corresponding Seed . For Raman scattering

- of polarized light by monocrystals one needs to set the orientations of the Incident light wavevector and Incident light polarization , as well as the orientations of the Scattered light wavevector and Scattered light polarization . If directions of wavevector and polarization of incident (or scattered) light are not perpendicular to each other, the polarization vectors will be automatically rotated to fulfill the orthogonality requirement. For this scattering process orientation averaging is not required. For Raman scattering

- of unpolarized light by polycrystals averaging over random crystal orientations is performed, where for each such crystal orientation a random orthogonal orientation of light polarization is considered. The only geometrical aspect remaining is the Angle between incident and scattered light . The orientation averaging conditions are defined by Number of crystal orientations and the Seed for the Average over crystal orientations , as well as the Number of polarization orientations and the Seed for the Planar average over polarizations . Default number of orientations are reduced to 5 to keep computational demands at comparable levels, given the combinatorial increase.

The Raman spectrum is recalculated and updated in the plot by pushing the Run button.

3 Thermodynamic Functions

Click on Analysis >> Thermodynamic Functions to open a dialog for selecting thermodynamic functions results from completed Phonon and *MT* jobs. Select one or more jobs to open new windows with the calculated thermodynamic functions as shown below. Atomic resolution is only offered by Phonon, therefore, analysing *MT* results only the first Tab for the Entire system is available. As of *MedeA* 3.4, additional Tabs for Atomic contributions and Thermal displacements of atoms as a function of temperature are available. To obtain atomic results for elder Phonon calculations, a restart of the corresponding jobs is required.
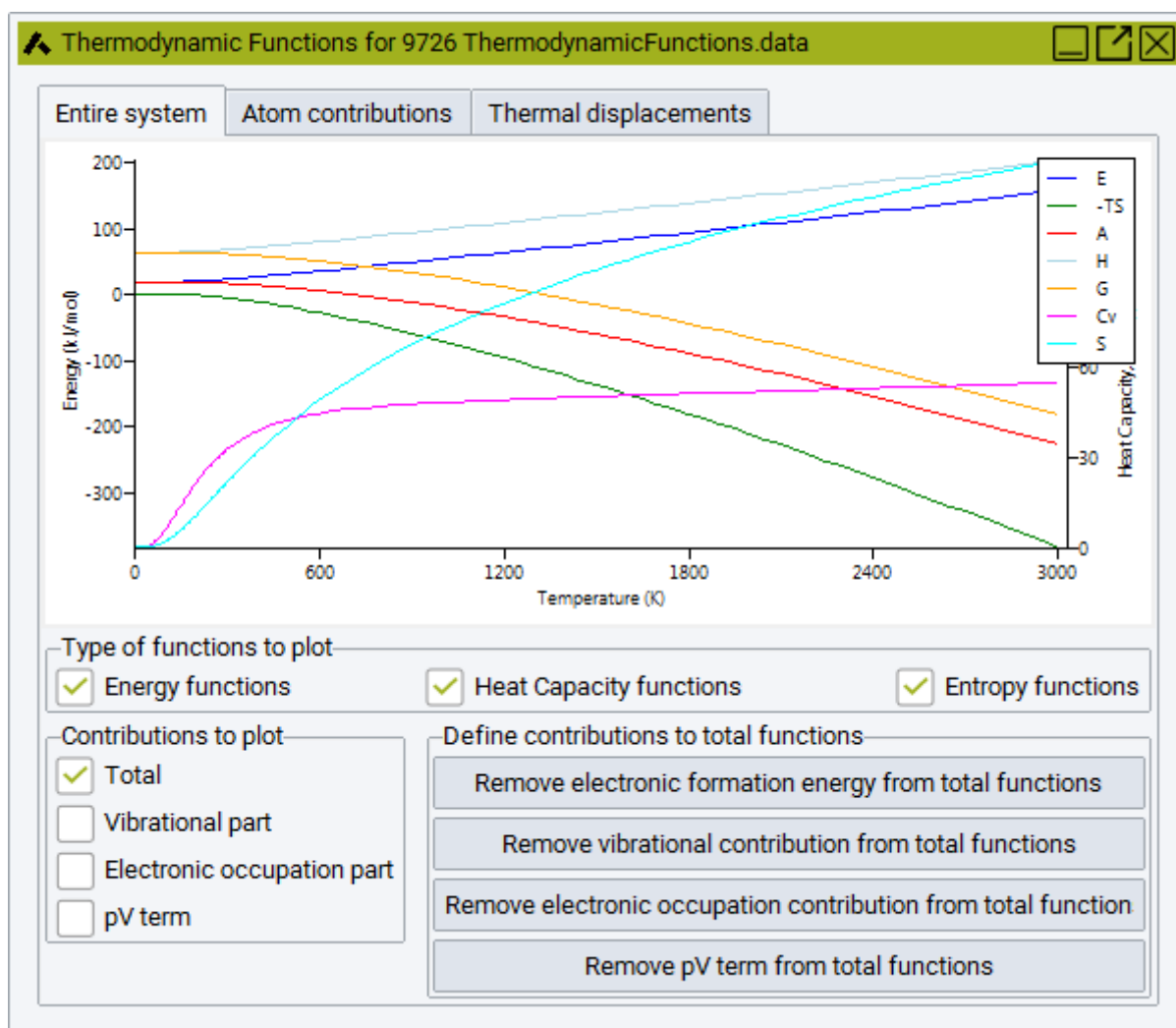
The thermodynamic functions windows in the Tabs for the Entire system are initially created with the total results for the energy functions, i.e. the internal energy (E), temperature times entropy (-TS), and the Helmholtz free energy (A). In case an external pressure is set for the underlying calculations, also the enthalpy (H) and Gibbs free energy (G) are shown.

Beneath the graph window there are a number of controls to customize the contents of the plot. Just below the graph window there is a row of options to control the Type of functions to plot :

- Energy functions : This toggles on and off the display of the energy related functions, which have alcreated been listed above, i.e. E, -TS, A, and by adding the pV term also H and G. These functions refer to the y-axis to the left of the graph. Individual functions can be displayed and hidden by selecting the legend fields to the right of the graph pane.

- Heat Capacity functions : This toggles on and off the display of the heat capacity functions under constant volume conditions (Cv), together with the Cv related legend entries to the right of the graph, which can again be used to display or hide individual components. Heat capacities refer to the axis to the right of the graph.

- Entropy functions : This toggles on and off the display of the entropy functions (S), which refer to the axis to the right of the graph.

Individual functions can be displayed and hidden by selecting the related legend fields.

Further down at the left side of the window there is a column of options to select the Contributions to plot :

- Total : This toggles on and off the display of the total functions, i.e. with the selected partial contributions added together. The display of the partial contributions can be controlled from the checkboxes

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below.

- Vibrational part : This toggles on and off the display of the vibrational contributions to the total functions, together with the legend entries (such as E_vib, -TS_vib, A_vib, H_vib, G_vib, Cv_vib or S_vib) to the right of the graph, which can be used to display or hide individual components.

- Electronic occupation part : This toggles on and off the display of the contributions of the electronic occupation to the total functions, together with the legend entries (such as E_elec, -TS_elec, A_elec, H_elec, G_elec, Cv_elec or S_elec) to the right of the graph, which can again be used to display or hide individual components.

- pV term : This toggles on and off the display of the pV term, which contributes to the total functions in case of finite external pressure.

To the right there are action buttons to add or remove these contributions to the total functions:

- Add electronic formation energy to total functions : This adds the electronic formation energy to the total energy related functions. The energy of formation is only available, if for the underlying Phonon or MT calculation the property Energy of formation has been selected from the Calculation Tab of the *MedeA VASP* interface, otherwise the formation energy is set to zero and there is no effect in the graph. After pushing this button, it becomes replaced by the button

- Remove electronic formation energy from total functions : This removes the electronic formation energy from the energy related total functions.

- Add vibrational contribution to total functions : This adds the vibrational contribution to all total functions, i.e. energy related ones, heat capacity and entropy. Vibrational contributions are always present, since they are the primary output of Phonon and MT calculations. After pushing this button, it becomes replaced by the button

- Remove vibrational contribution to total functions : This removes the vibrational contribution from all total functions.

- Add electronic occupation contribution to total functions : This adds to all functions the contribution of finite temperature occupation of excited electronic states close to the Fermi energy, as given by the Fermi-Dirac distribution. This is only available from Phonon calculations, if the option Temperature dependent electronic contributions (DOS) to thermodynamic functions (for metals) has been selected from the Calculation Tab of the *MedeA* Phonon interface, otherwise this button is greyed out and inactive. This contribution is currently unavailable from MT calculations. After pushing this button, it becomes replaced by the button

- Remove electronic occupation contribution to total functions : This removes the contribution of finite temperature occupation of excited electronic states from all total functions.

- Add pV term to total functions : This adds the pV term to the total energy related functions, thus plotting the enthalpy (H) and Gibbs free energy (G), in addition to other functions. If the underlying simulation applies a finite external pressure, the pV term is automatically added upon initially creating the plot. If an external pressure is not applied, the pV term might only be non-zero due to computational inaccuracies, and it is left to the user to decide, whether or not its addition is justified. Vibrational and electronic occupation contributions, i.e. H_vib, G_vib, H_elec and G_elec are plotted, if display of such contributions is selected. After pushing this button, it becomes replaced by the button

- Remove pV term from total functions : This removes pV term from the total energy related functions, i.e. all enthalpy and Gibbs free energy functions.

There are several options to export the thermodynamic functions to data files, all of which are accessible via a right-click on the graph pane. For all graphs, the picture can be exported to Postscript or tif format, and the underlying data can be exported to text or CSV format. The context-sensitive menu via the right mouse click enables us to increase or decrease line widths. The context-sensitive menu item Export selected data is a specific export feature which exports to text format all those functions selected for display in the graph pane. These right-click controls are available for all graph windows, also in other Tabs.
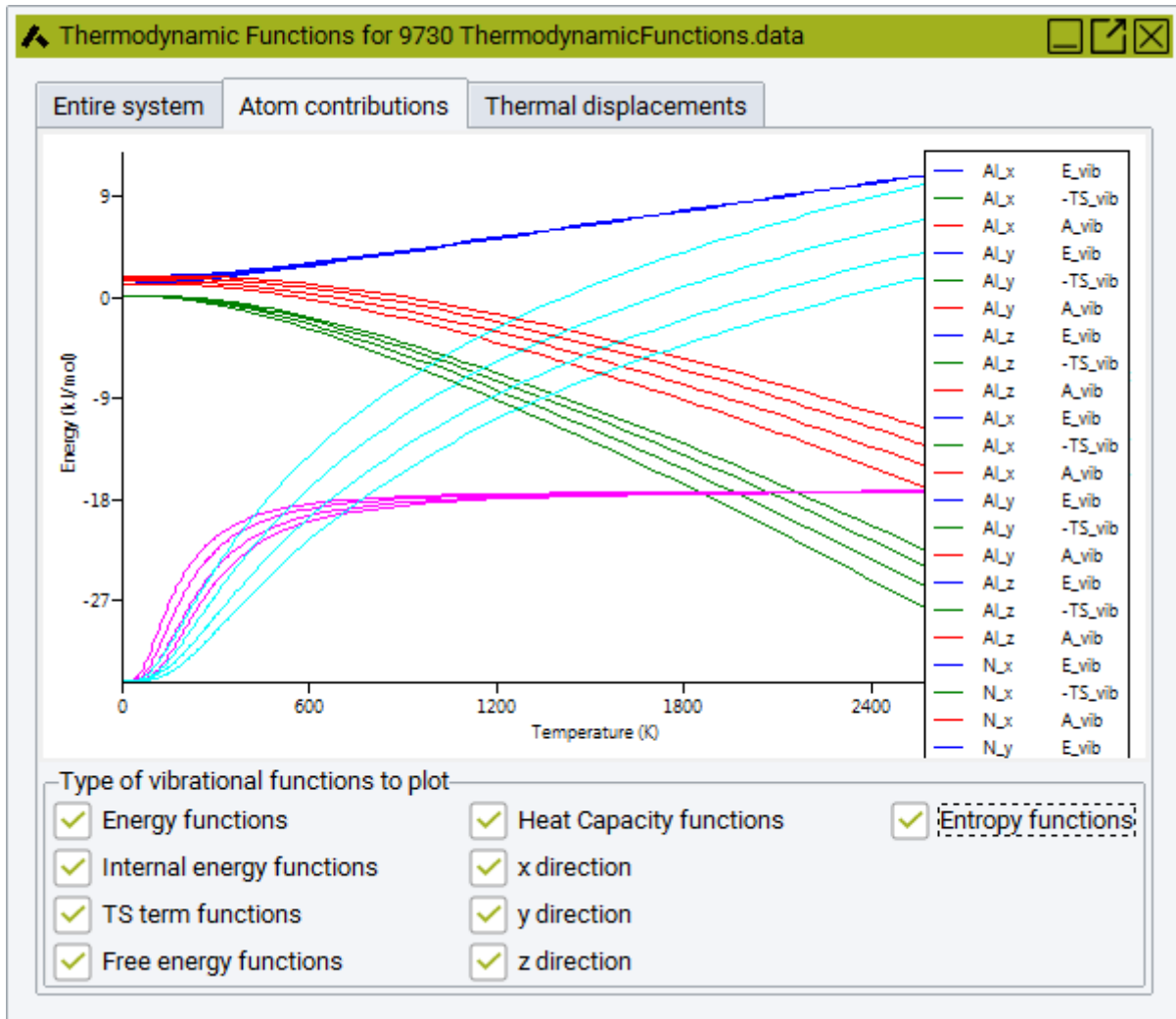
As mentioned in the beginning, for Phonon calculations further Tabs are available for analyzing results resolved for individual atoms. Selecting the Tab denoted Atomic contributions displays the solely vibrational contributions of each atom to the thermodynamic functions. Of course, any electronic contributions as well as pV terms are excluded from this analysis, since atomic contributions for those are unavailable.

Beneath this graph window there are a number of options to control the Type of functions to plot :

- Energy functions : This toggles on and off the display of atomic contributions to all energy related functions, which includes internal energy, -TS terms, and Helmholtz free energy contributions. These functions refer to the y-axis to the left of the graph. Individual types of energy contributions can be toggled on and off by the other three options of the first column of controls, namely for all atomic contributions to the

- Internal energy functions , for all atomic contributions to the

- TS term functions related to the entropy, as well as for all atomic contributions to the

- Free energy functions , adding internal energy and TS terms. In addition, the first row controls enable to display

- Heat Capacity functions : This toggles on and off the display of atomic contributions to the heat capacity functions under constant volume conditions (Cv), together with the Cv related legend entries to the right of the graph, which can be used to display or hide individual components. Heat capacities refer to the axis to the right of the graph. Furthermore, the top right control enables to display

- Entropy functions : This toggles on and off the display of atomic contributions to the entropy functions (S), which refer to the axis to the right of the graph. Finally, contributions of Cartesians directions can

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be selectively displayed by the controls

- x direction : toggles on and off atomic contributions to all selected functions in Cartesian x direction

- y direction : toggles on and off atomic contributions to all selected functions in Cartesian y direction

- z direction : toggles on and off atomic contributions to all selected functions in Cartesian z direction

All individual functions can be displayed and hidden by selecting the related legend fields to the right of the graph pane.
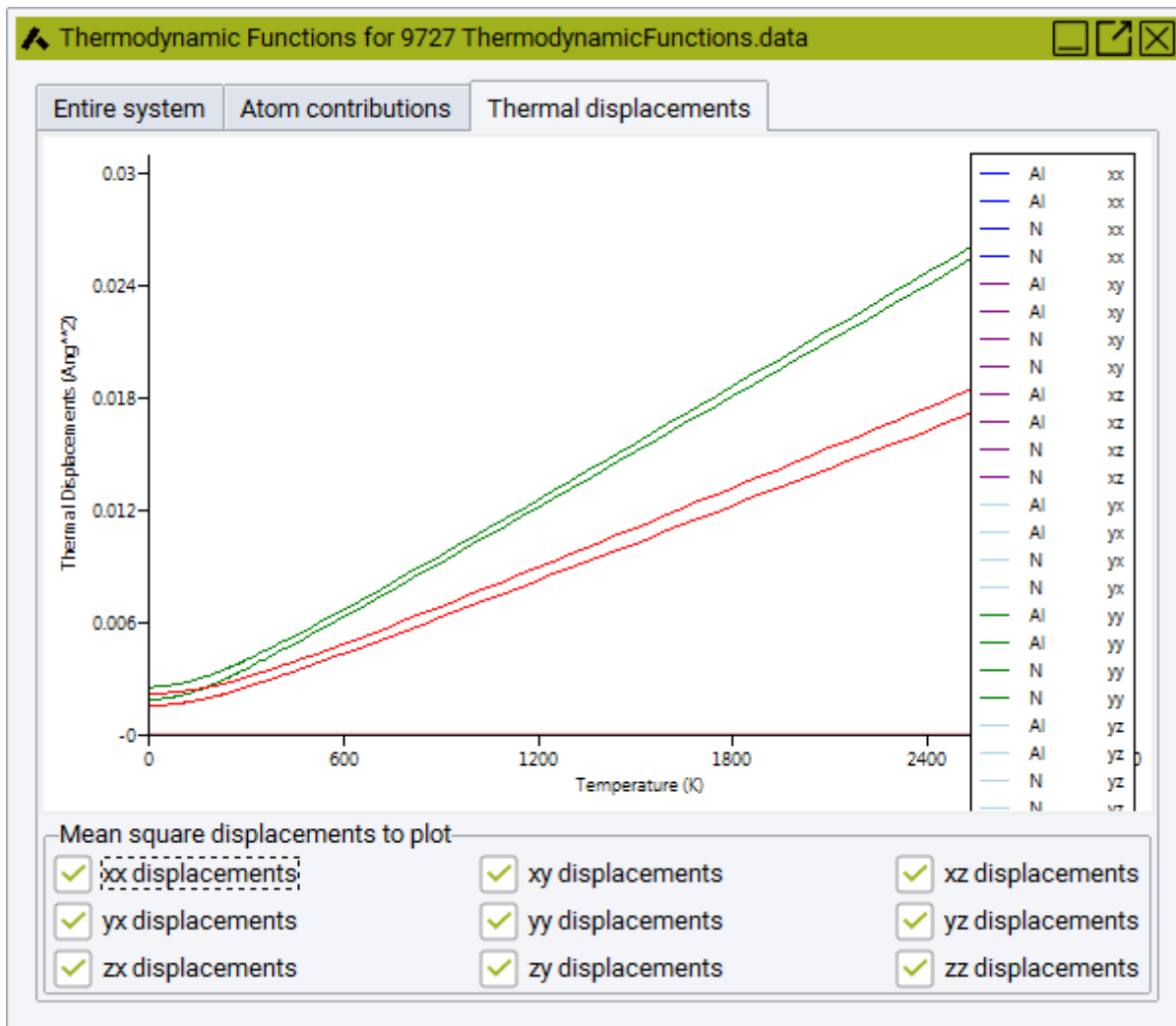
Selecting the Tab denoted Thermal displacements displays the tensor of mean square thermal displacements as a function of temperature for all atomic species. Individual tensor components for all atoms can be toggled on and off by the controls beneath the graph window, whereas individual components can be displayed and hidden by selecting the related legend fields.

4 Band Structure

Click on Analysis >> Band Structures to open a dialog for selecting results from completed jobs. Selecting one or more jobs to open a graphics window showing the corresponding band structure plots. A BandStructure menu entry shows up in the menu bar, given access to further options.

- Uncheck ☐ As Lines to see all calculated points along the path, as shown on the right side

Band structure for 28397 -- Stage_1: NaCl,PBE,BandStructure,1,VASP
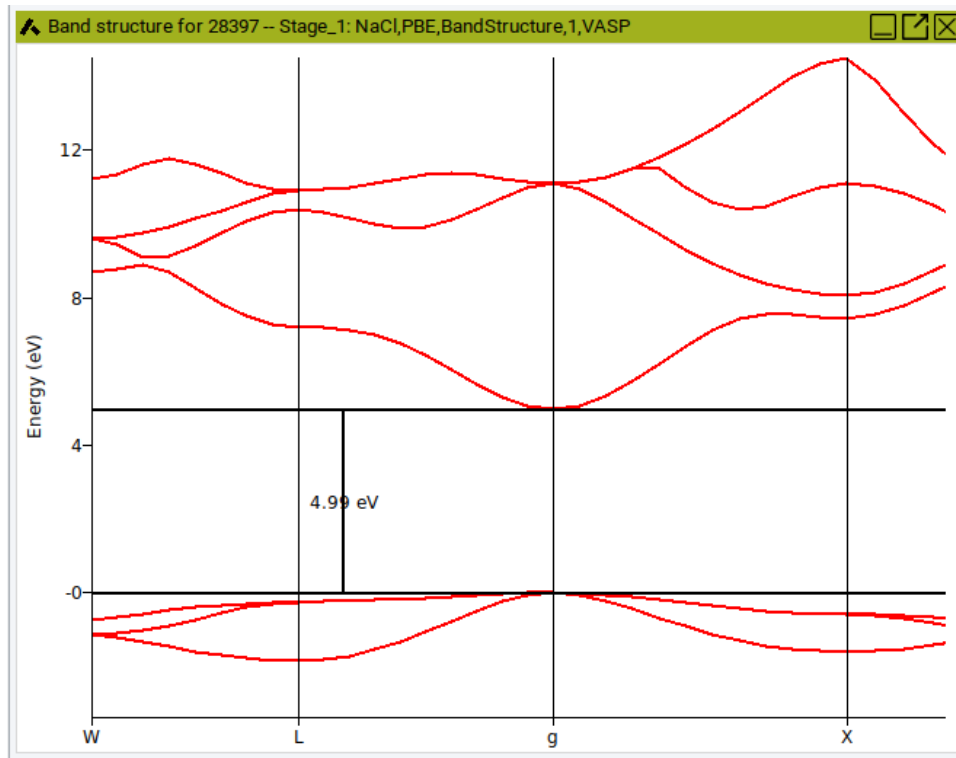
- Use ☑ Measuring lines to measure energy differences in the plot, you can move the lines by clicking on them and dragging them to a new position
- Left-click and hold to zoom into the plot
- Right-click and select Save as Postscript or Unzoom

5 Density of States

Click on Analysis >> Density of States to open a dialog for selecting results from completed jobs. Selecting one or more jobs to open a new window with the calculated density of states.
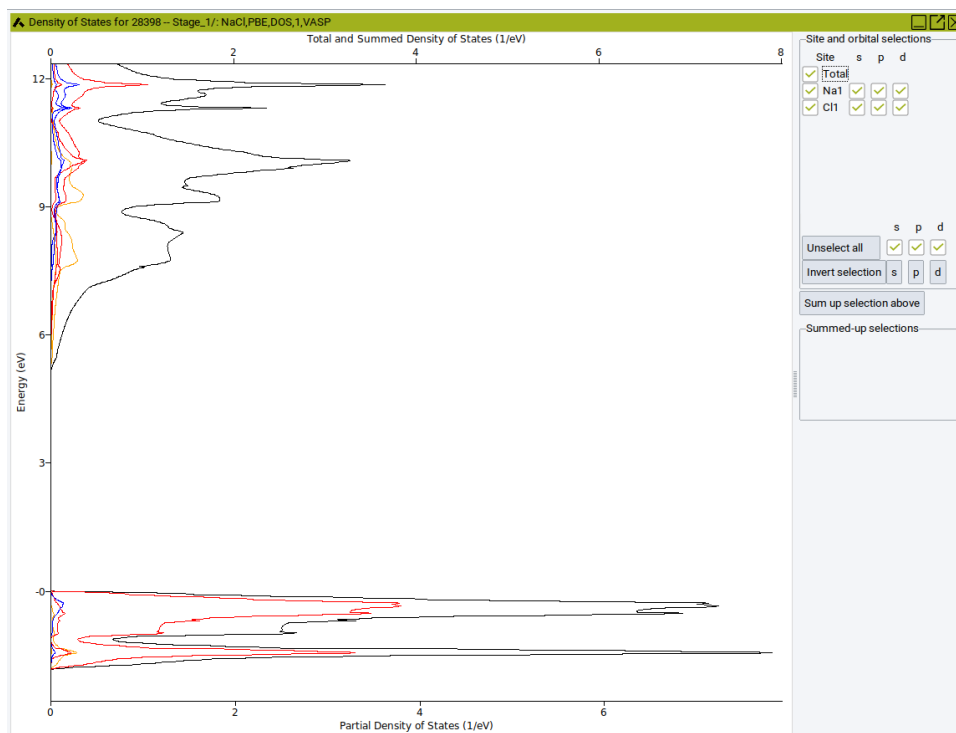
The color indicates the orbital or band: orange for s-states, red for p-states, blue for d-states, and black for the total DOS.

- On the right-hand side, select a field to display or hide the corresponding partial DOS

- Click on an Atom label (e.g. Cl) to display or hide the contribution of the selected atom.

- Sum up selection combines selected atoms or orbitals.

- Moving the mouse over a line , highlights the corresponding atom of group (in this case Cl).

Please note different scale: total density of states at the top, partial density of states at the bottom.

Note: Core electrons are not included in the density of states. The attribution of electrons to specific atoms in solids is done by projecting the electronic density into spheres around the atoms. The corresponding sphere radii are arbitrary parameters, therefore the partial atomic density needs to be interpreted with care. In *MedeA*, covalent radii for each element are used as default values. To change the sphere radii, use the Add to Input section of the VASP interface(see The VASP Manual [2] for more details on the RWIGS keyword).

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6 Optical Spectra

Click on Analysis >> Spectra >> Optical Response Functions to open a dialog for selecting optical property results from completed VASP jobs. Selecting one or more jobs to open new windows with the calculated optical spectra as shown below.

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[2] https://www.vasp.at/wiki/index.php/The_VASP_Manual
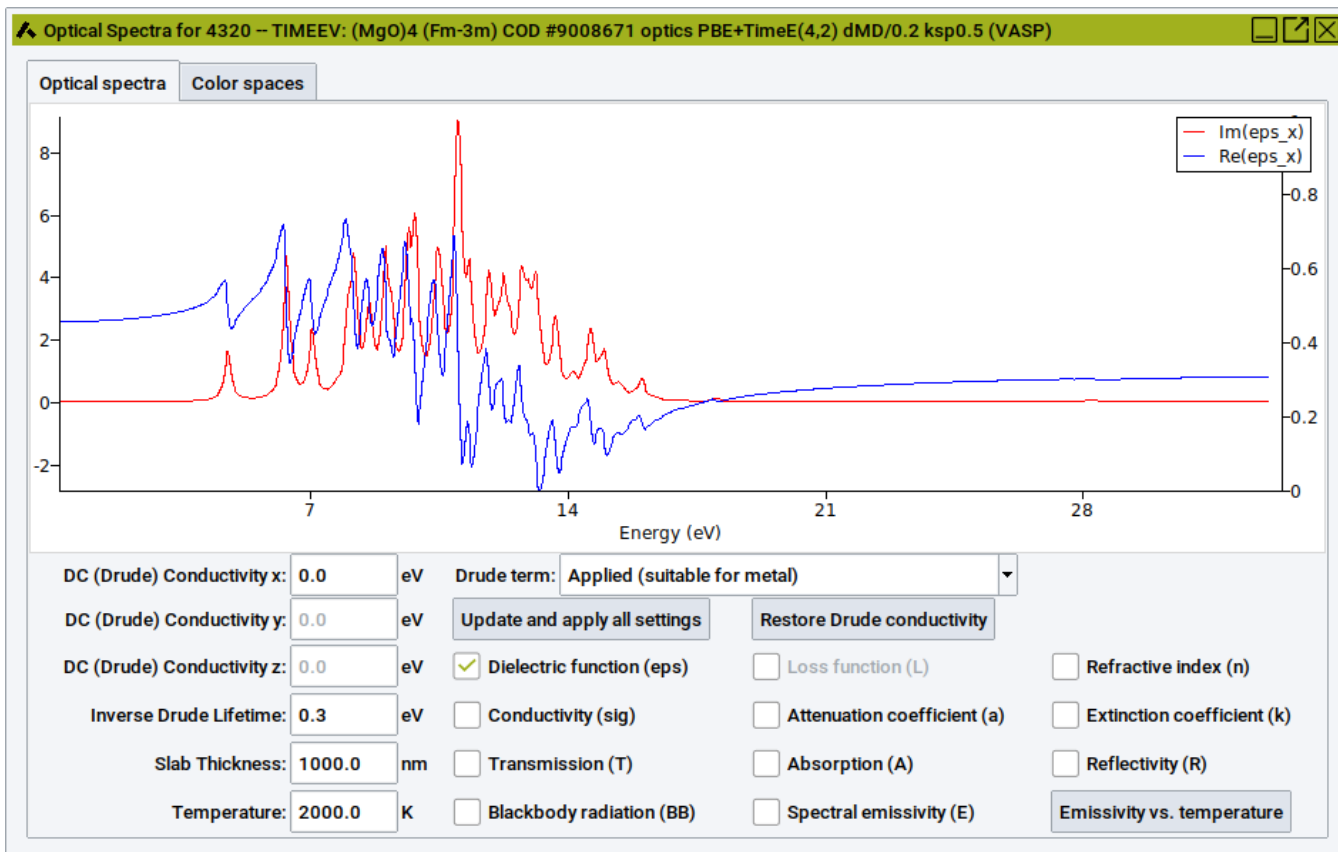
The optical spectra windows are initially created with the real and imaginary part of the dielectric functions, Im(eps) and Re(eps), plotted in the Optical Spectra Tab. In the case of optically anisotropic materials, components in different Cartesian directions, such as Im(eps_x), Im(eps_y) and Im(eps_z) as well as off-diagonal components are displayed. There are several options to add and remove optical functions for display in the graph pane using the checkboxes at the bottom right of the Optical Spectra window:

- Dielectric function (eps) : This toggles on and off the display of the real and imaginary part of the tensor elements of the dielectric function (ϵ). Individual components (depending on the symmetry of the system) can be displayed and hidden by selecting the legend fields to the right of the graph pane.

- Conductivity (sig) : This toggles on and off the display of the real and imaginary part of the optical conductivity tensor elements (σ) in units of eV, together with the legend entries Im(sig) and Re(sig) to the right of the graph, which can again be used to display or hide individual components.

- It is noted that dielectric function and conductivity tensor components refer to the scale to the left , which becomes highlighted in red color whenever the cursor touches one of these functions.

- Transmission (T) : This toggles the display of the transmission (T) together with the legend entries for individual toggling. The transmission is strongly affected by the Slab Thickness .

- Loss function (L) : The loss function is the imaginary part of the inverse of the tensor of the dielectric function. This feature is not supported by MedeA 3.3, hence grayed out.

- Attenuation coefficient (a) : This toggles the display of the attenuation coefficient together with the legend entries for individual toggling.

- Absorption (A) : This toggles the display of the absorption together with the legend entries for individual toggling.

- Refractive index (n) : This toggles the display of the refractive index (n), i.e. the real part of the complex index of refraction, together with the legend entries for individual toggling.

- Extinction coefficient (k) : This toggles the display of the extinction coefficient (k), i.e. the imaginary part of the complex index of refraction (sometimes denoted absorption index), together with the legend

entries for individual toggling.

- Reflectivity (R) : This toggles the display of the refractive index, together with the legend entries for individual toggling.

- It is noted that transmission, attenuation, absorption, and extinction coefficients as well as refractive index and Reflectivity refer to the scale to the right , which becomes highlighted in red color whenever the cursor touches one of these functions.

- Moving the mouse over a line highlights the line, the corresponding legend entry to the right, and the scale to be applied for this function (either left or right). Through the above checkboxes and legend entries, any combination of optical functions can be displayed together in one graph.

The last row of control elements are dedicated to display of emissivity and active radiation.

- Spectral emissivity (E) : This toggles the display of the spectral emissivity, together with the legend entries for individual toggling. The spectral emissivity is closely related to the absorption coefficient.

- Blackbody radiation (BB) : This toggles the display of the blackbody radiation, together with the legend entries for individual toggling. The blackbody radiation is determined for a given Temperature in Kelvin and does not depend on the material. The temperature can be set in the entry field to the left of the checkbox for display of the blackbody radiation.

- Note that spectral emissivity and blackbody radiation refer to the scale to the right .

- Pushing the Emissivity vs. temperature button to the right of the toggle for display of spectral emissivity brings up a graph window plotting the total emissivity as a function of temperature, up to the maximum temperature given in the entry field, as is shown below.
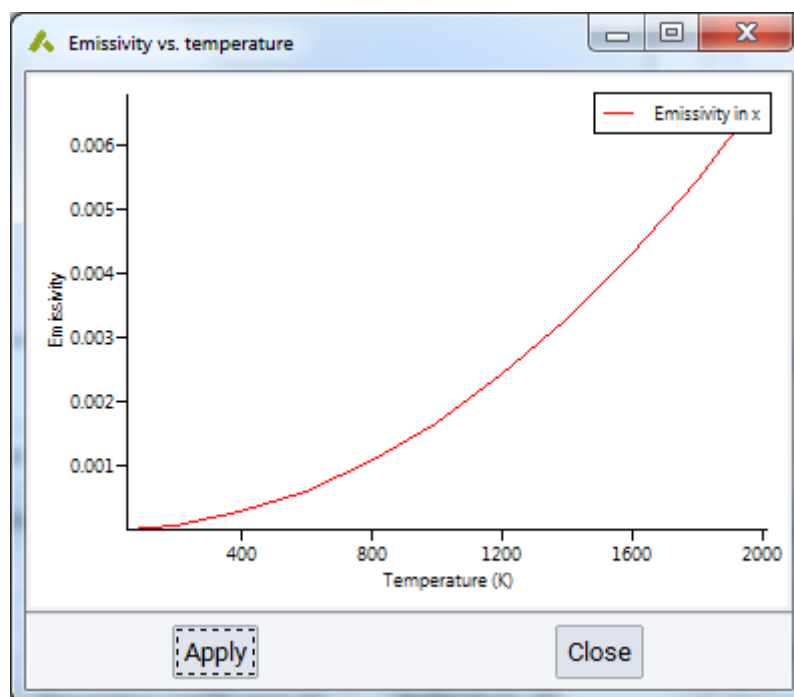
The optical functions are processed differently, depending on the existence of a band gap, i.e. depending on the metallic or insulating/semiconducting electronic structure of the system. The presence of a band gap is automatically detected by the underlying VASP calculation, and the information is provided beneath the graph on the right side, e.g. in the above example the Material is an insulator with a direct band gap = 5.00 eV .

For a metal, it informs that the Material is a metal with no band gap . In the case of metallic systems, the rather important intraband contribution is automatically added in an approximate manner using a Drude correction term mostly visible at relatively low frequencies. For insulating or semiconducting systems the Drude term is not applied. Although the behavior at low frequencies is automatically adjusted to the detected system type, it can also be manually added or removed by the choice:

- Drude term : which directly adapts all optical functions according to the two possible settings

  – Applied (suitable for metal)

  – Not applied (for insulator or semiconductor)

The Drude term requires two parameters, the (in general direction dependent) Drude conductivity and the Drude lifetime. The Drude conductivity is automatically obtained from the plasma frequency as calculated by VASP, but can be modified from the entry fields

- DC (Drude) Conductivity x

- DC (Drude) Conductivity y

- DC (Drude) Conductivity z

The Drude lifetime is an empirical parameter and can be adjusted from the entry field

- Inverse Drude Lifetime : The default value is 0.3 eV.

Any changes to the settings for the Drude term, as well as changes to the

- Slab Thickness in nm units

and changes to the

- Temperature in Kelvin units

need to be applied by pushing the Update and apply all settings button. To restore the default Drude conductivity values as derived from the plasma frequency values calculated from first principles, the button Restore Drude conductivity needs to be pushed.

There are several options to export the optical spectra to data files, all of which are accessible via a right-click on the graph pane. For all graphs, the picture can be exported to Postscript or tiff format, and the underlying data can be exported to text or CSV format. The context-sensitive menu via the right mouse click enables us to increase or decrease line widths and to change the energy/frequency/wavelength units. The context-sensitive menu item Export selected data is a specific export feature which exports to text format all those functions selected for display in the graph pane.

The second Tab of the optical spectra windows provides information on the Color spaces . Upon reflection and transmission (for optical anisotropic materials for different directions) a table provides the color space values of different Color matching functions , based on the CIE 1931 or CIE 1964 standards, as well as for Spectral power distributions of different light sources, i.e. Standard Illuminant D65 or the Fluorescent lamp FL2. The resulting RGB values are also included in the table. In addition, the RGB color values are shown by small canvas, demonstrating the predicted colors upon reflection and transmission (dependent on the Slab Thickness). For optical anisotropic materials color canvas for different Cartesian directions are shown.

	X	Y	Z	L*	a*	b*	C*	h0	sY	sCb	sCr	sR	sG	sB
Reflection	6.0	6.3	7.1	30.2	-0.0	-1.0	1.0	1.6	71	129	127	70	71	73
Transmission	83.2	87.5	91.2	94.9	-0.0	2.7	2.7	-1.6	240	125	130	243	240	235

Optical spectra   Color spaces

Spectral power distribution: Standard Illuminant D65   Color matching functions: CIE 1931

Reflection in x:

Transmission in x:

7 Difference Charge Density

MedeA allows visualizing the pseudo charge densities and charge density differences. Charge density differences are defined as the difference between the initial, atomic charge density distribution as used by VASP to initiate a calculation and the final electronic charge density distribution as it results from a self-consistent calculation of the electronic ground state. The latter is very useful to observe where electrons move during the SCF cycle.

- To compute electronic charge densities and differences using VASP, ☑ (Pseudo, difference, spin) charge density in the Properties field of the VASP Calculation panel

- To visualize the difference in charge density, click on Analysis >> Charge Densities >> Difference Charge Density to open a dialog with a list of calculated charge densities. Select one or more structures to visualize their charge densities

The analysis window appears as a split structure window, the left-hand side showing the structure, the right-hand side showing four panels, IsoSurface (3D) , Slice (2D) , Averages (1D) , and Points (0D) . By default an isosurface with an average value of the difference in charge density is shown.

In the IsoSurface (3D) tab you can:

- Specify the Iso value , using the slider or by typing in a value

- Choose a Color for the isosurface by clicking Choose color

- Type in a value to change the Transparency from invisible (0) to opaque (1)

- For quicker rotations and adjusting of the cell, the rendering quality can be modified by lowering the Precision from high to medium to very low

- Viewing Limits lets you display more than one unit cell of the structure. Click Update when making changes

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Note: To improve the spatial resolution of the Difference Charge Density increase the values of the VASP parameters *NGX*, *NGYF* and *NGZF*. You find these values in the *OUTCAR* file, increase them, preferably to a power of 2. Use Add to Input in the VASP panel to add a line like *NGXF=64*; *NGYF=64*; *NGZF=64* for increasing the computed default values.

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In the Slice (2D) tab you can:

- Select planes by giving their Miller indices or a Normal unit vector

- Change the Altitude of a given plane by moving the slider or by typing in a value

- Use the color scale to change the color spectrum

- Change the range of values covered by the color spectrum using the small black arrows on the right

- Right-click into the color scheme and select Edit section to change the values and colors used as upper/lower boundaries. Click Apply to apply after making changes

- Right-click into the color scheme and select Add section above/below to add an additional section. For each section, you can select a continuous spectrum of colors (ramp) or a constant value

- Edit as picture to get the current slice (without any superimposed cell boundaries and atoms), set the size to your specifications (either width or height) and save it as Bitmap, PNG or TIFF.

In the Averages (1D) tab you can:

- Select the axis normal to the averaged plane

- Integration range (in $\mathring{A}$) for the macroscopic averaging

- For further information push Help

In the Points (0D) tab you can:

- Add rows in a table with + and enter additional real space points in Fractional or Cartesian coordinates into the Table

- Calculate the values at these points by pushing Retrieve data

- For further information push Help

Example of Charge density difference for NaCl:
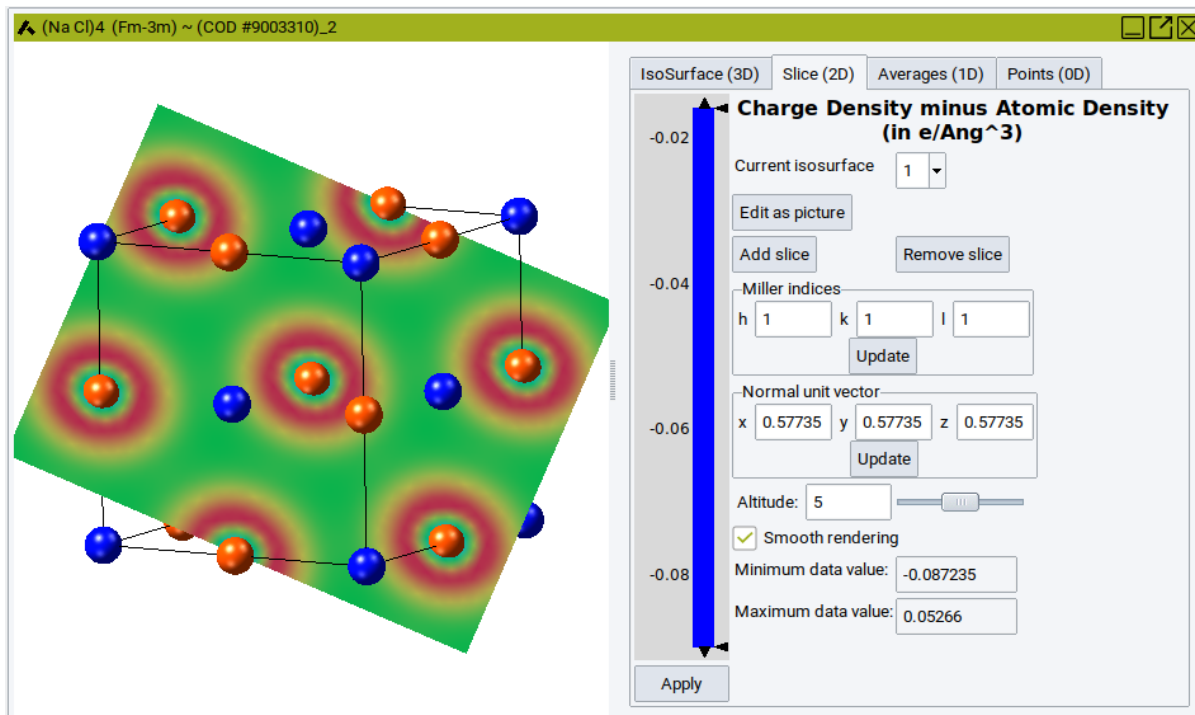
In the above example, a projection of the difference charge density onto the (111) plane is shown for NaCl. The range of the plot is from -0.087235 e$\mathring{A}$3 to 0.5266 e$\mathring{A}$3. The plot has three sections: The lowest section ranging from -0.09 to -0.016 is colored in blue. The section from -0.016 to 0.035 shows the variation of the

difference charge density in colors from blue to red, the highest section is all in red. Depending on the altitude of the slice, not the full range of the variation in difference charge density is visible.
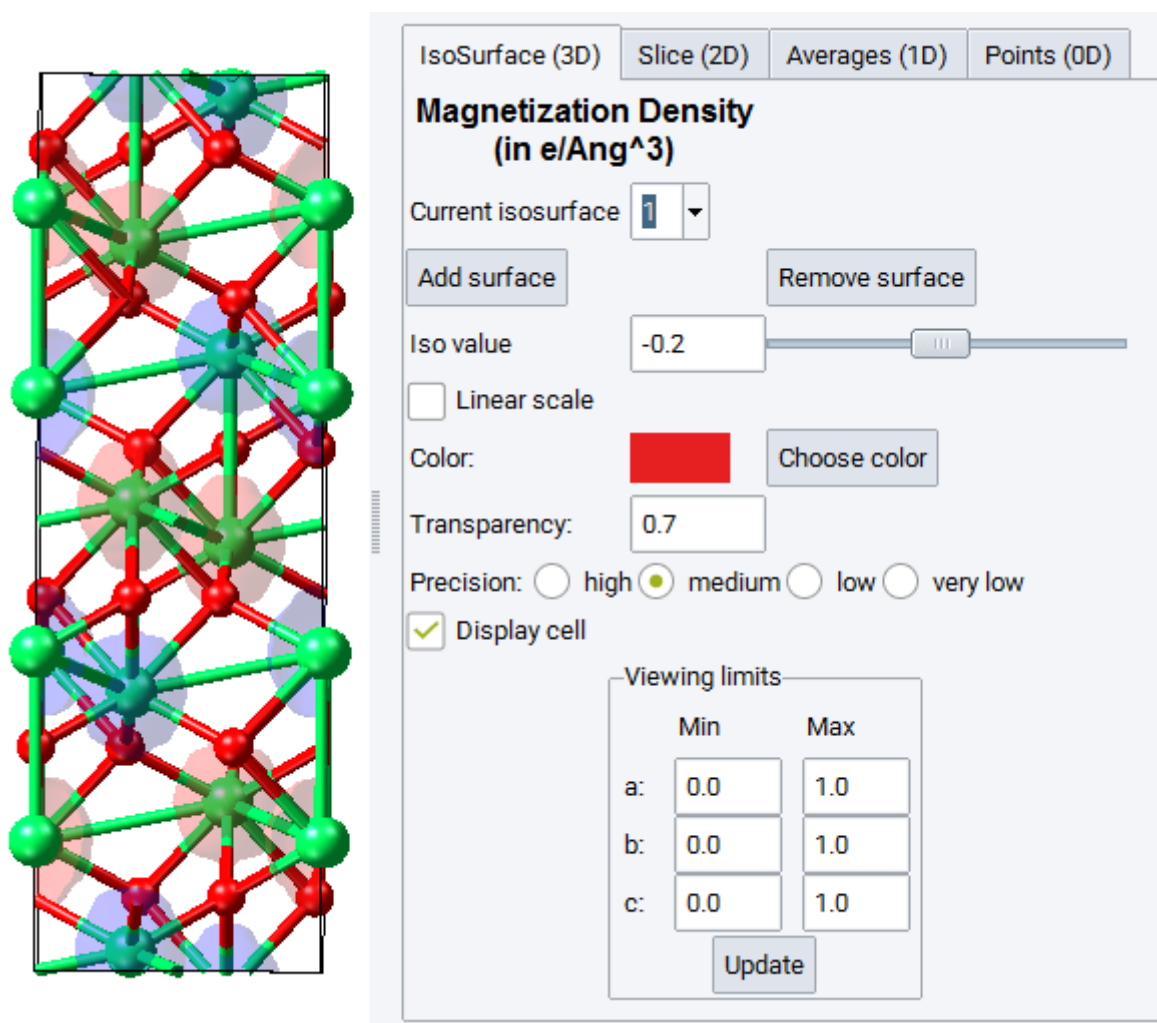
8 Magnetization Density

MedeA allows visualizing magnetization densities defined as difference between spin-up and spin-down electron density. To compute magnetization densities using VASP spin-polarized calculation, ☑ (Pseudo, difference, spin) charge density in the Properties field of the VASP Calculation panel

- To visualize a difference charge density, click on Analysis   >>   Magnetization Densities to open a dialog with a list of calculated charge densities. Select one or more structures to visualize their magnetization densities.

The Analysis window has the same options as explained in the previous section.

It allows you to display

Note: To improve the spatial resolution of the Magnetization density increase the values of the VASP parameters *NGXF,NGYF,NGZF*.

In the example above, the antiferromagnetic structure of Hematite (Fe2O3).

For structures with non-collinear magnetism, the analysis can be refined to x-, y- and z-direction.

In the Averages (1D) tab you can:

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- Select the `axis` normal to the averaged plane

- `Integration range` (in Å) for the macroscopic averaging

In the `Points (0D)` tab you can:

- Add rows in a table with `+` and enter additional real space points in Fractional or Cartesian coordinates into the Table

- Calculate the values of the magnetization density at these points by pushing `Retrieve data`

- For further information push `Help`

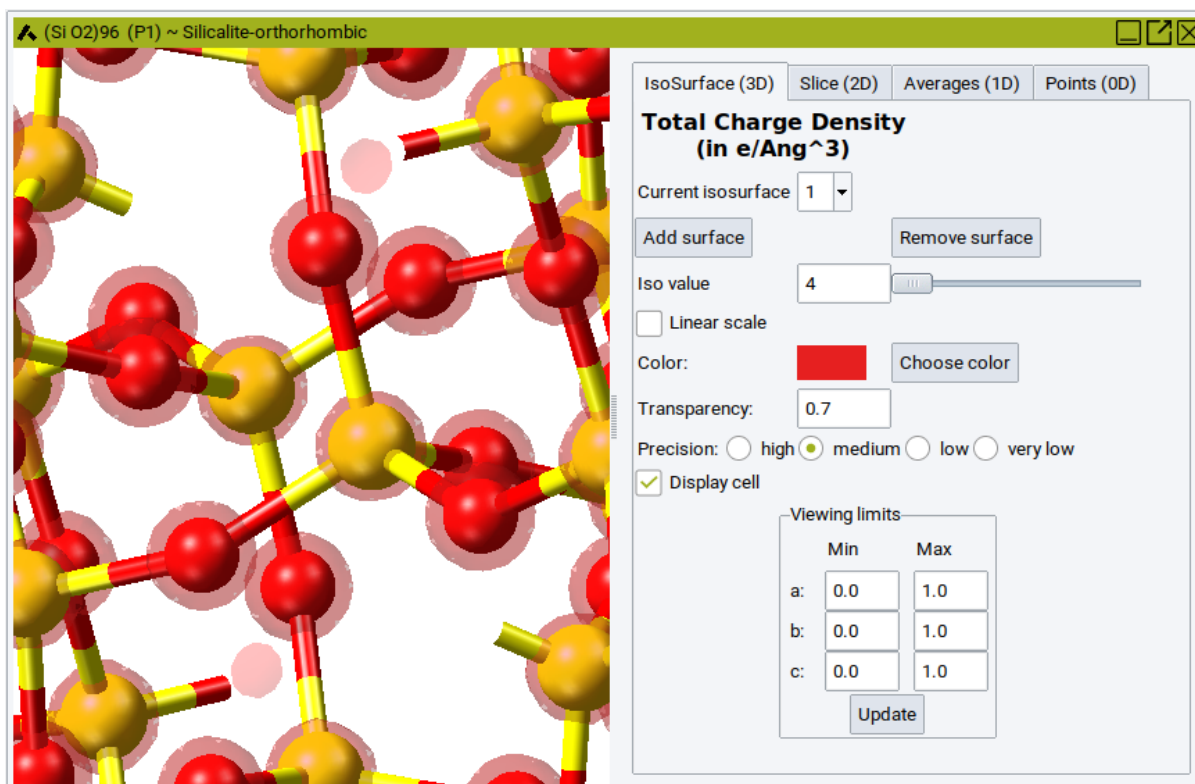# 9 Total Charge Density and Total Valence Charge Density

MedeA allows visualizing total charge density and total valence charge densities. The total charge density includes all electrons including the core, the total valence charge density includes all electrons not included in the core of the pseudo potential or PAW potential.

- To compute these electronic charge densities using VASP, ☑ `(Total, valence) charge density, Bader analysis` in the Properties field of the VASP `Calculation` panel

- To visualize a valence charge density, click on `Analysis` `>>` `Charge Densities` `>>` `Total Charge Densities` or `Analysis` `>>` `Charge Densities` `>>` `Total Valence Charge Densities` to open a dialog with a list of calculated charge densities. Select one or more structures to visualize their charge densities.

The analysis window appears as a split structure window, the left-hand side showing the structure, the right-hand side showing four panels, `IsoSurface (3D)` , `Slice (2D)` , `Averages (1D)` and `Points (0D)` . By default an isosurface with an average value of the total (valence) charge density is shown.

- Specify the `Iso value` , using the slider or by typing in a value

- Choose a Color for the isosurface by clicking `Choose color`

- Type in a value to change the `Transparency` from invisible (0) to opaque (1)

- For quicker rotations and adjusting of the cell, the rendering quality can be modified by lowering the `Precision` from high to medium to very low

- `Viewing Limits` lets you display more than one unit cell of the structure. Click `Update` when making changes

Note: To improve the spatial resolution of the Total Charge Density or Total Valence Charge density increase the values of the VASP parameters *NGXF,NGYF,NGZF*. You find these values in the *OUTCAR* file, increase them, preferably to a power of 2. Use `Add to Input` in the VASP panel to add a line like *NGXF=64*; *NGYF=64*; *NGZF=64* for increasing the computed default values.

In the Slice (2D) tab you can:

- Select planes by giving their Miller indices or a Normal unit vector

- Change the Altitude of a given plane by moving the slider or by typing in a value

- Use the color scale to change the color spectrum

- Change the range of values covered by the color spectrum using the small black arrows on the right

- Right-click into the color scheme and select Edit section to change the values and colors used as upper/lower boundaries. Click Apply to apply after making changes

- Right-click into the color scheme and select Add section above/below to add section. For each section you can select a continuous spectrum of colors (ramp) or a constant value.

- Edit as picture to get the current slice (without any superimposed cell boundaries and atoms), set the size to your specifications (either width or height) and save it as Bitmap, PNG, or TIFF.

In the Averages (1D) tab you can:

- Select the axis normal to the averaged plane

- Integration range (in Å) for the macroscopic averaging

In the Points (0D) tab you can:

- Add rows in a table with + and enter additional real space points in Fractional or Cartesian coordinates into the Table

- Calculate the values of the total (valence) charge density at these points by pushing Retrieve data

- For further information push Help

10 Pseudo Charge Density

MedeA allows visualizing pseudo charge densities used to construct the charge density differences. This includes all valence electrons not included in the core of the pseudo potential or PAW potential.

11 Electron Localization Function

The electron localization function [4], ELF, is used to identify binding and lone electron pairs in simple molecular systems. The *MedeA* interface for this feature is identical to the one for charge densities. The example below shows the graphene plane.
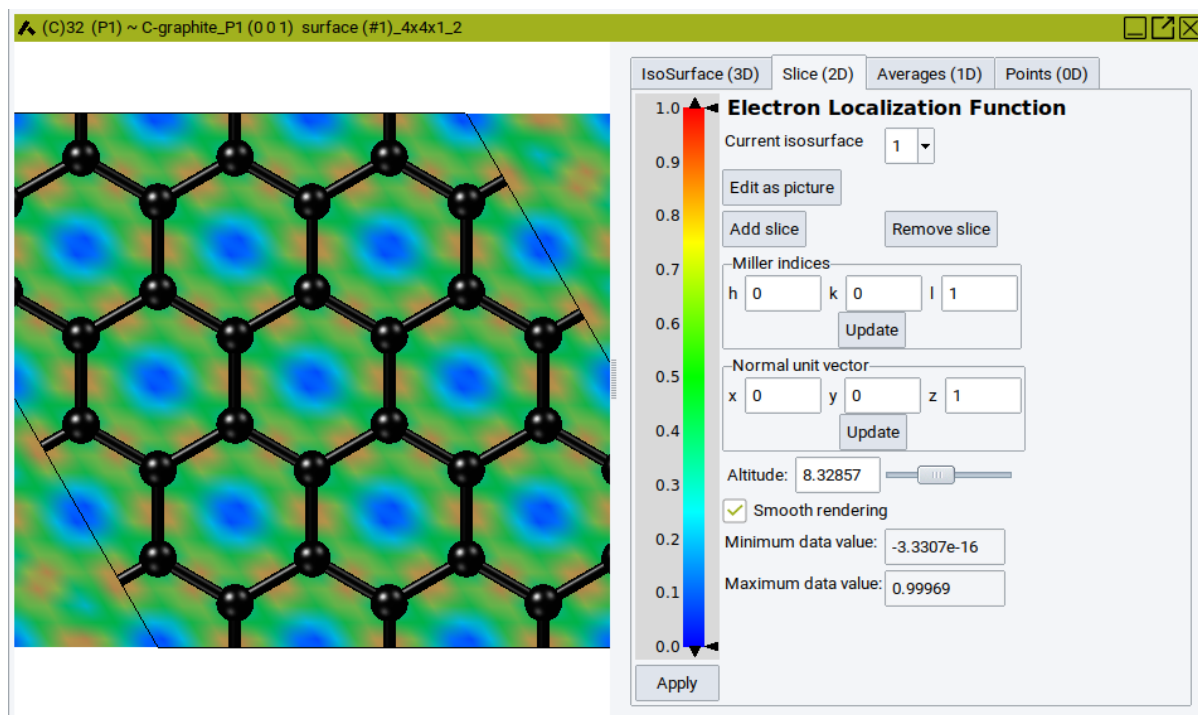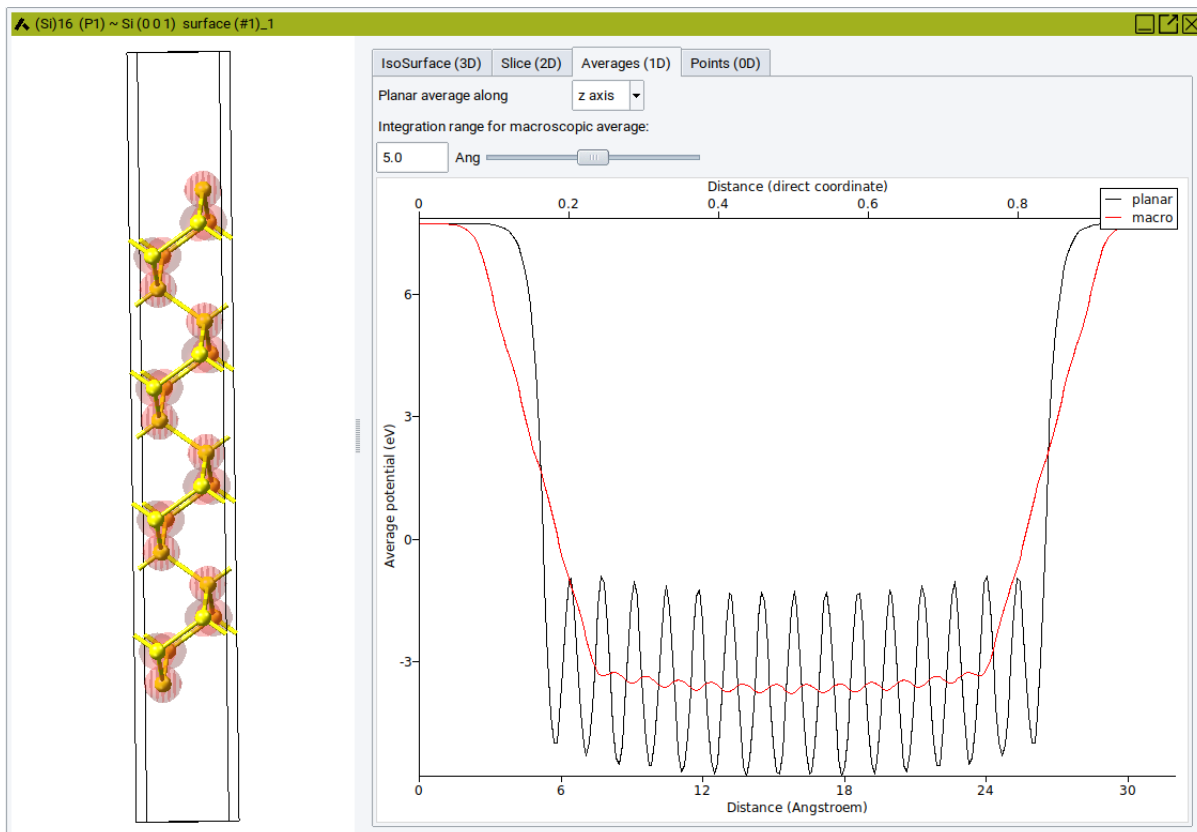

Note: To improve the spatial resolution of the electron localization function increases the values of the VASP parameters *NGX*, *NGY*, and *NGZ*. You find these values in the *OUTCAR* file, increase them, preferably to a power of 2. Use Add to Input in the VASP panel to add a line like *NGX=64*; *NGY=64*; *NGZ=64* for increasing the computed default values.

12 Total Local Potential

The *MedeA* interface for this feature is identical to the one for charge densities and ELF.

[4] A D Becke and K E Edgecombe, "A Simple Measure of Electron Localization in Atomic and Molecular Systems," *Journal of Physical Chemistry* 92, no. 9 (1990): 5397.

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The Averages (1D) tab plots the total potential averaged over a plane normal to the selected axis .

Select an appropriate Integration range for macroscopic average to compare the total local potential between specific regions.

Note: To improve the spatial resolution of the local potential increase the values of the VASP parameters *NGXF*, *NGYF*, and *NGZF*. You find these values in the OUTCAR file, increase them, preferably to a power of 2. Use Add to Input in the VASP panel to add a line like *NGXF=64*; *NGYF=64*; *NGZF=64* for increasing the computed default values.

13 Export Band Structure and DOS

Sometimes it is very convenient to have the information from a calculated band structure or DOS calculation in numerical format and calculate band centers or highlight a specific band or surface modes for a publication.

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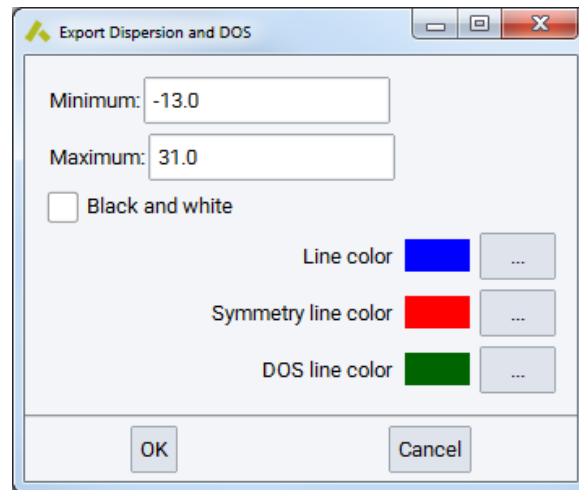
First, select a list of jobs, which have band structure or DOS calculated. You might see a warning message reminding you that the VASP GUI allows for selecting band structure and DOS independently.

Some of the jobs that you selected do not have dispersion data. For these jobs, only the DOS data will be exported.

You can restrict the export to a narrower energy range, by setting a Minimum (eV) and Maximum (eV) on the scale relative to the Fermi energy (different from the values in the original VASP output files). These bounds are applied to the results of all selected jobs.
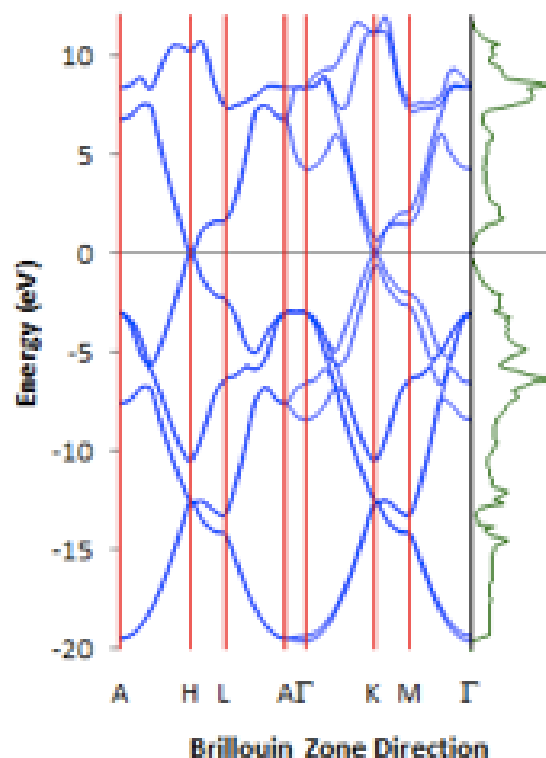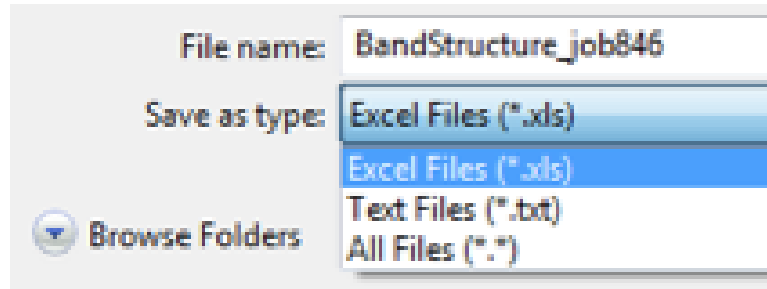

The color choices apply only to Excel and specify:

• Line color for bands

- vertical Symmetry line color and the

- color for the DOS line plotted on the right side of the band structure graph.

You can export the DOS values as a text file (*.txt*) or if Excel is installed, also into a spreadsheet (*.xls*) which contains the band structure as well. The default format is an Excel file (*.xls*).

Please note, that you can also get the numerical data for a selected Band Structure or Density of States plot in *MedeA* by right-clicking into the active graphics panel and choosing one of the export options from the pulldown menu.