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Set up and analyze VASP calculations with QuantumATK

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In this tutorial, you will explore how QuantumATK can be used as a graphical interface (GUI) for VASP calculations. In particular, you will learn how to easily create your structure and generate all the relevant VASP input files. Also, you will be able to analyze your VASP output files with QuantumATK, and plot the results.

Note that this tutorial is not a user guide to VASP, nor does QuantumWise provide access to the VASP code. It is assumed that the user has already obtained and installed VASP website from its official source, and is familiar with the code.

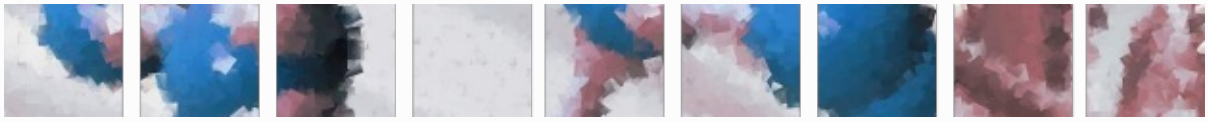
Contents:

- Analyze MD trajectories
- Visualize forces
- Visualize vibrational modes

Note

Click to read information about all input (➔) and output (➔) VASP files.

- ➔ POSCAR, INCAR, KPOINTS, POTCAR
- ➔ OUTCAR, CONTCAR, CHGCAR, DOSCAR, EIGENVAL, CHG, PARCHG, ELFCAR



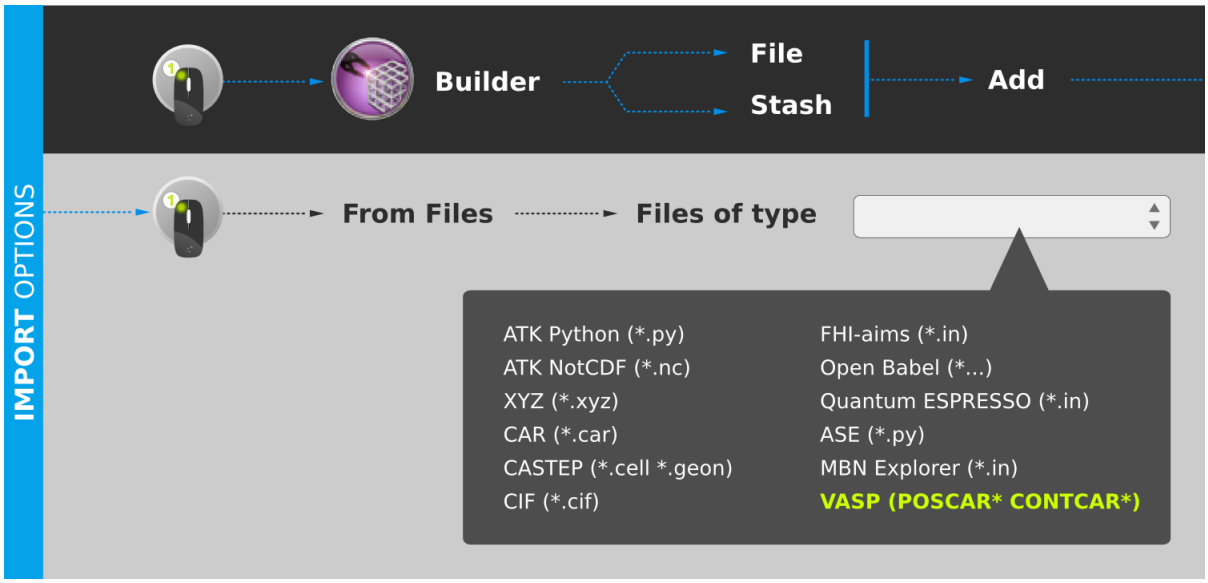
Important

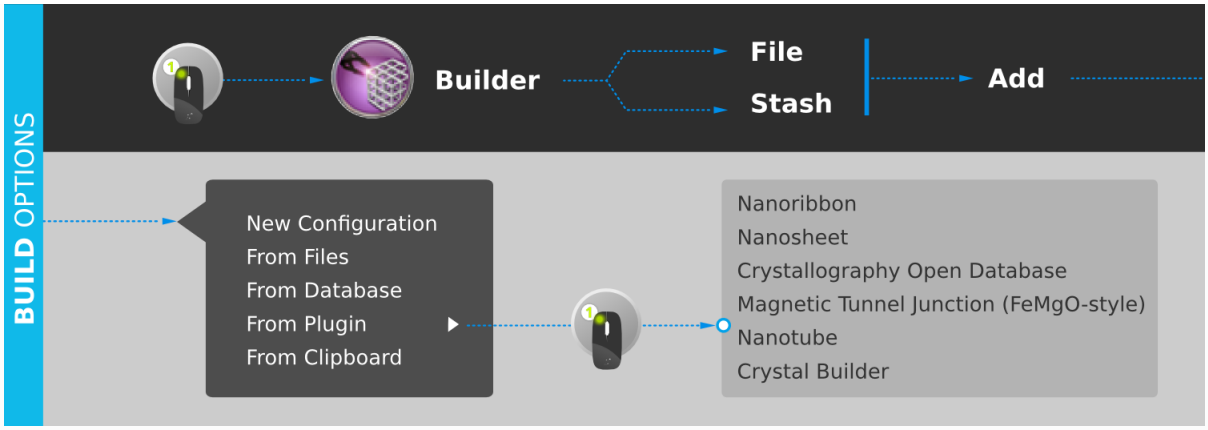
Read the The VASP Scripter AddOn tutorial in order to:

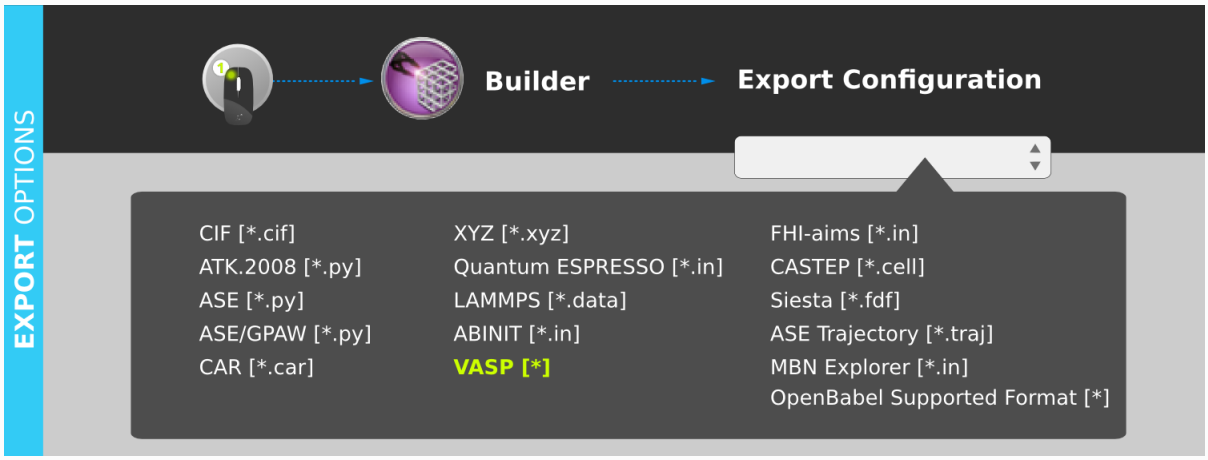
1. configure the VASP scripter;
2. install the VASP pseudopotential libraries.

Setting up the configuration using QuantumATK

You can use one of the many **import**, **build**, and **export** options as shown in the next pictures:



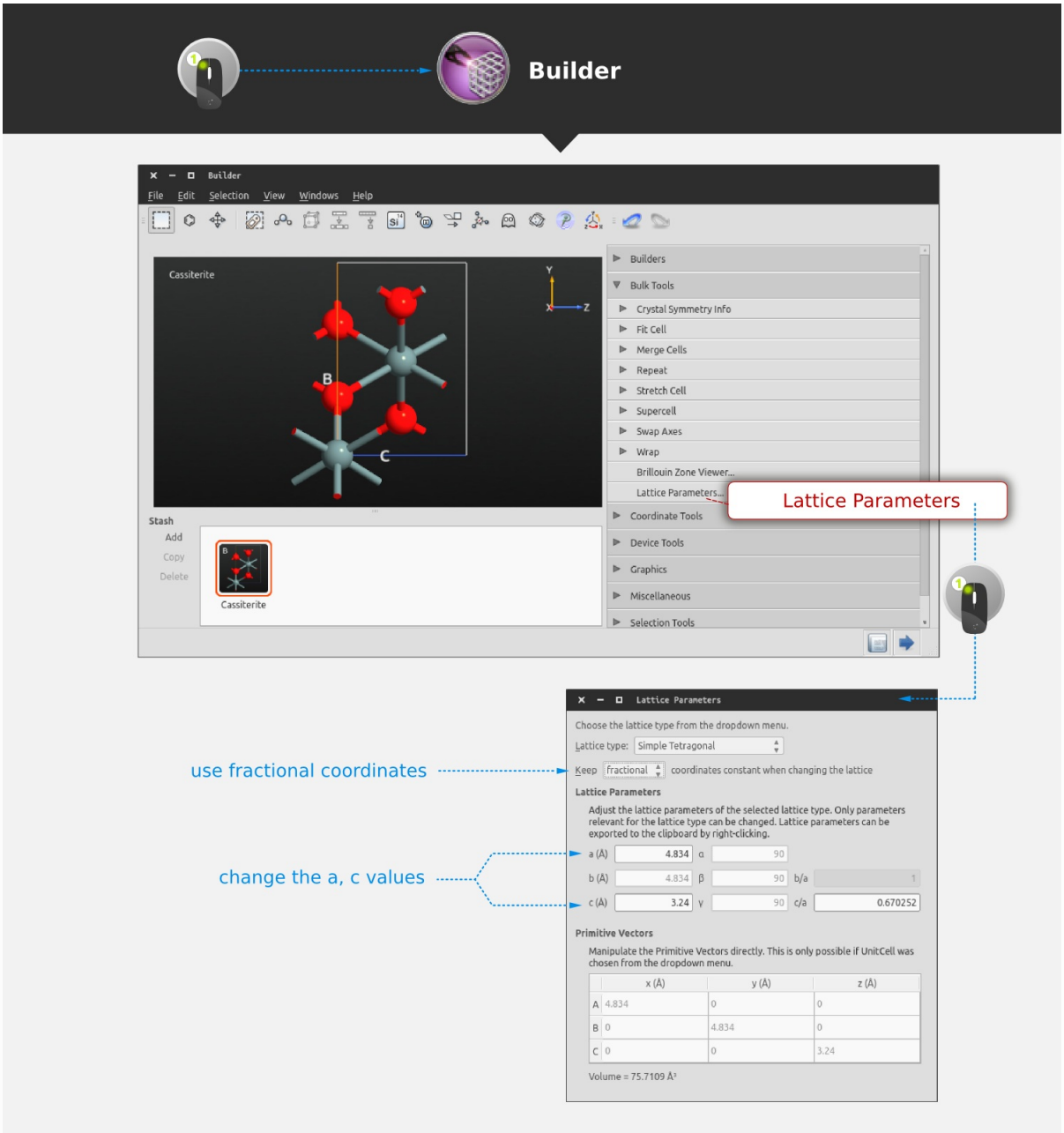




Note

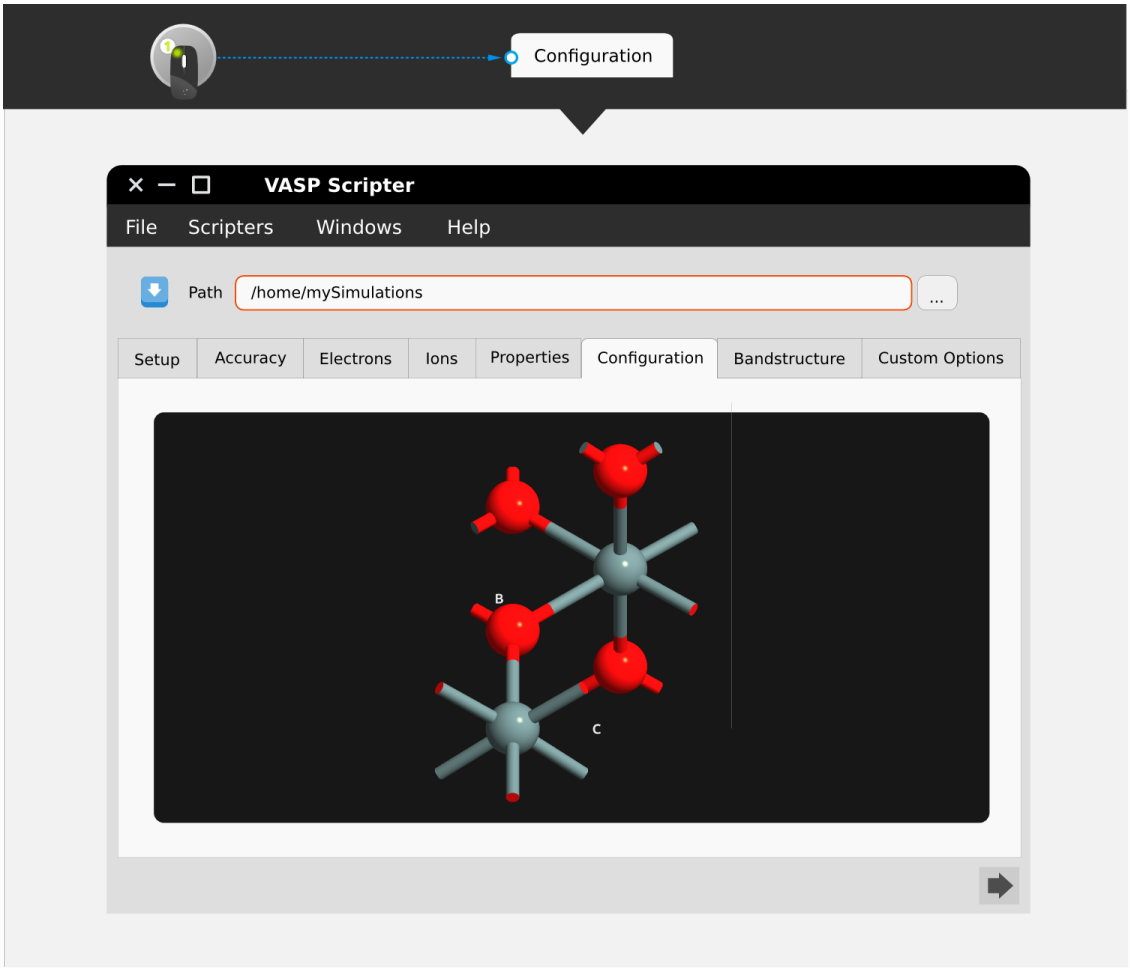
Note that whatever operation you will perform on your structure you will always be able to export the configuration to the POSCAR file format by File ▸ **Export Configuration**. Under the Save as type select VASP.

- Example: open the **Builder** and Add ▸ From Database ▸ **Cassiterite** (SnO_2). Modify the lattice paramenters to a=4.834 Å and c=3.244 Å in order to reproduce the results of Godinho et al.. From the Builder, open Bulk Tools ▸ **Lattice Parameters**, and keep *fractional coordinates* fixed and modify the a and c vectors:



Use the VASP Scripter to set up the calculation

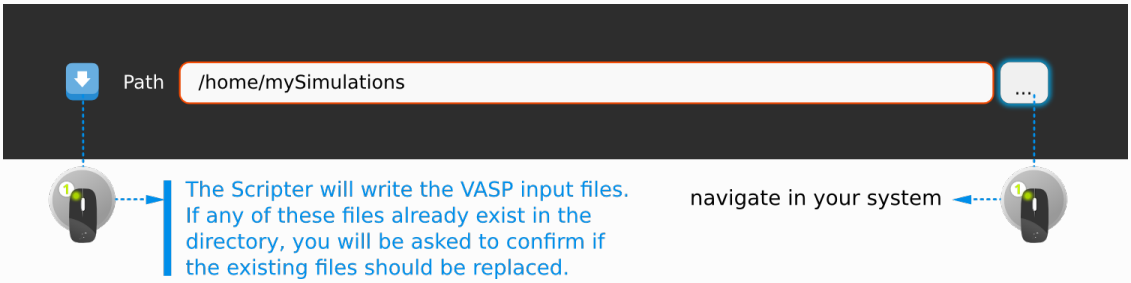
1. Open the VASP scripter: (from the main QuantumATK window) Custom Scripters ▸ Scripters ▸ **VASP Scripter**.
2. Once your structure is ready, drag 'n' drop it from the Stash in the VASP scripter. Then you will see the structure embedded in the **Configuration** tab of the VASP scripter:



3. Set up you simulation. For a detailed instruction on how the set up you simulation with the VASP Scripter, refer to the The VASP Scripter AddOn tutorial. In this example, we want to optimize the geometry of the bulk SnO_2 structure imported from QuantumATK. So, we choose Setup ▸ **Task** to **Structural optimization** and adjust all the parameters according to your needs.

> **Note**
>
> **Setting constraints:** If you may want to constrain some specific atoms during the geometry optimization. You can do that by assigning the tag name **constraints** to these atoms in the Builder through the Select ▸ **Tags** tool. The proper F and T flags will be added to the exported POSCAR.

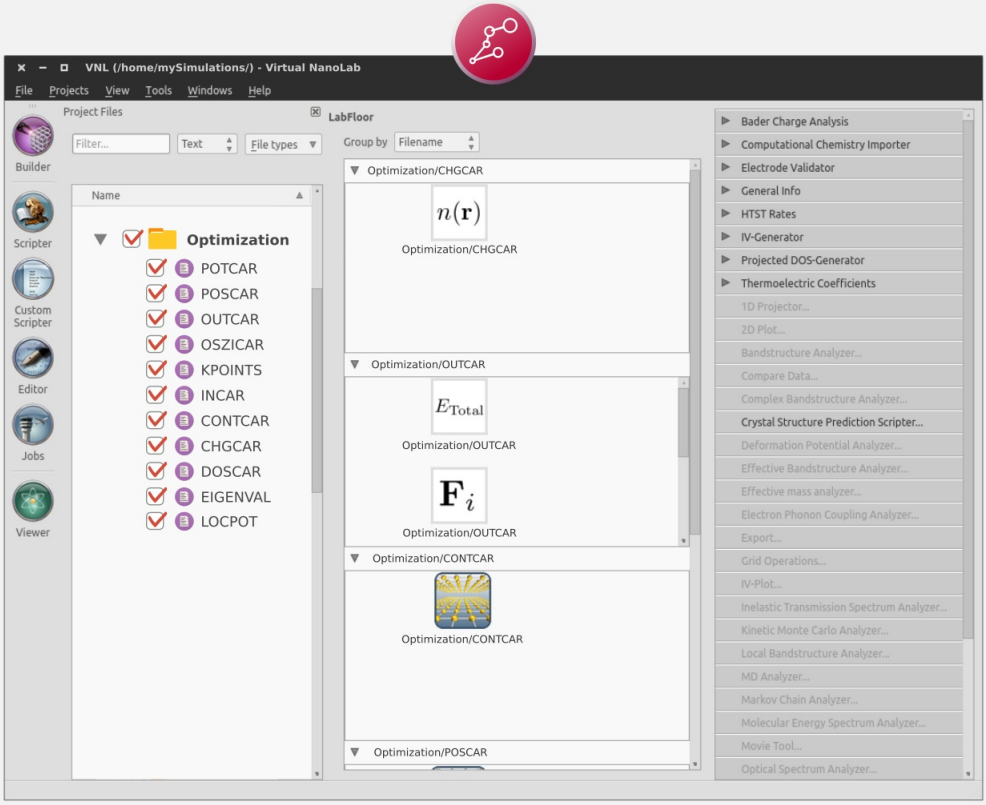
4. Choose the directory where to save the files and press **Save** to write the INCAR, POSCAR, KPOINTS and POTCAR files.



5. Run VASP!

Analyzing the results

- When the calculation is done and you have the VASP output files in the project directory, QuantumATK will automatically recognize their file format and add them to the LabFloor as shown below:

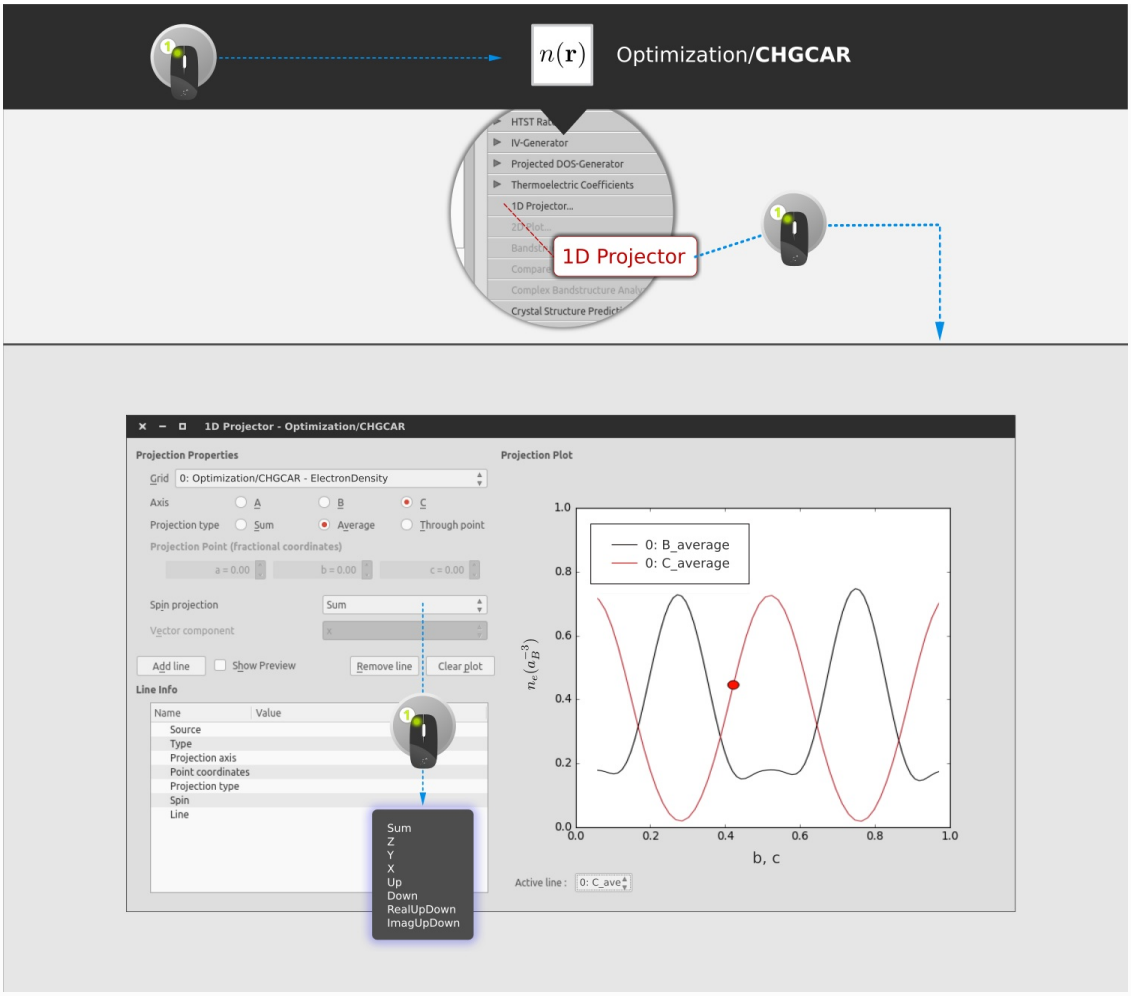


For example, from **CONTCAR** you can check the optimized structure by selecting it on the **LabFloor** and click on Show in 3D Viewer, or send it directly to the Builder for further modifications. Using **CHGCAR** you can inspect the charge density as described below by using different tools such as the **1D Projector**, the **Grid Operations** and the **3D Viewer** tools, which you can find in the right-hand side plugin panel.

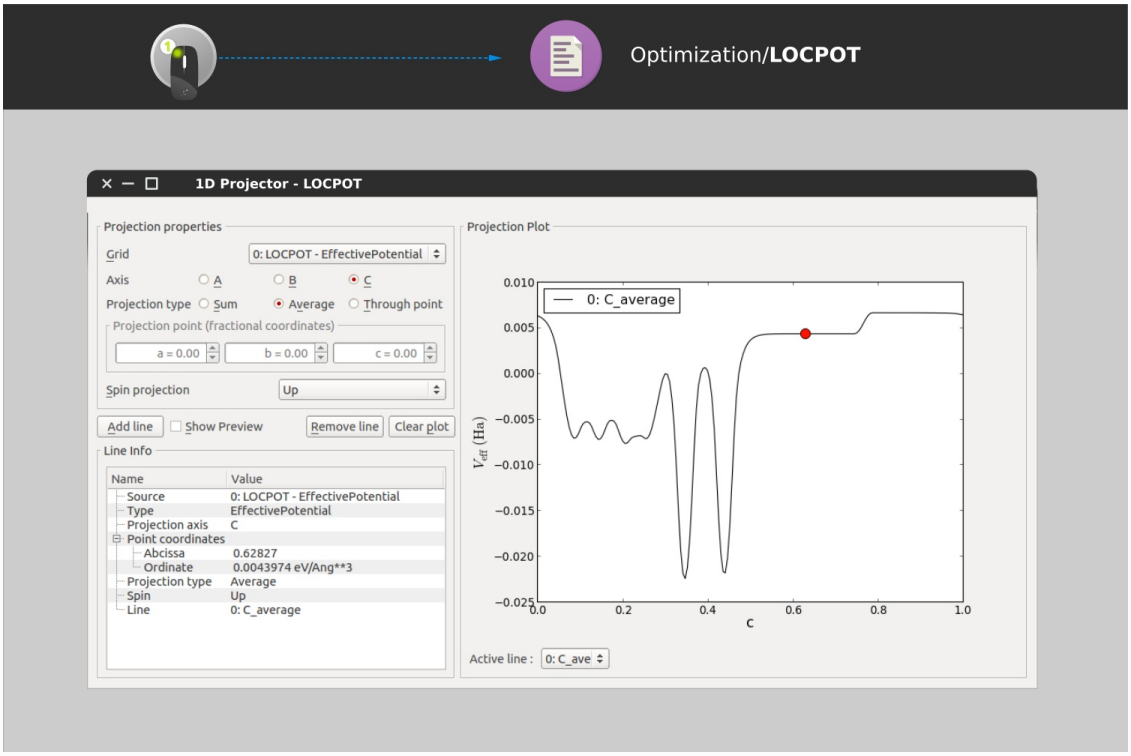
1D Projections of 3D grids

By using this tool you will be able to easily plot charge density projections of different types (sum, avarage or through a point) along the three axes (x,y,z). The window is interactive and by selecting a point on the graph you will have detailed information in the left-hand side of the window. This tool is pretty handy to analyze CHGCAR or LOCPOT files:

- select the **CHGCAR** element in the **LabFloor** and click the **1D Operations** button/bar.

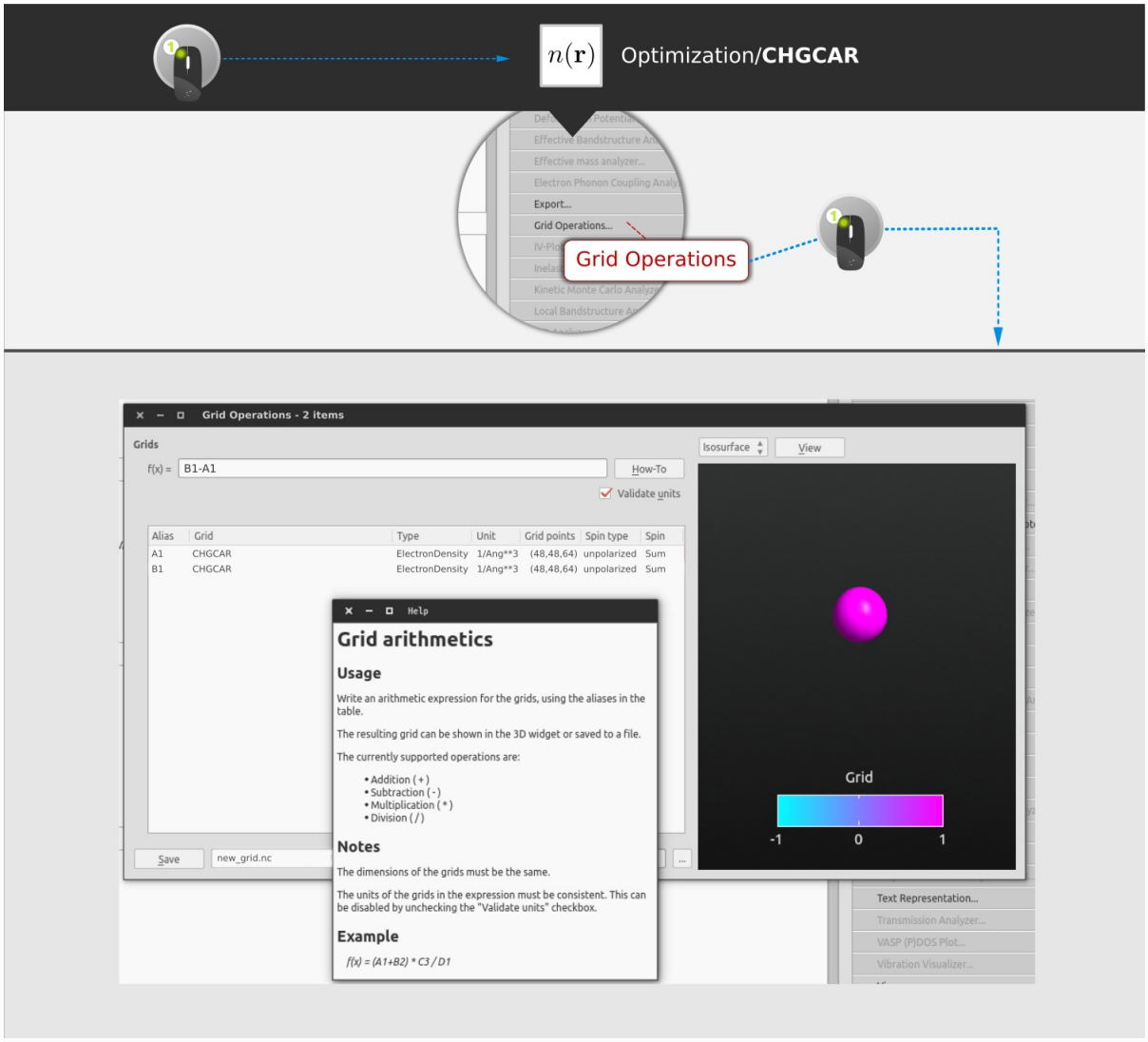


- If you have performed a potential simulation you can check the Local Potential property in the VASP Scripter (VASP keyword LVTOT = .TRUE.), the **LOCPOT** file is written by VASP and it will appear in the LabFloor. You can analyze the content of this file with the **1D Projector** or plot an isosurface or a plane cut in the **Viewer**. The figure below show the projection of the local potential along the C axis of a 2L-MgO/Fe(100) system. You can see that the dipole correction in the middle of the vacuum region has been applied.



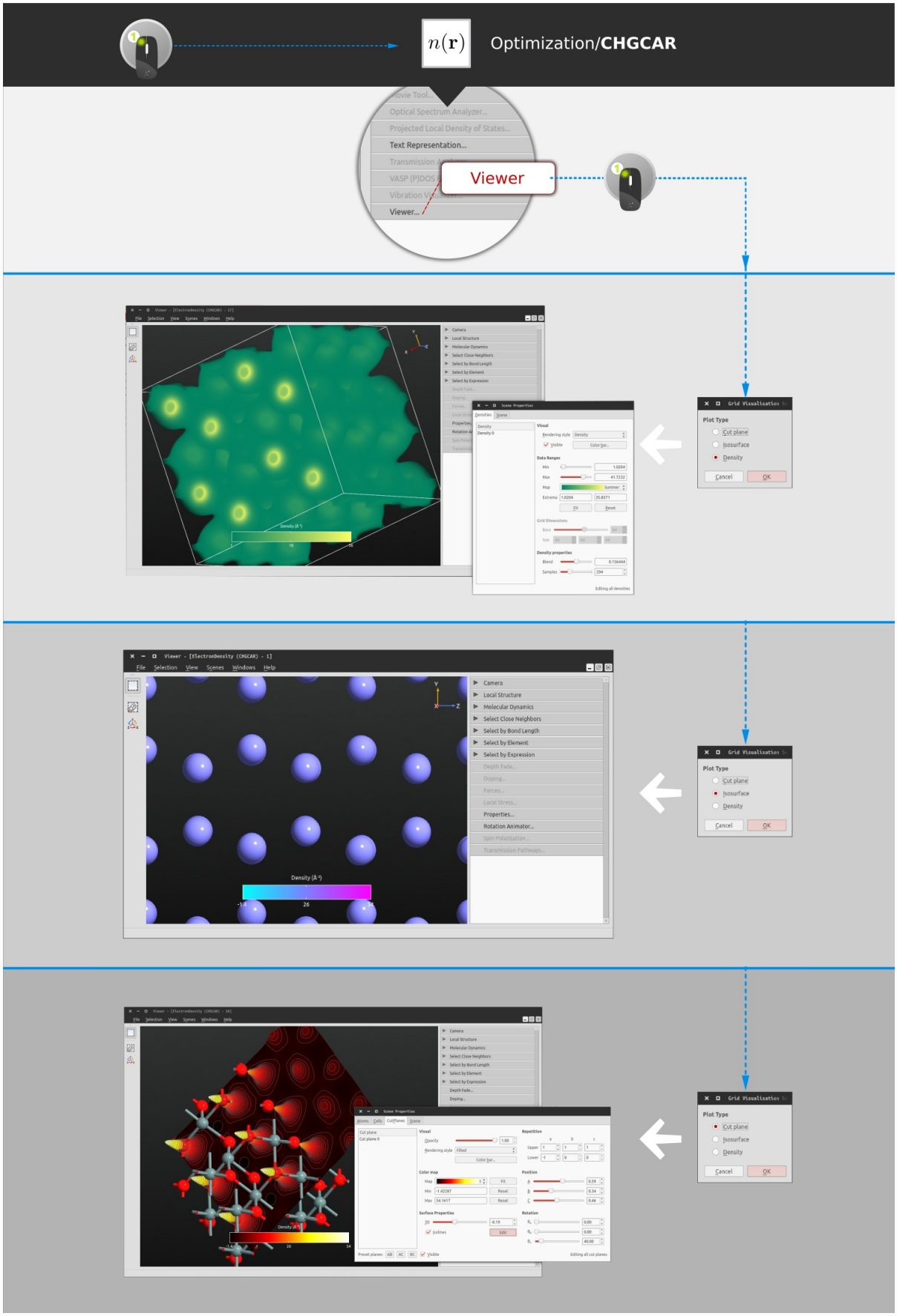
Operations with two or more 3D grids

This tool allows you to perform any kind of arithmetic operation with two or more **CHGCAR** files (or any other 3D grid). Just select the CHGCAR files from the **LabFloor** (by holding down Ctrl) and click on **Grid Operations**. A new window will open. Here you can write the arithmetic expression in the *f(x)* field (+, −, × and ÷ are allowed). A preview of the result is also showed. You can save the resulting grid in a NetCDF file for more detailed analysis (e.g. in the 1D projetor, or the 3D Viewer, see below). For example, this can be very useful to analyze the charge density difference of a system with and without a defect or before and after adsorption of a molecule/cluster on a surface and so on.



Visualize 3D grids as density, isosurface, or cut plane

This tool that allows you to display 3D grid data, such as the real-space charge density from **CHGCAR**, as isosurfaces or contour plots. Select the object from the **LabFloor**, click the **Viewer** button at the right and choose to plot an isosurface, a density or a plane cut. If your calculation is spin-polarized you will be able to plot the total charge density ($\uparrow + \downarrow$), the spin density difference ($\uparrow - \downarrow$) or only the spin-up ($\uparrow$) or spin-down ($\downarrow$) density.



Hint

You can Drag and Drop other elements from the LabFloor directly into this window and overlap the charge density plot with the structure contained in the CONTCAR file or even with the same CHGCAR

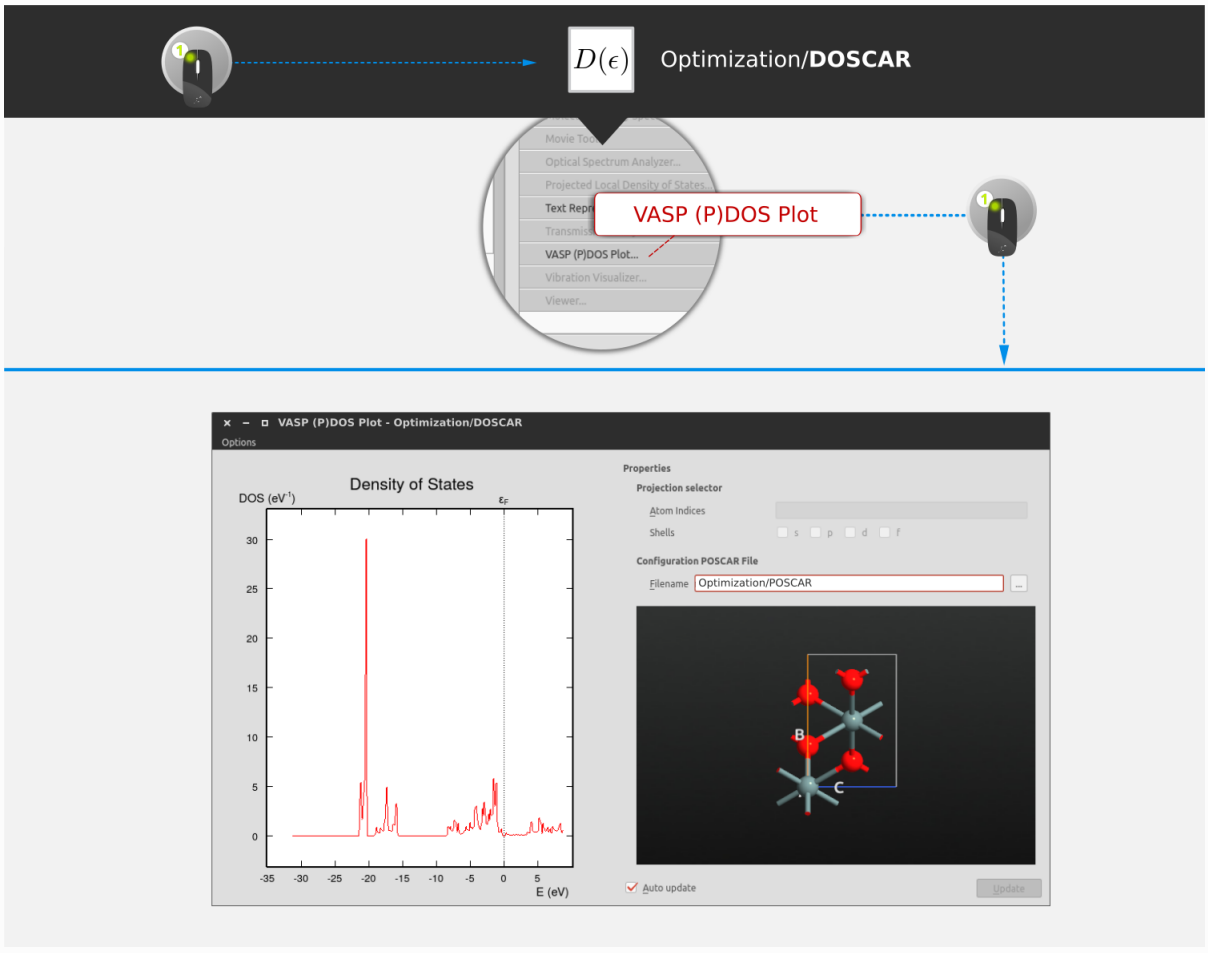
file to show a different plot type:

Click on Properties on the right-hand side of the Viewer window to have full control over all the aspects of the plot such as isovalue, positions of the cut planes, colors, … .

Plot density of states

- **Step A.** Open the **VASP Scripter** as described above and **drag 'n' drop** the **CONTCAR** file into it.
- **Step B.** Now select a self-consistent **Static run (SC)** from the list of tasks (in Setup tab).
- **Step C.** Eventually modify other parameters to run a well converged DOS calculation, e.g. increase the density of k-point sampling and the number of bands.
- **Step D.** Save the input files and run VASP!

At the end of the run, the DOSCAR file (and all the other output files) will appear on the LabFloor. Select the DOSCAR object and click on Show 2D Plot to generate the DOS plot.

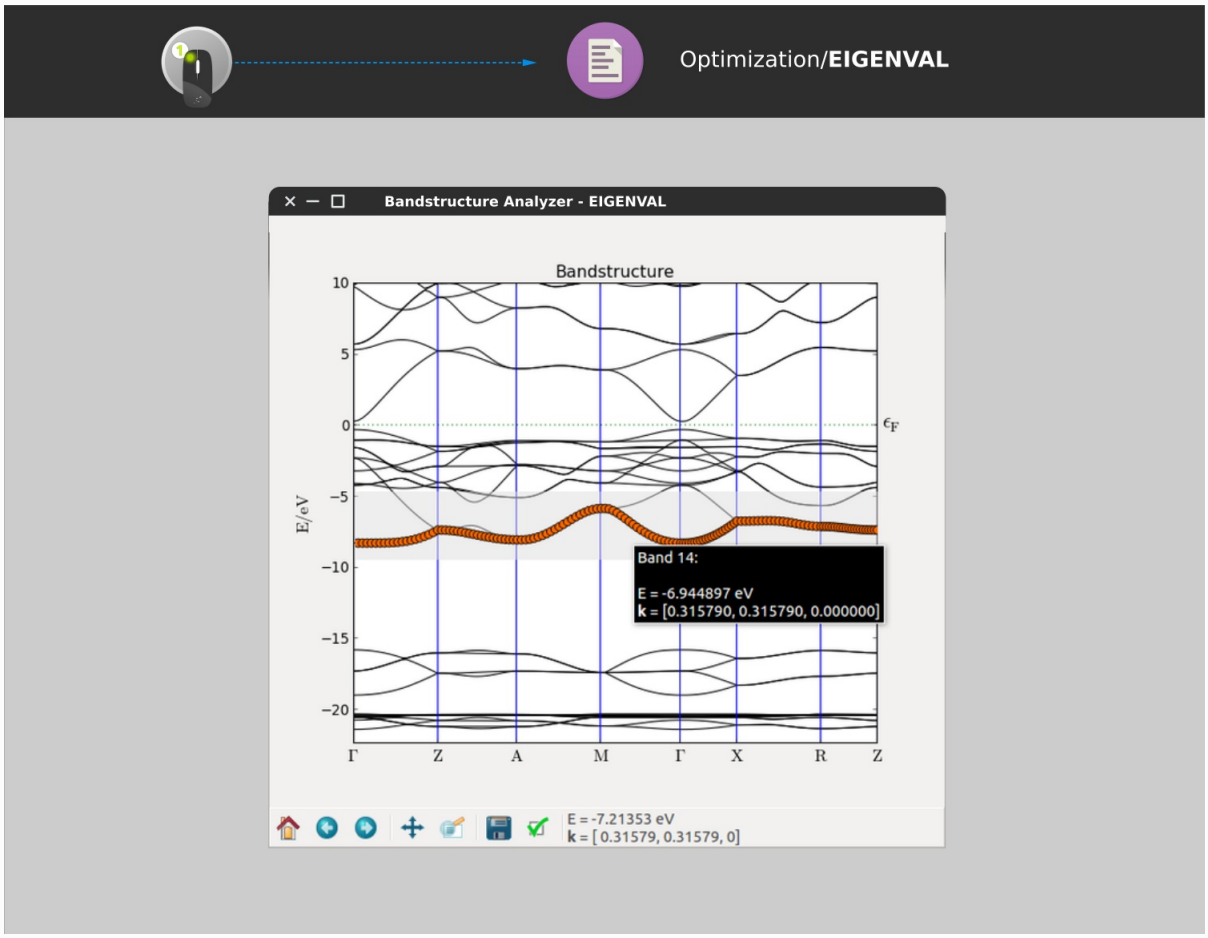


Plot bandstructure

- **Step A.** Once again, open the **VASP Scripter** and **drag 'n' drop** the **CONTCAR** file into it.
- **Step B.** From the list of (Setup tab) task, select **Bandstructure**.
- **Step C.** The Bandstructure tab is now active and you can set up the desired path in the Brillouin zone.

- **Step D.** Save the input files including the KPOINTS file and run VASP. Remember that in order to run a band structure calculation with VASP you have to use a preconverged CHGCAR file in the same directory!

From the LabFloor select the **EIGENVAL** object and click the Bandstructure analyzer in the plugin panel. A new interactive window will open. Here you can zoom into a small region of the plot and measure the band gap, for example.



Analyze MD trajectories

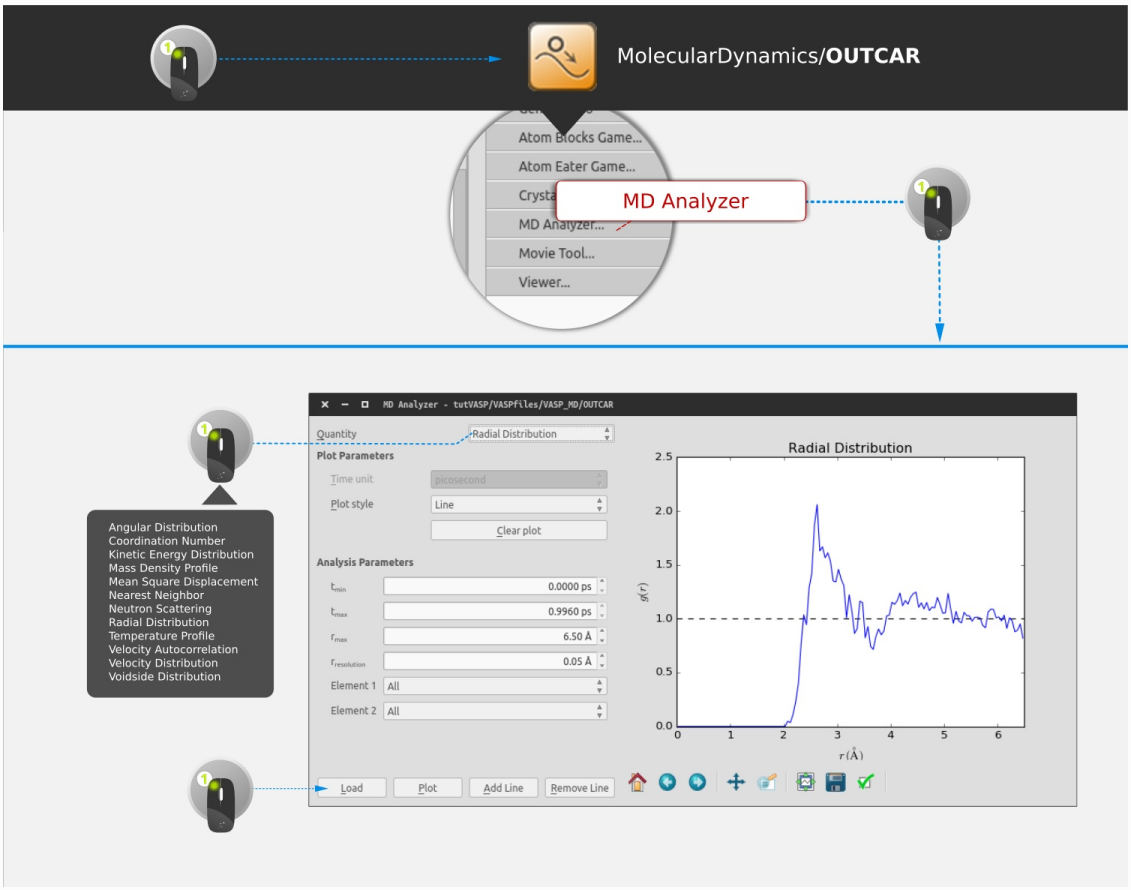
You can analyze your VASP molecular dynamics trajectory directly within QuantumATK. The information are read from the OUTCAR file, when selected the **MDTrajectory** object will be loaded in the LabFloor. Select this object and use either the **MD analyzer** or the **Movie Tool** plugin to analyze in detail you simulation.

- Using the **MD Analyzer**

  This tool will allow you to perform a series of analyses to your MD trajectory. See the Reference Manual for more details about each anlysis.

  - Angular distribution
  - Coordination number
  - Density profile
  - Kinetic energy distribution

- Mean square displacement
- Nearest neighbor
- Neutron scattering
- Partial structure factor
- Radial distribution
- Temperature profile
- Velocity autocorrelation
- Velocity distribution

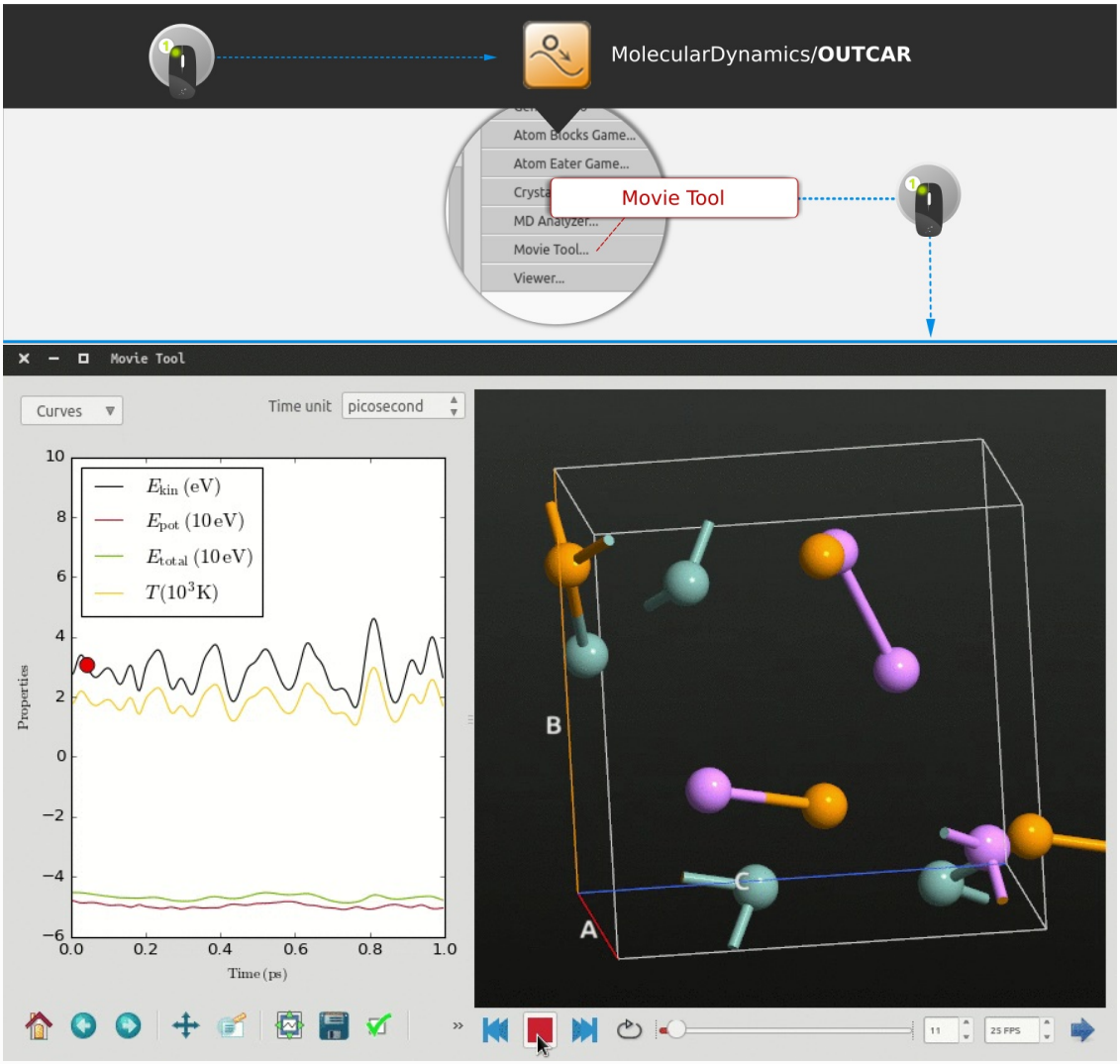


Note

You can perform these analysis for static configurations as well, i.e. with your POSCAR and CONTCAR configurations.

- Using the **Movie Tool**

  With this tool you can visualize all frames you MD trajectory. An interactive plot reporting energies and temperatures is showed on the left side.

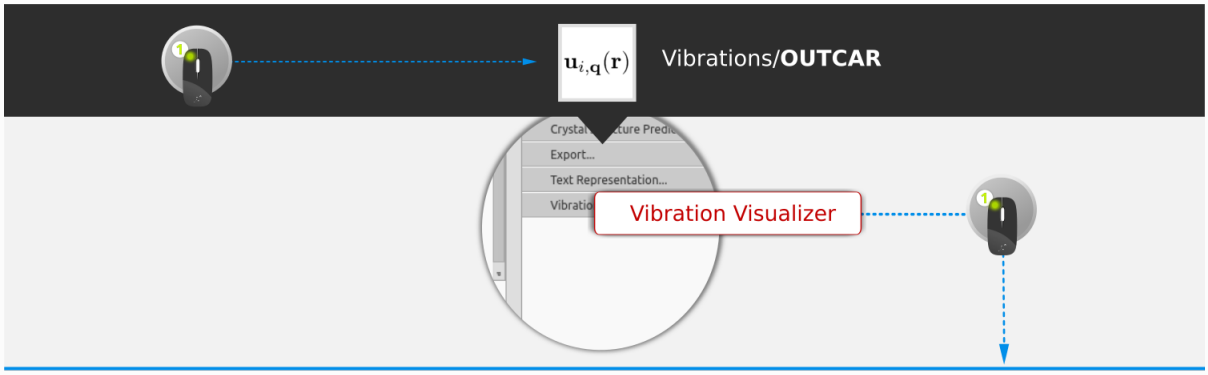


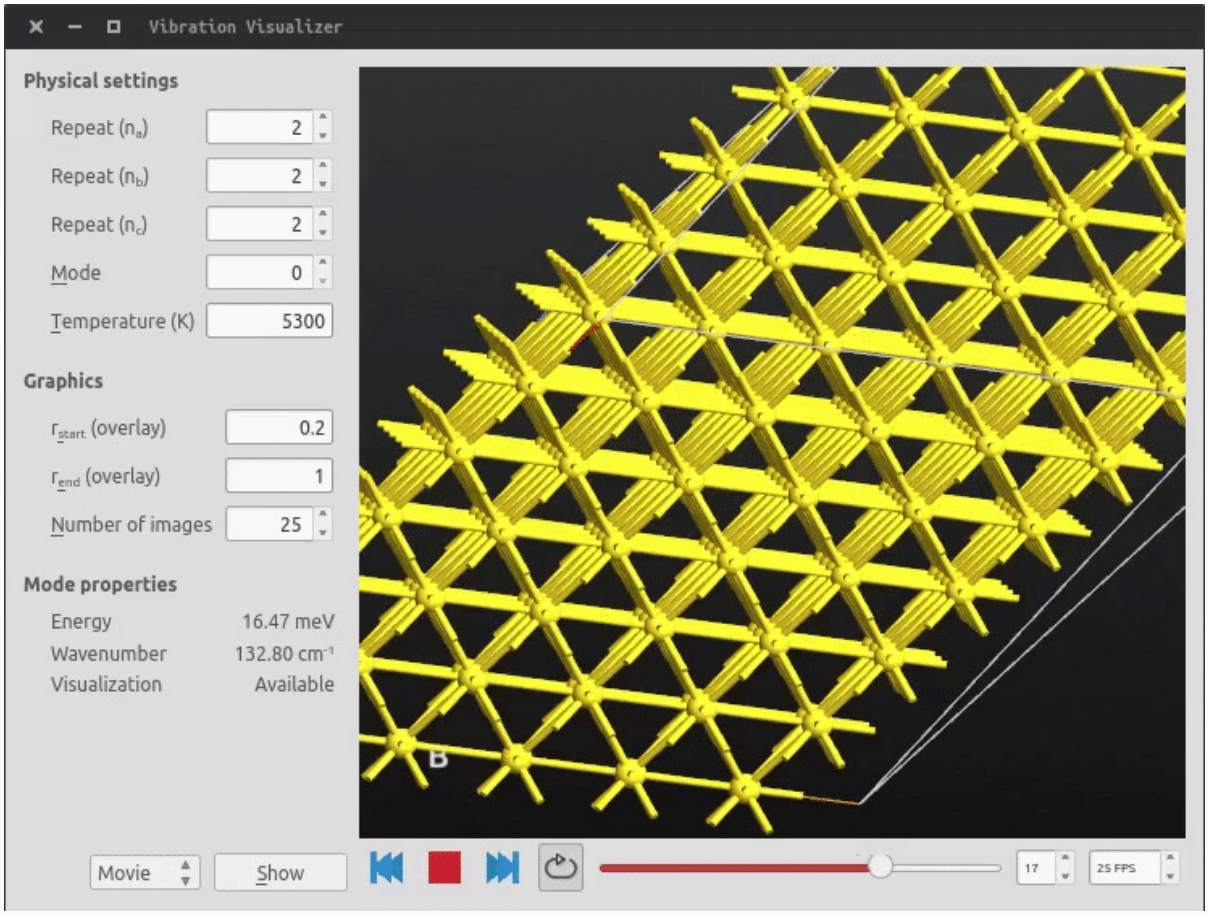
Tip

You can select any frame and use tha arrow on the bottom-right corner to export the corresponding configuration to the **Builder** or to the **Scripter** for further investigation.

Visualize vibrational modes

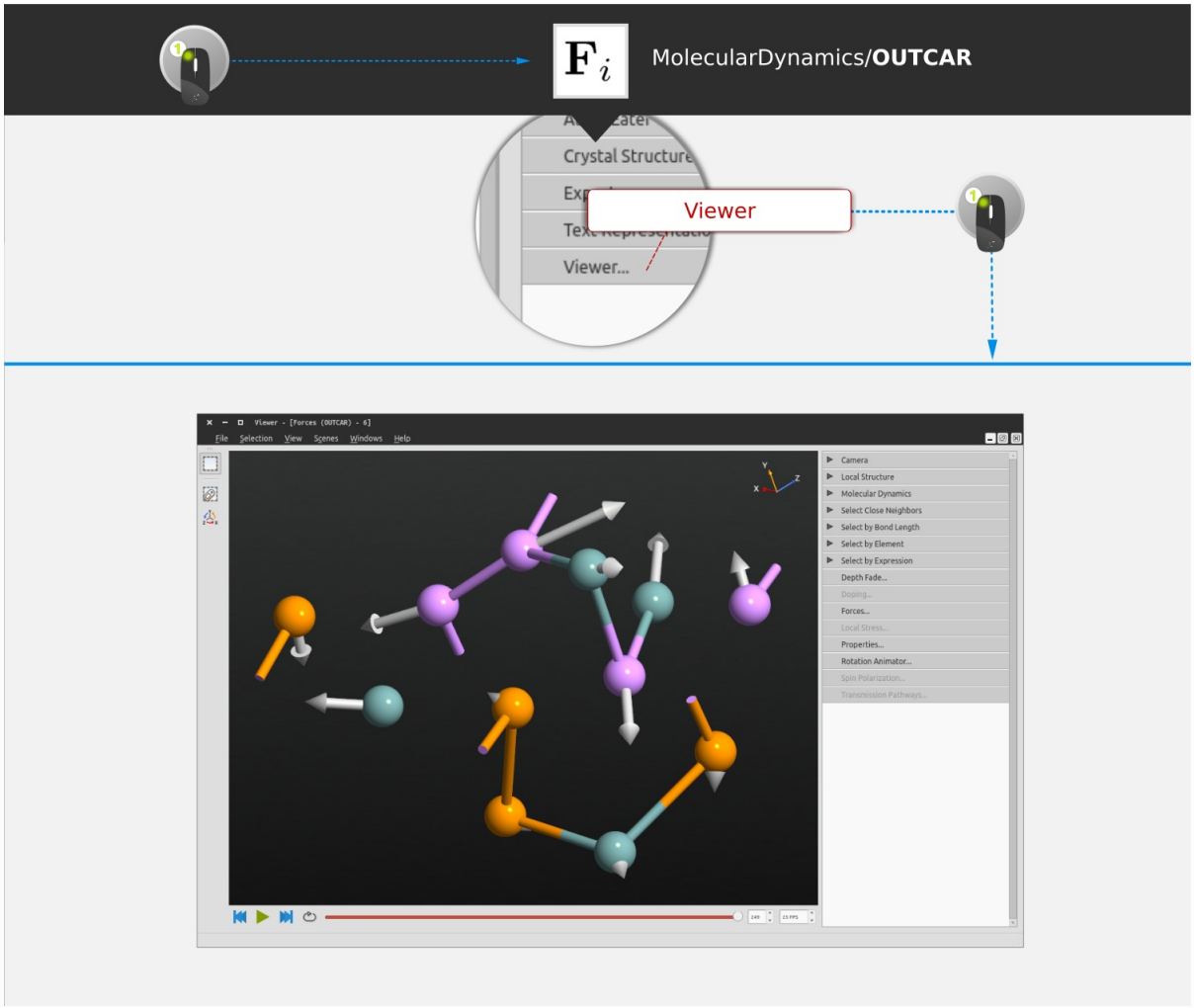
Select the VibrationalMode object present in your OUTCAR file and use the **Vibrational Visualizer** plugin to select a specific mode and visualize it in a new window. Here, you can select the mode, the number of repetitions for your structure, the visualization option, and other convenient parameters.





Visualize forces

If present in your OUTCAR file, forces can be visualized as arrows in the Viewer.



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