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Using QuantumATK to work with Nudged Elastic Band calculations in VASP

Using QuantumATK to work with Nudged Elastic Band calculations in VASP

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In this tutorial, you will learn how to set up a **Nudged Elastic Band (NEB)** calculation for **VASP** and how to analyze the output files by using **QuantumATK**, your graphical user interface for **VASP**!

ⓘ Attention

In particular, you will benefit from a new method for the creation of high quality initial reaction paths. This method is based on **image-dependent pair potentials (IDPP)** ^[1] and it is now implemented in **QuantumATK**. Using this can reduce the total computational time by a factor of 2 to 10, compared to the most commonly used technique of linear interpolation!

ⓘ Note

If you are not familiar with the **VASP Scripter**, first check out the more general [Set up and analyze VASP calculations with QuantumATK](#) for a full description of how to set up and analyze **VASP** calculations with **QuantumATK**.

Introduction

This tutorial closely follows the NEB tutorial for **QuantumATK/ATK** [How to calculate reaction barriers using the Nudged Elastic Band \(NEB\) method](#). and covers the following steps:

- optimize the bulk Pt from scratch using VASP;
- construct the end-points for the “*exchange diffusion*” process of a Pt adatom on Pt(100) using **QuantumATK** and optimize them with VASP;
- construct the initial guess for the NEB path for the same process;

- set up and run the NEB calculations with VASP;
- analyze the VASP output files with QuantumATK.

The tutorial covers the same topic discussed in the VASP tutorial “[Collective jumps of a Pt adatom on fcc-Pt \(001\): Nudged Elastic Band Calculation](#)”, although here the system geometry is slightly different. There you can find more informations about VASP keywords and other input files.

Note

This tutorial is not a guide to VASP, nor does Synopsys QuantumATK provide access to the VASP code. It is assumed that you have already obtained and installed VASP from its official source (www.vasp.at) and that you are familiar with the code.

Note

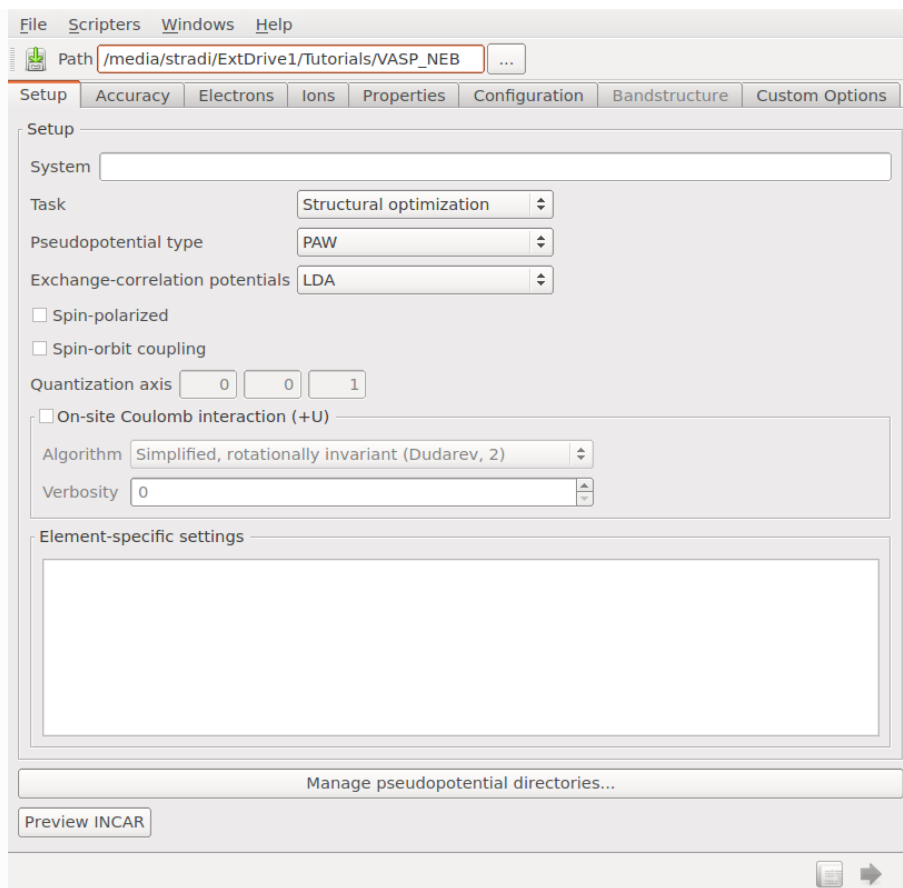
To use the advanced VASP functionalities in QuantumATK you need a specific “*ATKVASP*” license feature. If the POSCAR icons are greyed out on the LabFloor, it means you are missing this feature in your license file - in this case, contact us for options using this [link](#).

Creating the initial and final configurations

To create the initial and final configurations, you can follow similar steps as those described in the NEB tutorial for QuantumATK/ATK “[How to calculate reaction barriers using the Nudged Elastic Band \(NEB\) method](#)”. Thus, here we will be brief and just focus on the differences due to the use of VASP instead of ATK-classical as calculation engine.

Setting up the VASP input for optimizing the bulk Pt

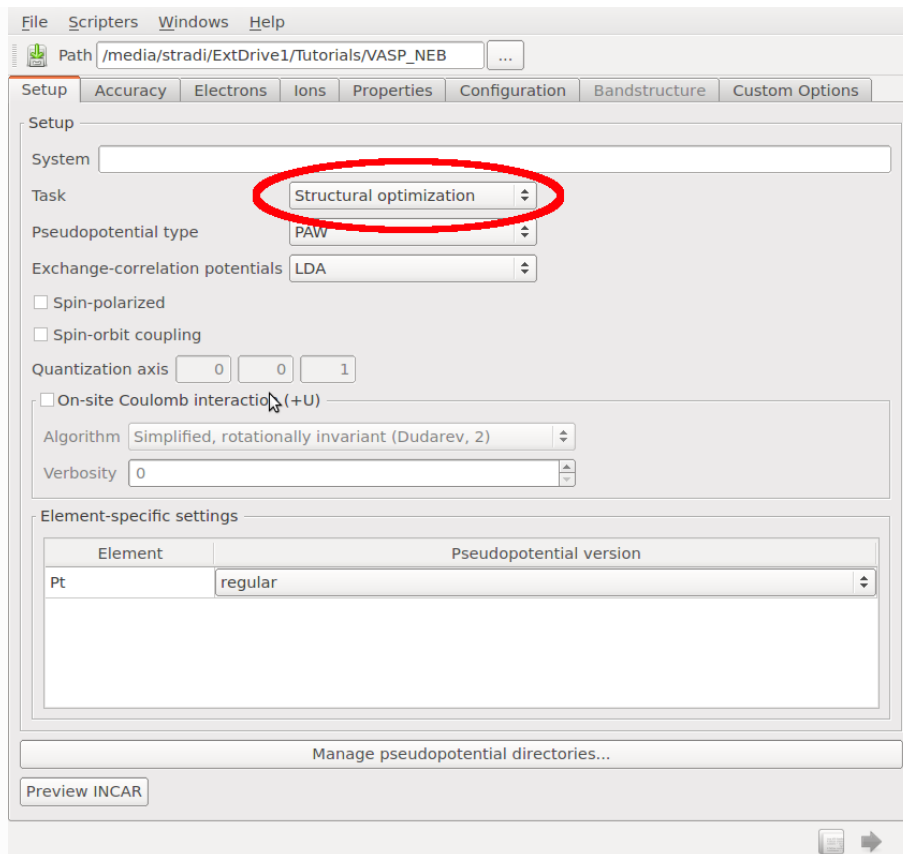
1. Once you have created the bulk structure of Pt as described in the tutorial [How to calculate reaction barriers using the Nudged Elastic Band \(NEB\) method](#), click on Tools ► Custom Scripter in the main QuantumATK window. The Custom scripter panel will open up. Select Scripters ► VASP scripter. The VASP scripter window will show up.



Drag and drop the initial configuration from the **Stash** directly into the **VASP Scripter**.

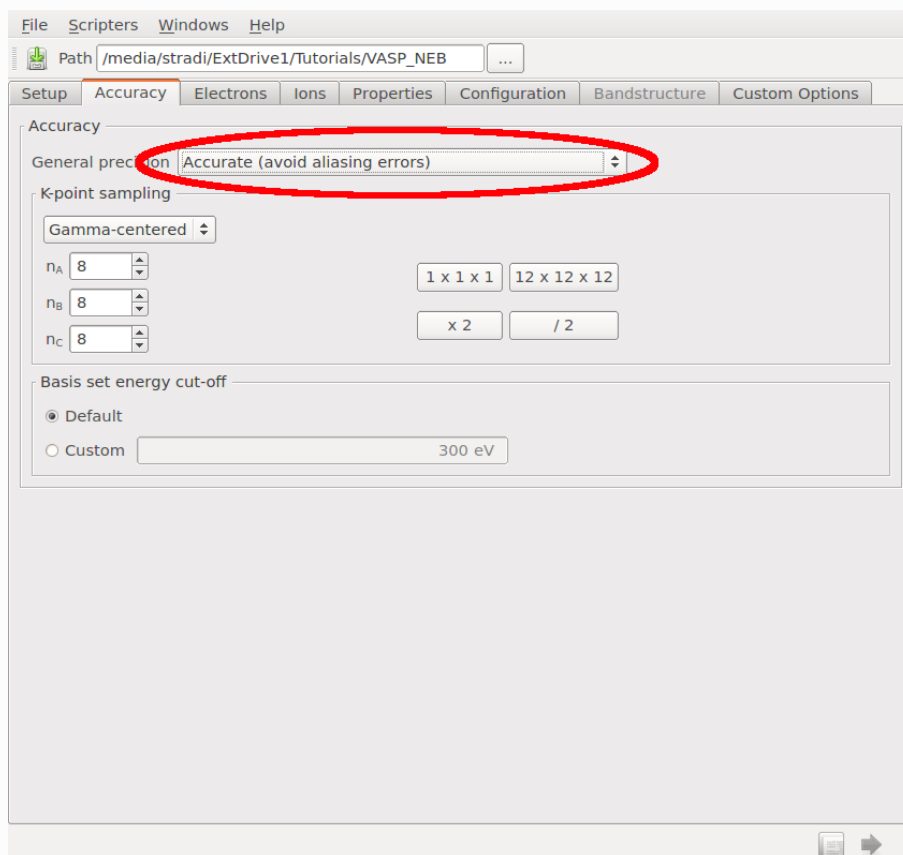
2. If it is not already selected, in the **Setup** tab select:

- Task: *Structural Optimization*



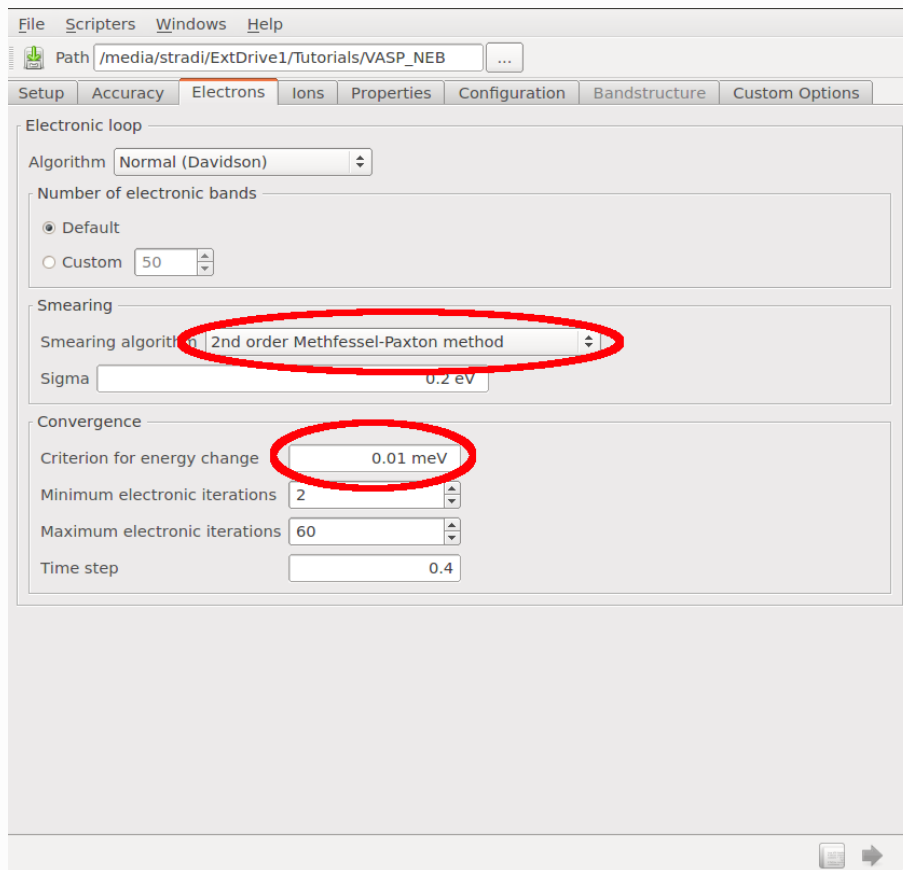
3. In the Accuracy tab select:

- General precision: *Accurate*

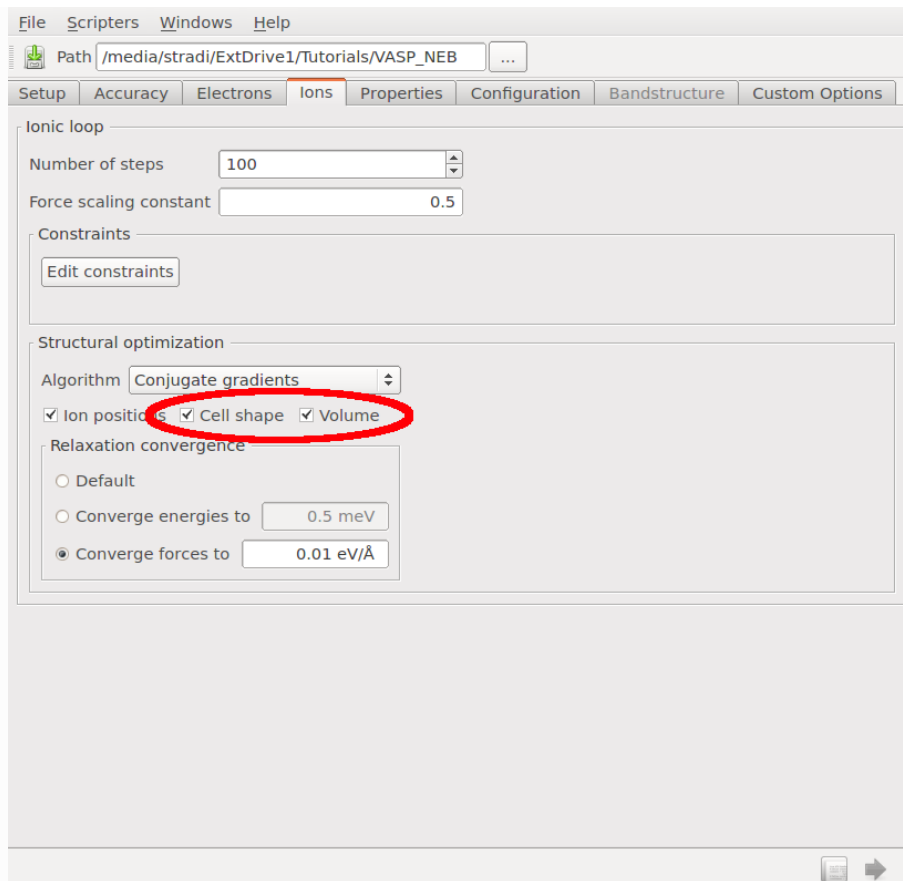


4. In the **Electrons** tab select:

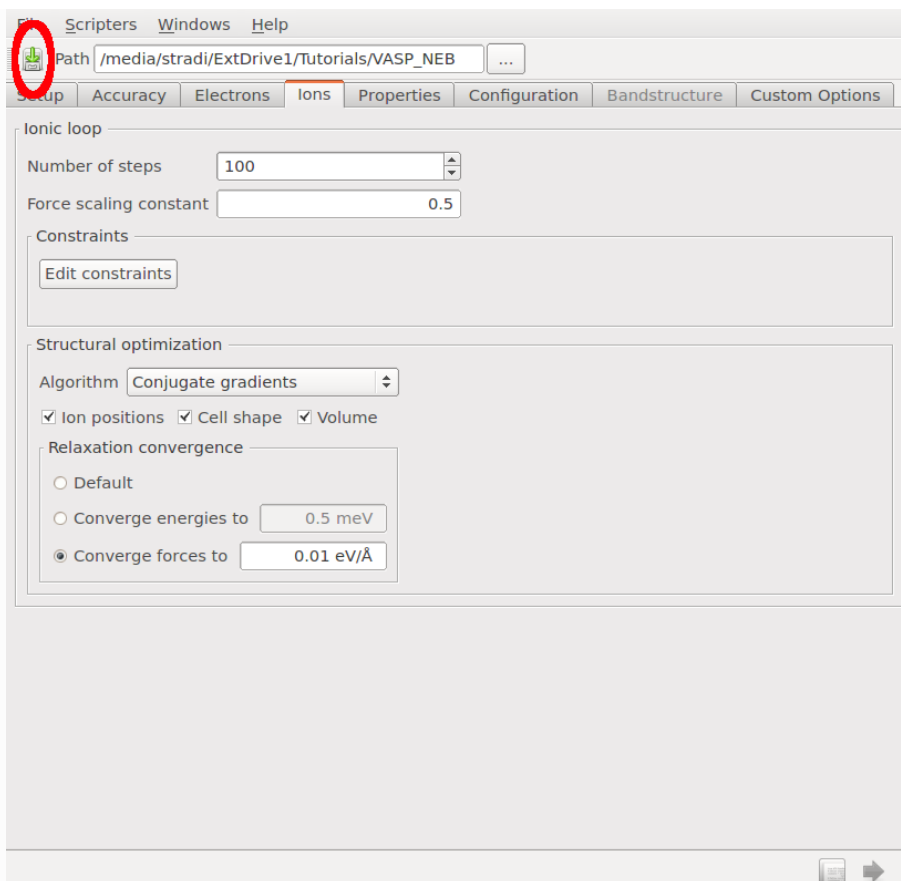
- Smearing algorithm: *2nd order Methfessel-Paxton method*
- Criterion for energy change: *0.01 meV*



5. In the **Ions** tab, tick on the *Cell shape* and *Volume* options to allow for the structural optimization of the cell.

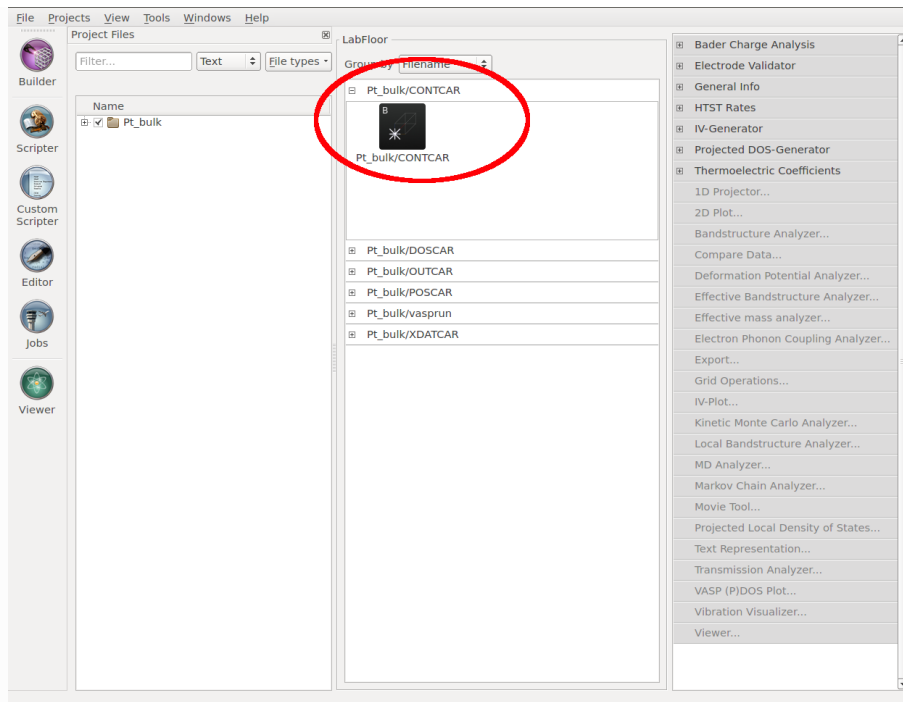


6. Once you are done, press the **Save** icon (see the image below) to save the four input files INCAR, POSCAR, KPOINTS and POTCAR in the selected directory. Then, run VASP and wait for the output files.

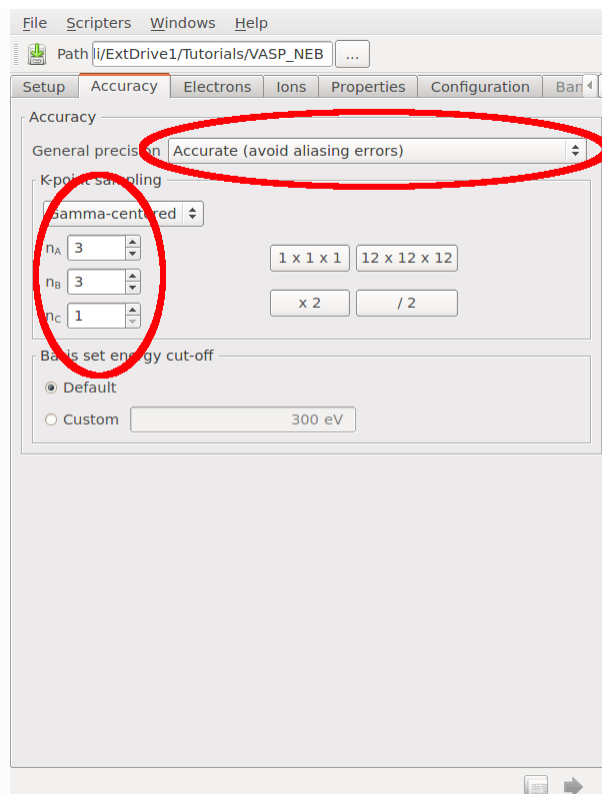


Creating and optimizing the end-points

1. Once the bulk optimization is finished, the VASP output files will appear in the **LabFloor** main window. Select the CONTCAR file containing the optimized configuration, and drag and drop it into the **Builder** to construct the geometries of the initial and final end-points starting from bulk Pt as discussed in the tutorial [How to calculate reaction barriers using the Nudged Elastic Band \(NEB\) method](#).



2. Once you have constructed the two configurations, open again the **VASP Scripter** and drag and drop the initial configuration into the scripter.
3. In the **Setup** tab select:
 - Task: *Structural Optimization*
4. In the **Accuracy** tab select:
 - General precision: *Accurate*
 - K-point mesh: 3x3x1

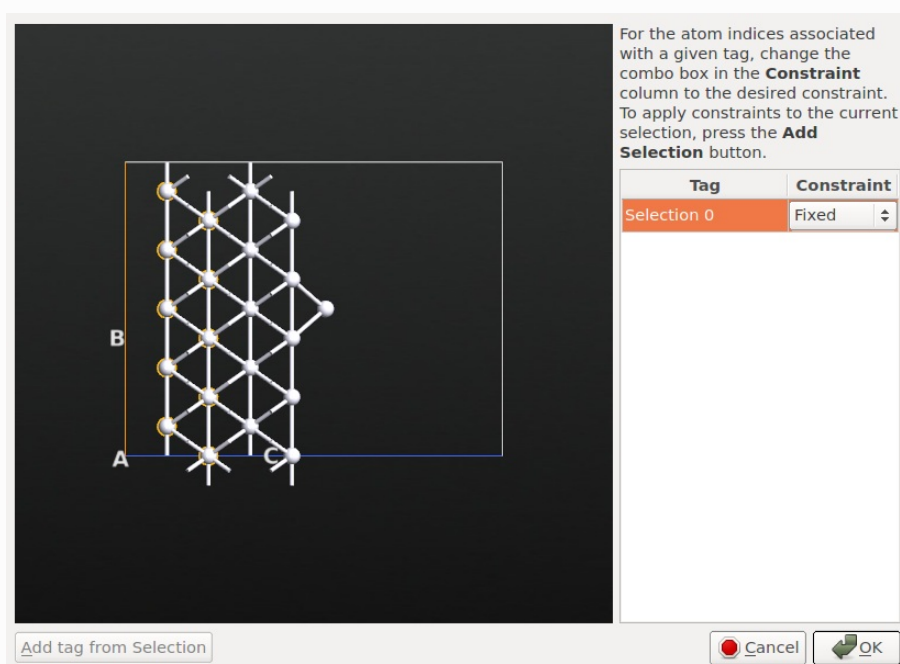


5. In the **Electrons** tab select:

- Smearing algorithm: *2nd order Methfessel-Paxton method*

6. In the **Ions** tag, select **Edit Constrains** and constrain the coordinates of the Pt(100) bottommost two layers as follows (see also the figure below):

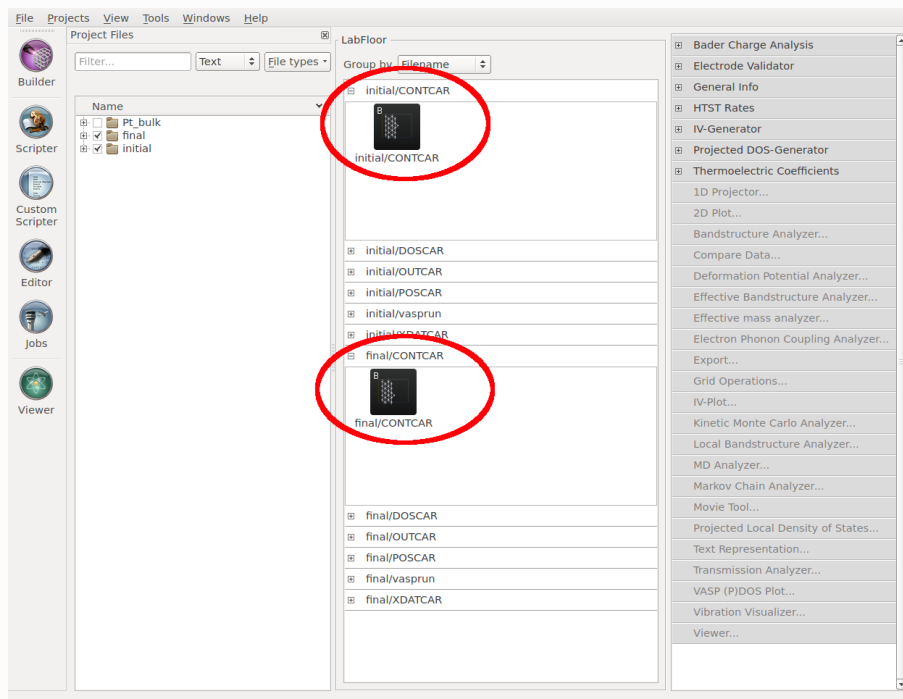
- Select the bottommost two layers;
- Click **Add tag from selection**;
- Change the constrain of the tagged atoms to *"Fixed"*.



Once you are done, save the files and run VASP. Then, repeat the same steps for the final end-point.

Constructing the NEB path

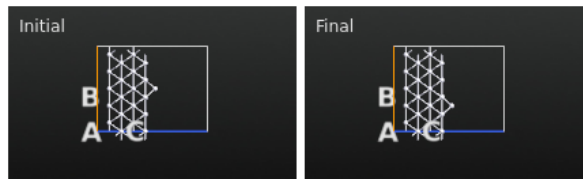
1. Drag and drop the optimized configurations of the initial and final end-point contained in the respective CONTCAR files into the **Builder**.



2. In the **Builder**, use the **Nudged Elastic Band** plugin to setup the initial guess for the NEB path using the IDPP method ^[1]. Set the maximum distance to have 7 images. For more details about the options available in the NEB plugin and how to modify your NEB object check the [How to calculate reaction barriers using the Nudged Elastic Band \(NEB\) method](#) tutorial.

Nudged Elastic Band

The NEB consists of the initial and final configurations plus a number of intermediate configurations. To generate a NEB, drop two configurations to the drop zones **Initial** and **Final** - then press **Create**.




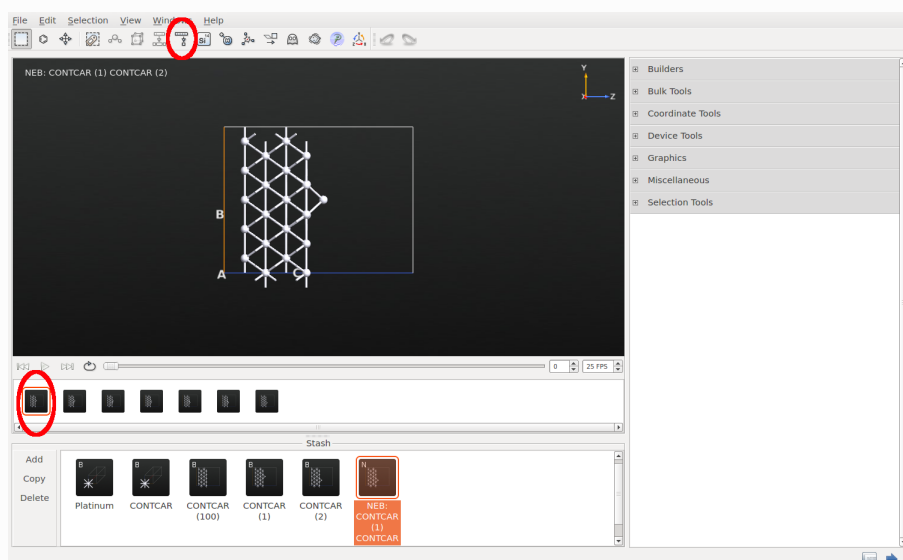
The intermediate configurations are interpolations between the initial and final configuration. The initial, final, and intermediate configurations are called *images*. Below you can choose the **Method** used to generate the NEB, as well as the **Maximum distance** between the images.

Constraints	
Method	Image Dependent Pair Potential
Maximum distance	0.60 Å
Distance	3.4 Å
Number of Images	7
Create	

Note

In order to be consistent with the constrain settings, remember to constrain the two bottommost layers also during the generation of the NEB path guess! You can do it by clicking on the **Constrain** button (see the image above) in the **Nudged Elastic Band** plugin.

- Once the initial guess for the NEB path has been created, select the newly created NEB configuration in the **Stash**. The sequence of images will show up in the **Builder** main window. Select the first image and click on the  icon on the top bar of the **Builder** to extract the selected image from the sequence. Repeat the procedure also for the last image of the sequence.



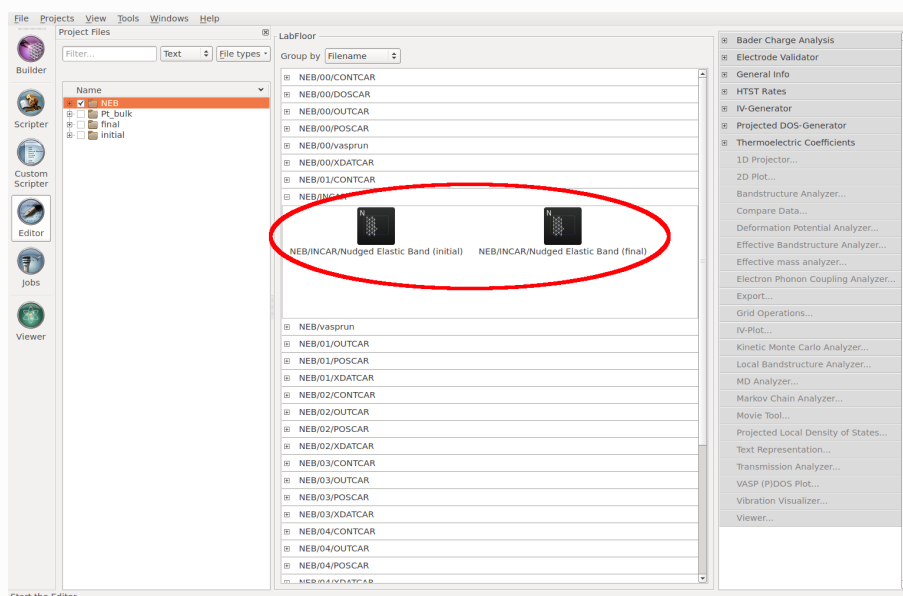
Setting up the NEB calculation

- Drag and drop the NEB configuration object from the **Stash** to the **VASP Scripter**.

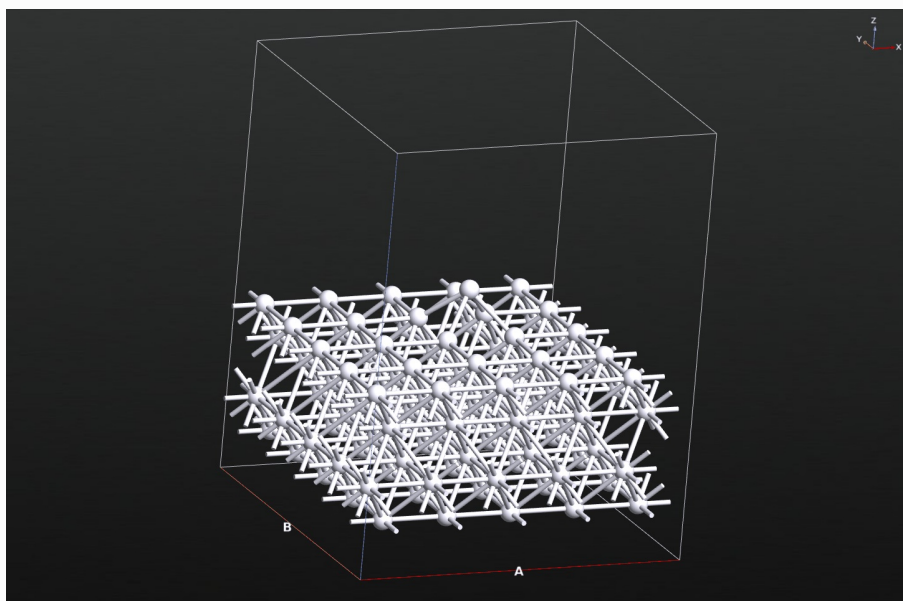
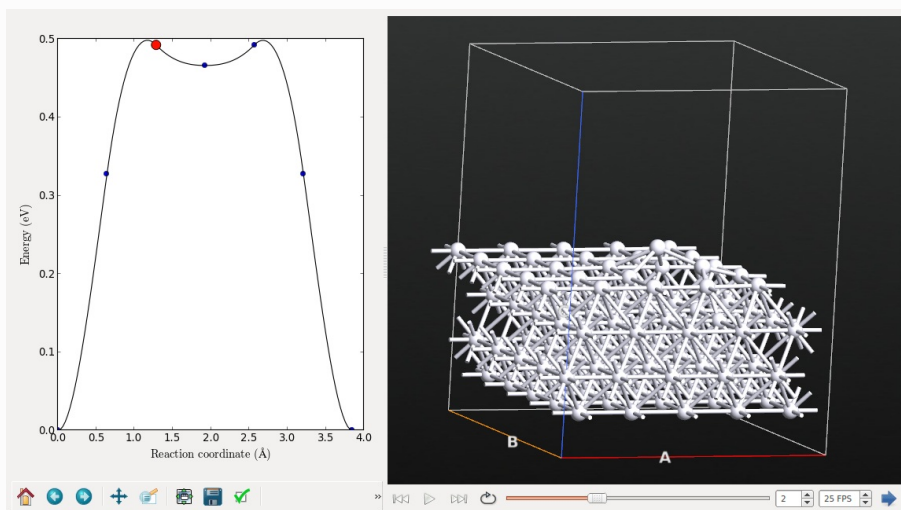
2. In the **Setup** tab, the only available task is NEB.
3. In the **Precision** tab, select:
 - General precision: *Accurate*
 - K-point mesh: 3x3x1
4. In the **Electrons** tab select:
 - Smearing algorithm: *2nd order Methfessel-Paxton method*
5. Create a new, empty directory inside the current project, and select this for the path where to save the VASP input files. Press **Save** to generate the INCAR, KPOINTS, POTCAR files and the 00, 01, 02, 03, 04, 05 and 06 directories, each one containing the POSCAR file of the corresponding image.
6. Leave the **VASP Scripter** window open and go back to the **Builder**. Drag and drop the configuration of the first image of the NEB path that you extracted previously from the **Stash** to the **VASP Scripter**.
7. In the **Setup** tab select:
 - Task: *Static run (SC)*
8. Save the INCAR, KPOINTS, POTCAR and POSCAR files in the 00 directory of the NEB path. The program will ask if you want to overwrite the existing input files. Press *Yes*.
9. Repeat steps 6-8 for the configuration of the last image of the NEB path that you extracted previously and save the files in the 06 directory.
10. Run the VASP calculation in the directory of the INCAR file.
11. Go to the 00 directory and run the VASP calculation in there. Then do the same in the 06 directory.

Analyzing the results


1. When all the VASP calculations are done, the output files in each of the image directories will appear on the LabFloor, and can be analyzed as usual with the various tools in **QuantumATK**.
2. In the **LabFloor**, select the INCAR file of the NEB calculation. Two configurations are now present, corresponding to the initial guess (*initial*) and the optimized path (*final*) of the NEB calculation.



3. To visualize the optimized NEB path, select the *final*/configuration and click on the **Movie Tool** in the **Panel plugins** on the right-hand side of the **LabFloor**. The following windows will show up showing the NEB path. The calculated barrier is in good agreement with the results published in the literature [\[2\]](#).



Tip

The window on the right side of the **Movie Tool** is interactive! It is possible to export the selected image for further analysis by left-clicking on it with the mouse and using the  icon in the menu that appears.

References

[1] (1,2)

S. Smidstrup, A. Pedersen, K. Stokbro, and H. Jónsson. Improved initial guess for minimum energy path calculations. *J. Chem. Phys.*, 140:214106, 2014. doi:10.1063/1.4878664.

[2]

P. J. Feibelman. Surface diffusion mechanism versus electric field: pt/pt(100). *Phys. Rev. B*, 64:125403, 2001. doi:10.1103/PhysRevB.64.125403.

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