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How to calculate reaction barriers using the Nudged Elastic Band (NEB) method

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In this tutorial you will learn how to calculate reaction barriers for a reaction with well-defined initial and final states. As an example, we will use the diffusion of a single platinum ad-atom on a Pt(100) surface, but the methodology can be used in any situation where you can define an initial and final state of the system, connected by movement of one or more atoms.

Specifically, in this tutorial you will:

- create the Pt(100) surface with a Pt ad-atom;
- create a high-quality initial NEB path and run the NEB calculation;
- analyze the results and compare with the literature.

In order to have more details about the parameters used to construct and optimize the NEB object, you can check the `NudgedElasticBand` and `OptimizeNudgedElasticBand` pages in the manual.

Note

The NEB method employed in this tutorial requires the *a priori* knowledge of the initial and final configurations of the reaction, which is often a non-trivial task. However, other powerful methods, such as the Adaptive Kinetic Monte Carlo (AKMC) tool, allow study of reaction barriers in a system from just a user-defined initial state, as shown in Adaptive Kinetic Monte Carlo Simulation of Pt on Pt(100).

Prerequisites

This tutorial is an introduction to the NEB functionality in QuantumATK and only requires basic familiarity with the QuantumATK interface. This can be achieved via the following basic tutorials and guides:

- How to use QuantumATK for fast and easy atomic scale modelling
- Introduction to the Workflow Builder
- Introduction
- Organize your data in the Nanolab data view
- Geometry optimization: CO/Pd(100)
- Job Manager for local execution of QuantumATK scripts

Create the initial and final states for the NEB

In this section you will set-up the structure of a Pt ad-atom on Pt(100), which will be used as the initial and final configurations in the NEB calculations. First, you will relax bulk platinum with the chosen calculator to ensure the Pt(100) slab does not have an inherent strain.

Relax bulk platinum

Open **QuantumATK** and create a new project (f.ex. *Pt_Pt100_NEB*). Relax bulk platinum with a **ForceFieldCalculator** using the *EAM_Pt_2004* parameter set and default optimization parameters. This simulation runs in a few seconds. If needed, you can download the workflow for this calculation here: Pt_bulk_workflow.hdf5.

Tip

Tutorial on geometry optimization: Geometry optimization: CO/Pd(100)

Create the initial state - a Pt(100) surface with a Pt ad-atom

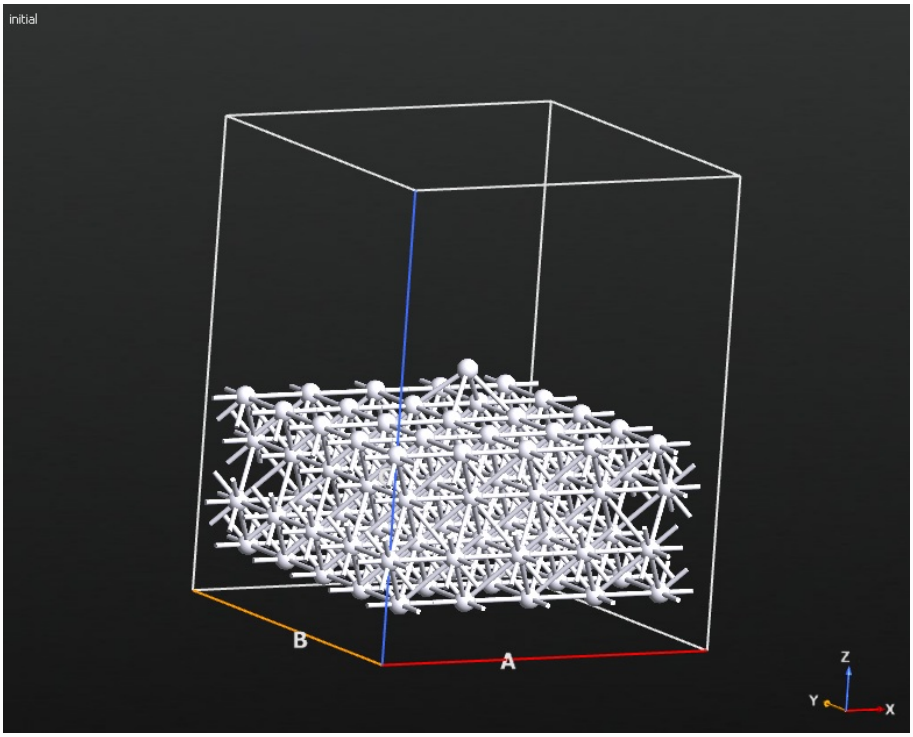
1. Use the relaxed platinum bulk configuration to construct a 5×5 (100) slab with a thickness of 4 layers, using the **Surface (cleave)** tool in the **Builder**.

   Tip

   A guide to the **Surface (cleave)** tool: Cleave tool guide

1. In the **Stash**, right-click with the mouse on the newly created *Pt_bulk (100)* object and select *Duplicate*. Then, right-click on the newly created *Pt_bulk (100) (1)* object and select *Rename* to change its name to *initial*.
2. Click on the icon to open the **Camera** panel, and orient the system along the XY direction.
3. While holding down the `CTRL` button on your keyboard, use the left mouse button to select a square of four Pt atoms of the Pt(100) topmost layer. Then add an extra atom in between them by clicking on the icon.
4. Select the new Pt atom, and click on Coordinate Tools ▸ Translate in the **Panel plugins** on the right-hand side of the screen. Define the translation vector as 1.6 in the z-direction to move the atom about 1.6 Å above the surface plane.

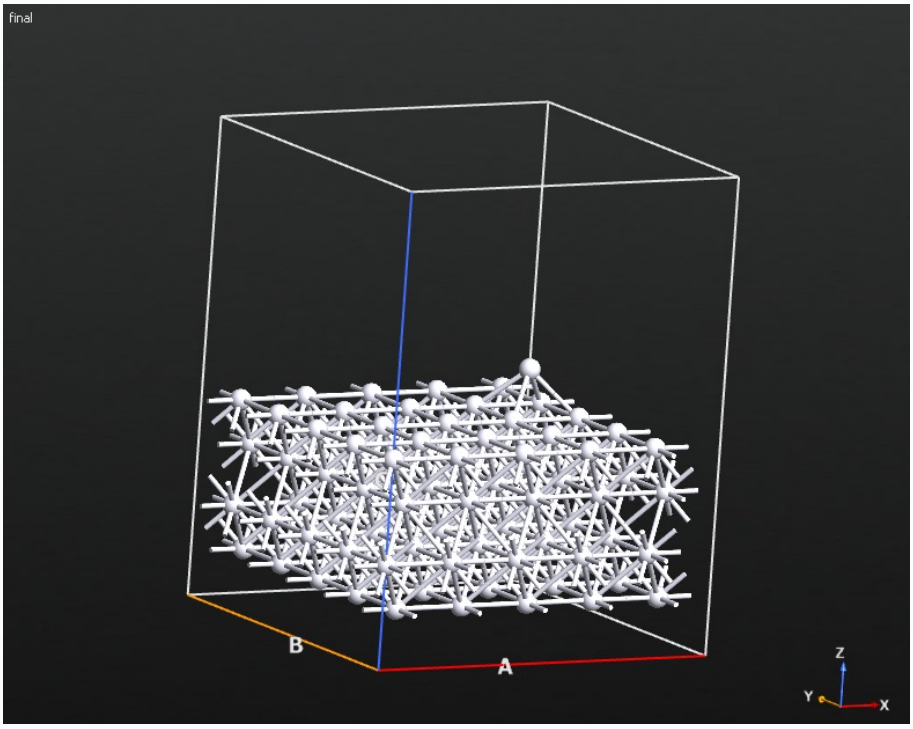
The structure you have just obtained for a Pt ad-atom on Pt(100) will be used as the initial configuration for the NEB calculations performed in this tutorial.



Create the final configuration for the direct jump process

In this section, you will set up the final configuration for the most direct diffusion process possible for a Pt ad-atom on Pt(100), in which the ad-atom jumps directly between neighboring four-fold hollow sites of the Pt(100) surface.

1. In the **Stash**, duplicate the *initial* configuration and change its name to *final_jump*
2. Select the *final_jump* configuration in the **Stash**, select the Pt ad-atom and click Coordinate Tools ▸ Translate.
3. In the **Translate Panel**, translate the Pt ad-atom 2.77195 Å in the x or y-direction.
4. In this way, you have obtained the final configuration for the NEB calculation of the direct jump diffusion process.



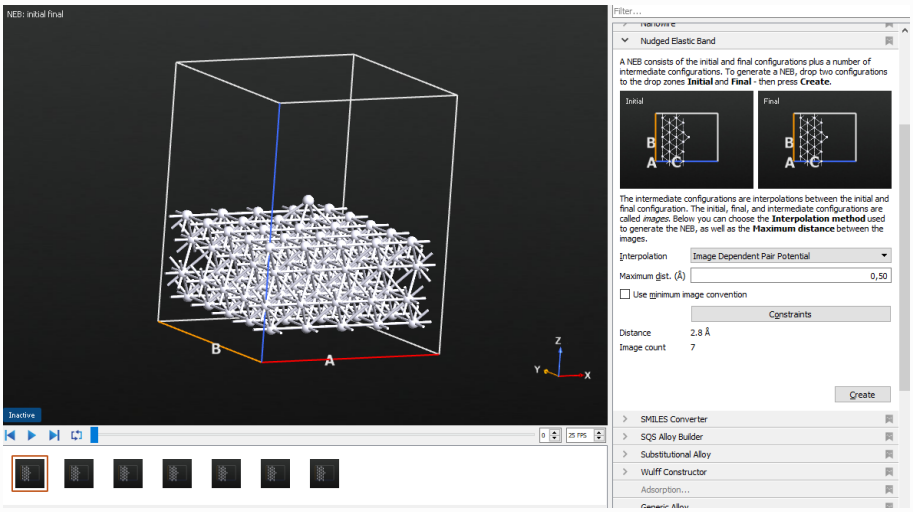
Relax the initial and final configurations

To ensure we get the best possible initial guess for the reaction path between the initial and final states, we need to relax them before constructing it. Use the same calculator as before to relax the two slabs with an ad-atom to a tolerance of *0.01 eV/Å*, and using *FIXED* atom constraints on the bottom two layers of the slab. You can use this workflow to do it: relax_initial_and_final_WF.hdf5

Set up and run the NEB calculations

Construct the NEB path

1. In the **Builder**, click on Builders ▸ Nudged Elastic Band and drag and drop the relaxed *initial* and *final* configurations into the left and right panels.
2. In the **Nudged Elastic Band** panel, set the **Interpolation** to *Image dependent Pair Potential*. Click *Create* to create an object in the **Stash** named *NEB: initial final*, containing the initial and final configurations as well as the interpolated configurations along the reaction path.



Note

The *image dependent pair potential (IDPP)* [1] implemented in **QuantumATK** provides high quality initial guesses for the NEB reaction path compared to the more commonly employed linear interpolation method. For complex reaction paths, the improvement in terms of number of required iterations and speed can be substantial.

Run the NEB calculations

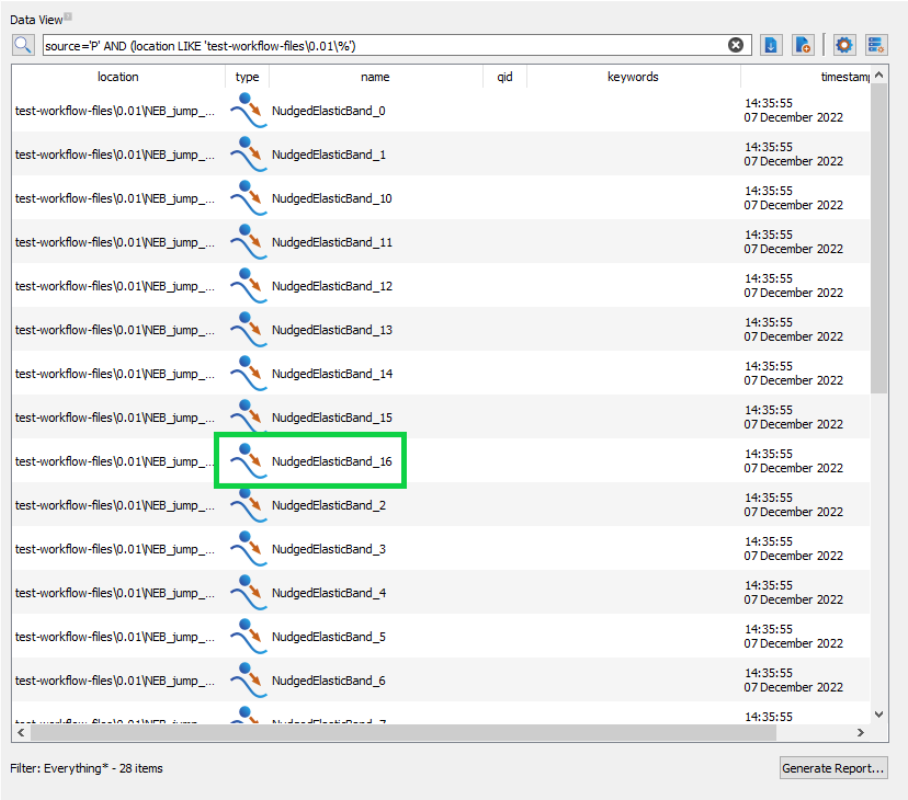
1. Click on the icon and send the *NEB: initial final* configuration to the **Workflow Builder**.
2. In the **Workflow Builder**, change the output **Filename** at the bottom of the middle panel to `NEB_Pt-jump.hdf5`.
3. Add the following blocks to the **Build** panel by double clicking on the corresponding icons in the **QuantumATK** tab in the right-hand panel:
   - Under **Calculators**: *Set ForceFieldCalculator*
   - Under **Optimization and Dynamics**: *OptimizeNudgedElasticBand*
4. Double-click on the *Set ForceFieldCalculator* block and select the *EAM_Pt_2004* parameter set again.
5. Double-click on the *OptimizeNudgedElasticBand* block, set the **Force tolerance** to *0.01 eV/Å* and set *FIXED* constraints on the bottom two layers.

6. Send the workflow to the **Job Manager** as a script and save the script as `NEB_Pt-jump.py`. This script runs in a few seconds, it can run locally.

You should now have a workflow identical to this one: NEB_jump_workflow.hdf5

Analyze the results

Once you have run the NEB calculations for the direct jump diffusion process, many new objects should appear in the **Data View** section of **QuantumATK NanoLab**. There is a `NudgedElasticBand` object for each step in the optimization. They are stored in the file you defined before, here called *NEB_Pt-jump.hdf5*.



1. Select the last NEB trajectory, i.e. the one with the highest number, which contains the optimized NEB path for the direct jump process. Then, double-click on it to open it in the **Movie Tool**.
2. On the left, the **Movie Tool** shows the energy of each image, referenced to the energy of the first image. On the right is the corresponding atomic configuration of each image. You can now see the energy barrier for this diffusion process as the highest point in the plot on the left, and see the corresponding transition state configuration on the right by moving the cursor so the vertical gray line is at the transition state.

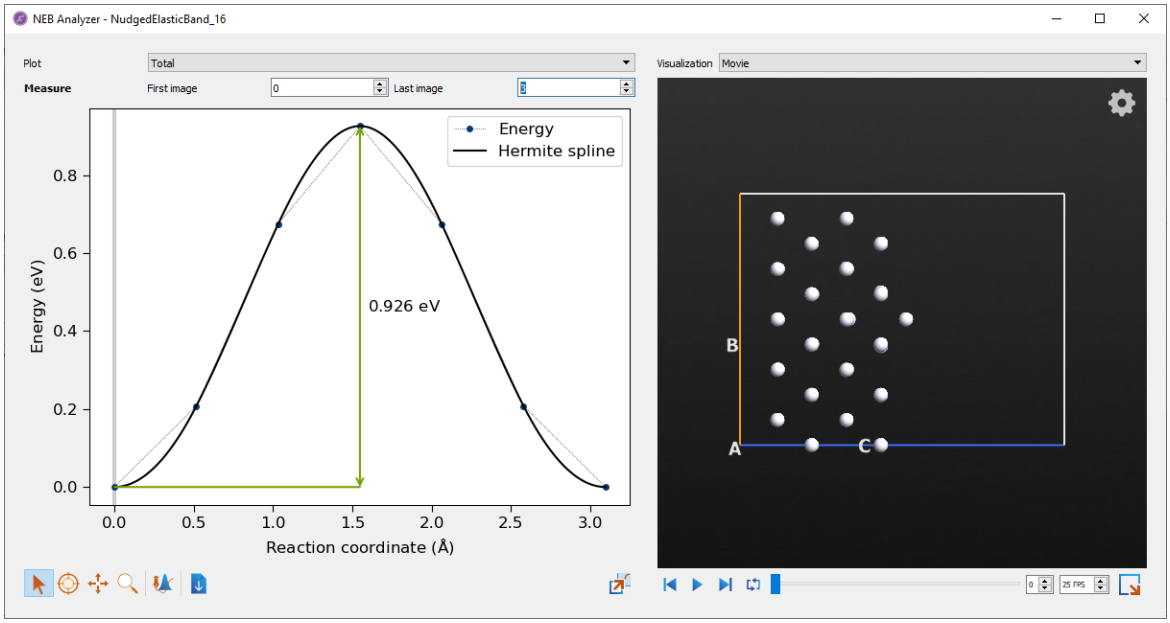


Fig. 11 Calculated reaction path for the direct jump diffusion process.¶

Note

As it can be seen in the tutorial at Adaptive Kinetic Monte Carlo Simulation of Pt on Pt(100), the AKMC method finds this path, among others, without any *a priori* knowledge of the potential energy surface of the system.

Summary

Throughout this tutorial, you have used a **ForceField** calculator and the **NanoLab** graphical user interface to set up, simulate and analyze the direct jump diffusion path for a Pt ad-atom on a Pt(100) surface. You can also repeat this tutorial with DFT by replacing the **Set ForceFieldCalculator** blocks with **Set LCAOCalculator** blocks, to compare directly with the DFT results reported in the literature [2].

References

[1]
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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