slab_creator

Release v1

Kazem Zhour

Mar 28, 2024

CONTENTS:

The Slab Creator script (slab_creator.py) facilitates the creation of slab structures with different orientations.

CHAPTER

ONE

USAGE

To use the script, follow these steps:

1. Launch the script by running the slab_creator.py file.
2. Provide the path to the CONTCAR file containing the bulk structure.
3. Enter the Miller indices for the desired slab orientation.
4. Specify the minimum slab size and minimum vacuum size in Angstroms.
5. Choose whether to apply LLL reduction (orthogonalize) to the slab.
6. Choose whether to force the slab to be perpendicular to the c-axis.

The generated slab will be saved in VASP format with the specified Miller indices in the filename (e.g., POSCAR100.vasp). Additionally, the script will visualize the slab structure using the ASE package in the gui version of the code.

CHAPTER

TWO

EXAMPLES

Here's an example of how to run the script:

python slab_creator.py

Follow the on-screen instructions to provide the required inputs and generate the slab structure.

Or you can run the GUI version of the code in the gui directory:

python slab_creator+gui.py

then fill the required variables.

CHAPTER

THREE

DEPENDENCIES

The Slab Creator (slab_creator.py) script requires the following dependencies:

- pymatgen: A Python library for materials analysis.

pip install pymatgen

- ase: Another Python library for materials analysis (required only for the GUI version of the script).

pip install ase

- tkinter: The standard Python interface to the Tk GUI toolkit (required only for the GUI version of the script).

CHAPTER

FOUR

INDICES AND TABLES

- genindex
- modindex
- search