SlabGen: An Integrated Platform for Systematic Surface Generation, Visualization, and DFT Workflow Preparation

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Why Surfaces?

Almost every interaction between a material and its environment happens at the surface.

- **Catalysis** — reaction rates depend on which crystal face is exposed
- **Corrosion** — certain surfaces degrade faster than others
- **Thin films and coatings** — growth behavior depends on surface termination
- **Crystal growth** — equilibrium shape is dictated by surface energies

Understanding surfaces computationally starts with a deceptively simple task: cutting a slab from a bulk crystal along a chosen crystallographic plane.

The Problem

In practice, generating surface slabs is tedious and error-prone.

The typical workflow today looks like this:

1. Write a Python script using pymatgen's `SlabGenerator`
2. Manually inspect the output for correctness
3. Repeat for every Miller index and termination you care about
4. Separately write VASP input files by hand

Common mistakes along the way:

- Wrong surface termination (different atomic layer exposed than intended)
- Polar surfaces that produce unphysical dipoles
- Atom stretching and distortion at high-index orientations like (2,1,0) or (3,1,1)
- No easy way to see what you've generated without loading it into VESTA or another tool

  There is no single tool that connects structure sourcing, slab generation, visualization, screening, and DFT preparation into one workflow.

SlabGen

SlabGen is an open-source desktop application that integrates the full surface science workflow in one place.

Input: Bulk crystal structure from the Materials Project database or a local file (VASP POSCAR, CIF)

What it does:

- Generates surface slabs for any Miller index (h,k,l)
- Interactive 3D visualization — rotate, zoom, inspect
- Screens all symmetrically distinct surfaces at once
- Prepares complete VASP DFT input file sets (POSCAR, INCAR, KPOINTS)

Built with: Python, PyQt5, pymatgen, matplotlib

Available at: github.com/shahabafshar/SlabGen (MIT license)

The Two-Step Algorithm

Direct slab generation at high Miller indices can produce distorted structures where atoms are stretched or compressed unnaturally. SlabGen avoids this with a two-step approach:

Step 1 — Orient and replicate

Take the bulk crystal and rotate it so the desired (h,k,l) plane aligns with the z-axis. Then replicate along z to build up slab thickness.

```
SlabGenerator(structure, miller_index=(h,k,l), min_vac=0)
→ oriented slab
→ make_supercell([1, 1, z_reps])
```

Step 2 — Add vacuum and terminations

Apply a second SlabGenerator pass with (0,0,1) — now a trivial cut — to add vacuum spacing and enumerate all possible surface terminations.

```
SlabGenerator(oriented_slab, miller_index=(0,0,1), min_vac=vacuum)
→ final slab(s) with vacuum and correct terminations
```

This separation keeps the geometry clean even for high-index surfaces.

Live Demo

Workflow to demonstrate:

1. Search "Mo2C" in the Materials Project panel — select a structure — bulk crystal appears in the 3D viewer
2. Set Miller index to (0,0,1), Z Reps = 3, Vacuum = 15 A — click **Generate Slabs** — slab appears, rotate it around
3. Click **Screen All Surfaces** — the screening dialog runs with a progress bar — results table fills in with all symmetrically distinct surfaces
4. Select an interesting surface from the table — click **Load in Main** — it appears in the 3D viewer
5. Click **Prepare DFT Inputs** — adjust ENCUT, ISMEAR, dipole correction — preview the INCAR — generate all files to a directory

Estimated time: 3 minutes

If the demo fails, switch to the pre-recorded video or static screenshots.

The Interface

Layout:

Section	What it does
Top panel	Search Materials Project by formula, or upload a local POSCAR/CIF file
Slab options	Set Miller indices (h,k,l), slab thickness (Z reps), vacuum, centering
Advanced	Toggle all terminations, surface comparison, screening
Middle	Generated slabs list (left) + interactive 3D viewer (right)
Bottom	Export slab as VASP/CIF, or generate full DFT input sets

The 3D viewer uses Jmol colors and element-scaled atom sizes. Atoms render in front of the unit cell wireframe for clarity.

Surface Screening

SlabGen can screen all symmetrically distinct surfaces for a material in a single pass.

How it works:

- Uses pymatgen's `get_symmetrically_distinct_miller_indices()` to find all unique orientations up to a maximum Miller index

- For each orientation, generates all possible terminations using the two-step algorithm
- Reports: Miller index, shift (termination), atom count, surface area, symmetry, composition
- Runs in a background thread — the GUI stays responsive

Output:

- Sortable results table (green = symmetric slab, yellow = asymmetric)
- One-click CSV export for further analysis
- Any surface can be loaded directly back into the main window

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DFT Input Generation

For any generated slab, SlabGen produces a complete set of VASP input files ready for HPC submission.

Generated files:

File	Contents
POSCAR	Slab structure
INCAR	Relaxation parameters (ISIF=2 for slabs, automatic dipole correction)
KPOINTS	Gamma-centered mesh with k_z = 1 along the vacuum direction
POTCAR.spec	Element list for pseudopotential selection
job.sh	SLURM submission script template

Key settings are configurable through the GUI:

ENCUT, ISMEAR/SIGMA, EDIFFG, ISIF (slab vs. bulk), dipole correction toggle. An INCAR preview updates live as you adjust parameters.

Case Study: Mo2C

Molybdenum carbide (Mo2C) is a material of interest for heterogeneous catalysis and hard coating applications. Its surface properties are not fully characterized.

We used SlabGen to systematically study Mo2C surfaces:

1. **Loaded** Mo2C from the Materials Project database
2. **Screened** all symmetrically distinct surfaces up to max Miller index 2
3. **Identified** all unique terminations, flagged symmetric vs. asymmetric slabs

4. **Generated** VASP input sets for selected surfaces
5. **Submitted** slab and bulk reference calculations to ISU HPC

Screening Results: Mo2C

Key observations:

- Number of unique Miller indices found: ___
- Total number of distinct terminations: ___
- Symmetric slabs: ___
- Asymmetric slabs (requiring dipole correction): ___

Some Miller indices produce multiple terminations with very different surface compositions — the (h,k,l) alone doesn't fully define a surface. The termination (shift value) matters.

Surface Energies

Surface energy tells us how much energy it costs to create a unit area of surface:

$$\gamma = \frac{E_{\text{slab}} - n \cdot E_{\text{bulk}}}{2A}$$

Surface	Atoms	Area (A^2)	Energy (J/m^2)
(0,0,1)	___	___	___
(1,0,0)	___	___	___
(1,1,0)	___	___	___
(1,1,1)	___	___	___

Lower surface energy = more thermodynamically stable surface = more likely to appear on the equilibrium crystal shape.

Wulff Construction

The Wulff construction predicts the equilibrium crystal shape from surface energies. Surfaces with lower energy occupy larger fractions of the crystal facets.

Area fractions:

Facet	Fraction
(0,0,1)	___
(1,0,0)	___
(1,1,0)	___
(1,1,1)	___

This shape represents the minimum-energy morphology of a Mo2C nanoparticle — a prediction that can be compared against TEM observations.

What SlabGen Enables

Before SlabGen: Write custom scripts for each material. Manually track Miller indices, terminations, file paths. Debug stretching artifacts. Generate DFT inputs separately. Takes hours to days per material.

With SlabGen: Load a structure, screen all surfaces in minutes, visualize them interactively, generate DFT-ready input sets with a few clicks. The entire pipeline from crystal structure to HPC submission fits in one session.

This matters because systematic surface studies — where you want to compare many surfaces of the same material — were previously impractical for most research groups due to the scripting overhead.

Future Directions

- **Surface energy database** — collect and compare surface energies across materials
- **Adsorption site identification** — find high-symmetry sites on generated surfaces for catalysis studies
- **Multi-code support** — extend DFT output beyond VASP to Quantum ESPRESSO, CP2K, and others
- **Convergence testing** — automated slab thickness and vacuum convergence workflows
- **Web interface** — make SlabGen accessible without local installation

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- Iowa State University
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SlabGen is open source and freely available:

github.com/shahabafshar/SlabGen

Questions?