SlabGen: Systematic Surface Generation, Screening, and DFT Preparation

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14th Annual GPSS Research Conference | February 20, 2026

The Problem

Surfaces govern much of how materials interact with their environment, including catalytic activity, corrosion, coatings, and film growth.

Studying surfaces from first principles means building slab models: periodic structures cut from a bulk crystal along a chosen plane, then relaxed with DFT. The idea is straightforward. **The practical workflow is not.**

- Each material and orientation demands its own script
- Unphysical polar terminations and missing surface cuts go unnoticed
- Geometric distortion at high-index planes
- Fragmented toolchain: Materials Project → pymatgen scripts → VESTA → manual VASP input prep

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SlabGen

An open-source GUI that handles the full surface workflow in one place.

Load a crystal from the Materials Project or a local file **Generate** slabs for any Miller index using a two-step orient-then-replicate strategy that avoids distortion **Visualize** in interactive 3D: rotate, zoom, compare terminations **Screen** all symmetrically distinct orientations at once. Catalogs every termination, flags symmetric vs. asymmetric **Prepare** ready-to-submit VASP file sets (INCAR, KPOINTS, POSCAR, job script) with automatic dipole corrections

Built with Python, PyQt5, and pymatgen. Open source, MIT license.

Case Study: Pt Validation + Mo_2C

Platinum (validation):

- Predicted surface energy ordering γ(111) < γ(100) < γ(110), consistent with experiment and prior computational work
- 9 orientations, 1 termination each, all symmetric, as expected for FCC

Mo_2C (where SlabGen's screening power matters):

- **19** orientations, **44** unique terminations: 34 symmetric, 10 asymmetric
- (1,1,1) alone has 6 distinct terminations. The Miller index doesn't fully define a surface
- All 44 terminations screened and VASP inputs generated in a single interactive session

Surface energy: $\gamma = (E_{slab} - n \cdot E_{bulk}) \ / \ 2A$

Takeaway

SlabGen turns days of scripting into minutes of guided interaction.

It makes systematic surface studies practical. Screen every surface of a material, visualize them, and go straight to DFT, all without writing a single line of code.

Open source: github.com/shahabafshar/SlabGen

Thank you.