



SlabGen

**An Interactive Platform for Automated Surface Slab
Generation, Screening, and DFT Workflow Preparation**

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Motivation

Why surface slab modeling matters

- Surface properties govern catalytic activity, corrosion resistance, and thin-film growth
- DFT slab calculations require careful construction: proper terminations, vacuum thickness, and dipole corrections
- Manual slab setup is tedious and error-prone -- systematic screening of multiple orientations is impractical by hand
- No existing tool integrates structure retrieval, slab generation, screening, and DFT input preparation in a single GUI

SlabGen automates the entire pipeline from bulk crystal to DFT-ready slab models.

Background

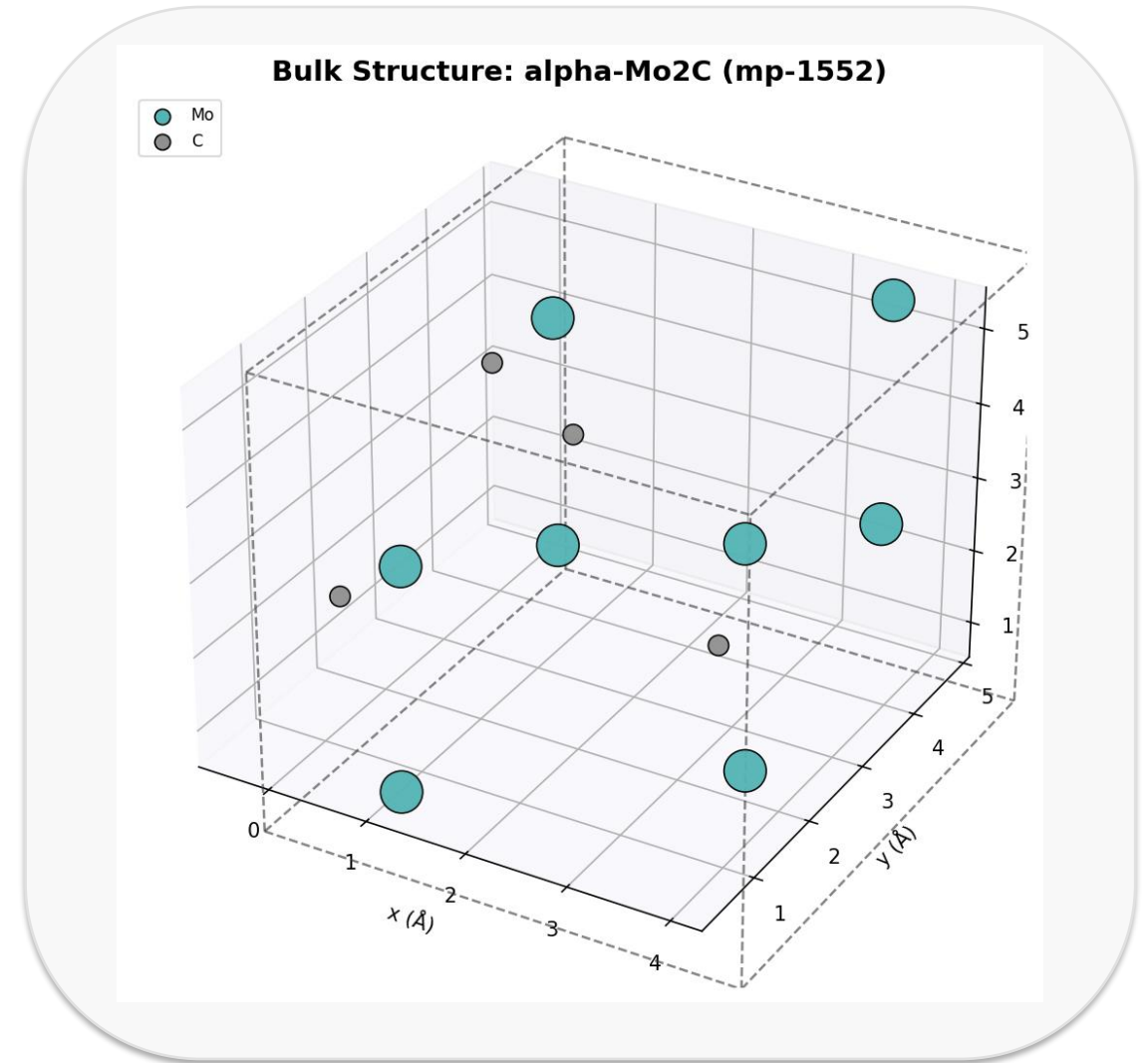
Key concepts in computational surface science

Surface Slab Model

- Miller indices (h,k,l) define the crystallographic plane for cutting
- Terminations: different atomic layers exposed at the surface (same orientation, different cuts)
- Vacuum layer separates periodic slab images in DFT
- Symmetric slabs avoid spurious dipole moments; asymmetric slabs need dipole correction

DFT for Surfaces

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



SlabGen Architecture

Technology Stack

- Python + pymatgen (materials analysis)
- PySide6 / Qt6 (cross-platform GUI)
- matplotlib (embedded 3D visualization)
- Materials Project API (structure database)

Modular Design

core/slab_generator.py

Slab generation + oriented replication

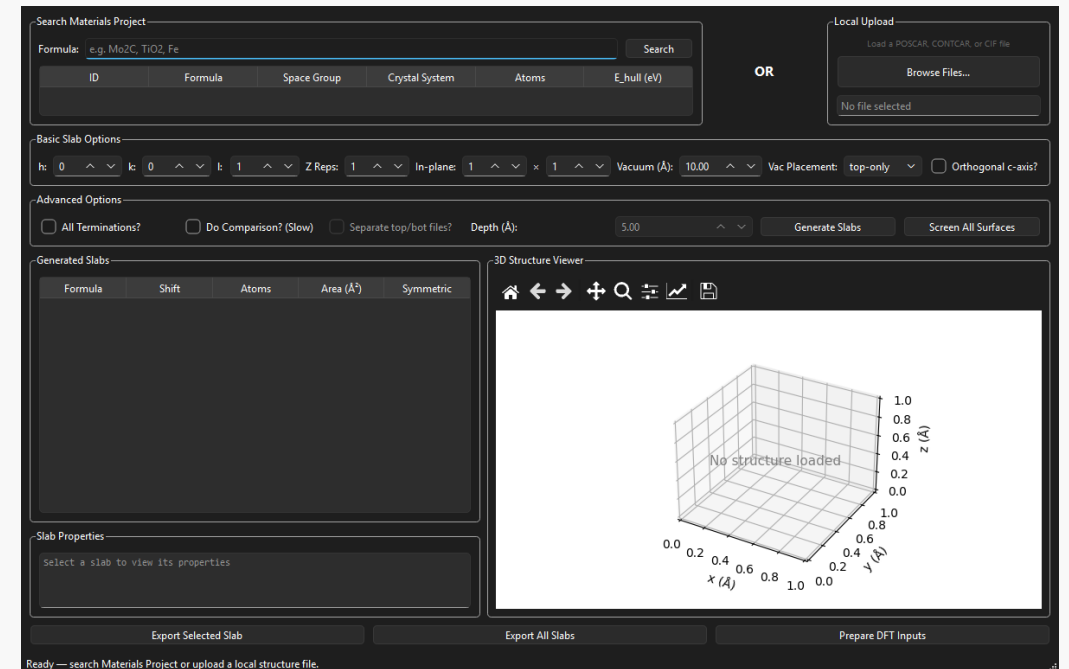
core/screening.py

Batch Miller index screening

core/dft_inputs.py

VASP input file generation

core/visualization.py



Key Algorithm: oriented_slab_replication

Two-stage approach avoids atom-stretching artifacts

Stage 1: Orient

Rotate bulk crystal so target (h,k,l) plane aligns with the z -axis, then replicate along z to desired thickness.



Stage 2: Generate

Apply SlabGenerator with $(0,0,1)$ on oriented structure to add vacuum and enumerate all unique terminations.

Why two stages?

- Direct SlabGenerator on arbitrary (h,k,l) can produce distorted atomic positions for complex unit cells
- Pre-orienting + z -replication ensures physical atom spacing is preserved before vacuum is applied
- Enables correct slab models for any crystal system (cubic, orthorhombic, hexagonal, ...)

Demo: Structure Retrieval from Materials Project

Search & Select

1. Enter chemical formula (Mo_2C)
2. Query Materials Project API
3. Browse results: ID, space group, crystal system, atoms
4. Select structure to load into 3D viewer

Selected: mp-1552

- Alpha- Mo_2C (Pbcn, orthorhombic)
- 12 atoms per unit cell
- Ground-state polymorph ($E_{\text{hull}} = 0$)

The screenshot displays the Materials Project web interface. At the top, the 'Search Materials Project' section shows the formula 'Mo2C' entered in the search bar. Below this, a table lists search results with columns for ID, Formula, Space Group, Crystal System, Atoms, and E_{hull} (eV). The first result is 'mp-1552' with the formula 'Mo2C', space group 'Pbcn', crystal system 'Orthorhombic', 12 atoms, and E_{hull} 'N/A'. To the right of the search bar is a 'Local Upload' section with a 'Browse Files...' button and a 'No file selected' message. Below the search results, the 'Basic Slab Options' section includes input fields for 'h' (0), 'k' (0), 'l' (1), 'Z Repts' (1), 'In-plane' (1 x 1), 'Vacuum (Å)' (10.00), 'Vac Placement' (top-only), and a checkbox for 'Orthogonal c-axis?'. The 'Advanced Options' section has checkboxes for 'All Terminations?' (unchecked), 'Do Comparison? (Slow)' (unchecked), and 'Separate top/bot files?' (unchecked), along with a 'Depth (Å)' input field set to 5.00. There are 'Generate Slabs' and 'Screen All Surfaces' buttons. Below these, the 'Generated Slabs' table is empty. The '3D Structure Viewer' section shows a 3D model of the crystal structure with Mo atoms represented by teal spheres and C atoms by grey spheres. The axes are labeled x (Å), y (Å), and z (Å). At the bottom, there are buttons for 'Export Selected Slab', 'Export All Slabs', and 'Prepare DFT Inputs'. The status bar at the very bottom reads 'Selected mp-1552 — Mo2C (12 atoms)'.

ID	Formula	Space Group	Crystal System	Atoms	E_{hull} (eV)
3 mp-1552	Mo2C	Pbcn	Orthorhombic	12	N/A

Basic Slab Options

h: 0 k: 0 l: 1 Z Repts: 1 In-plane: 1 x 1 Vacuum (Å): 10.00 Vac Placement: top-only ☐ Orthogonal c-axis?

Advanced Options

☐ All Terminations? ☐ Do Comparison? (Slow) ☐ Separate top/bot files? Depth (Å): 5.00 Generate Slabs Screen All Surfaces

Generated Slabs

Formula	Shift	Atoms	Area (Å²)	Symmetric
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3D Structure Viewer

Mo C

Selected mp-1552 — Mo2C (12 atoms)

Demo: Slab Generation -- Mo₂C (1,1,1)

Search Materials Project

Formula:

OR

Local Upload
Load a POSCAR, CONTCAR, or CIF file

No file selected

Basic Slab Options

h: k: l: Z Reps: In-plane: × Vacuum (Å): Vac Placement: ☐ Orthogonal c-axis?

Advanced Options

☒ All Terminations? ☐ Do Comparison? (Slow) ☐ Separate top/bot files? Depth (Å):

Generated Slabs

	Formula	Shift	Atoms	Area (Å ²)	Symmetric
1	Mo2C	0.0000	36	49.20	Yes
2	Mo2C	0.0427	36	49.20	No
3	Mo2C	0.0848	36	49.20	No
4	Mo2C	0.1116	36	49.20	No
5	Mo2C	0.1366	36	49.20	No
6	Mo2C	0.1667	36	49.20	Yes

Slab Properties

Formula: Mo2C
Num atoms: 36
Surface area: 49.20 Å²
Slab thickness: 16.59 Å

3D Structure Viewer

Export Selected Slab Export All Slabs Prepare DFT Inputs

Generated 6 slab(s) for (1,1,1).

Parameters

- Miller indices: (1, 1, 1)
- Z repetitions: 3
- Vacuum: 15 Å
- All terminations: enabled

Results

- 6 unique terminations
- 36 atoms per slab
- 49.20 Å² surface area
- 2 symmetric + 4 asymmetric

Demo: Slab Inspection & 3D Visualization

Search Materials Project

Formula:

OR

Local Upload
Load a POSCAR, CONTCAR, or CIF file

No file selected

ID	Formula	Space Group	Crystal System	Atoms	E_hull (eV)	
3	mp-1552	Mo2C	Pbcn	Orthorhombic	12	N/A

Basic Slab Options

h: k: l: Z Reps: In-plane: x Vacuum (Å): Vac Placement: ☐ Orthogonal c-axis?

Advanced Options

☒ All Terminations? ☐ Do Comparison? (Slow) ☐ Separate top/bot files? Depth (Å):

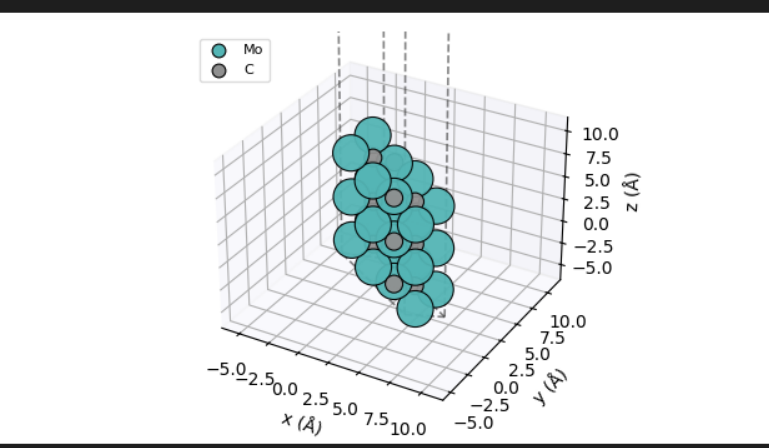
Generated Slabs

	Formula	Shift	Atoms	Area (Å ²)	Symmetric
1	Mo2C	0.0000	36	49.20	Yes
2	Mo2C	0.0427	36	49.20	No
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Slab Properties

Formula: Mo2C
Num atoms: 36
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3D Structure Viewer



Export Selected Slab Export All Slabs Prepare DFT Inputs

Generated 6 slab(s) for (1,1,1).

Slab Properties

Formula: Mo₂C

Atoms: 36

Surface area: 49.20 Å²

Slab thickness: 16.59 Å

Symmetric: Yes (shift 0.0)

3D Viewer Features

- Interactive rotation and zoom
- Jmol color scheme (element-based)
- Lattice box with axis labels
- Updates on slab selection

Demo: Systematic Surface Screening

Screening Parameters

Max Miller Index: ^ v Z Reps: ^ v Vacuum (Å): ^ v Placement: v ☐ Ortho c-axis?

Run Screening 100% Done. 20 terminations across 7 surfaces.

	Miller Index	Shift	Atoms	Surface Area (Å ²)	Symmetric	Formula
1	(1,1,1)	0	36	49.2	Yes	Mo ₂ C
2	(1,1,1)	0.0427	36	49.2	No	Mo ₂ C
3	(1,1,1)	0.0848	36	49.2	No	Mo ₂ C
4	(1,1,1)	0.1116	36	49.2	No	Mo ₂ C
5	(1,1,1)	0.1366	36	49.2	No	Mo ₂ C
6	(1,1,1)	0.1667	36	49.2	Yes	Mo ₂ C
7	(1,1,0)	0.0015	36	42.58	Yes	Mo ₂ C
8	(1,1,0)	0.0708	36	42.58	No	Mo ₂ C
9	(1,0,1)	0	36	40.01	Yes	Mo ₂ C
10	(1,0,1)	0.0835	36	40.01	No	Mo ₂ C
11	(1,0,1)	0.1667	36	40.01	Yes	Mo ₂ C
12	(1,0,0)	0.0424	36	31.53	No	Mo ₂ C
13	(0,1,1)	0	36	37.76	Yes	Mo ₂ C
14	(0,1,1)	0.0283	36	37.76	No	Mo ₂ C

Export to CSV Export All as POSCAR Load Selected in Main Window Close

Batch Screening

- All symmetrically distinct Miller indices up to max index
- Runs in background thread (GUI stays responsive)
- Progress bar with live updates

Mo₂C Results (max index 1)

- 7 surface orientations
- 20 unique terminations
- Color-coded: green = symmetric, yellow = asymmetric

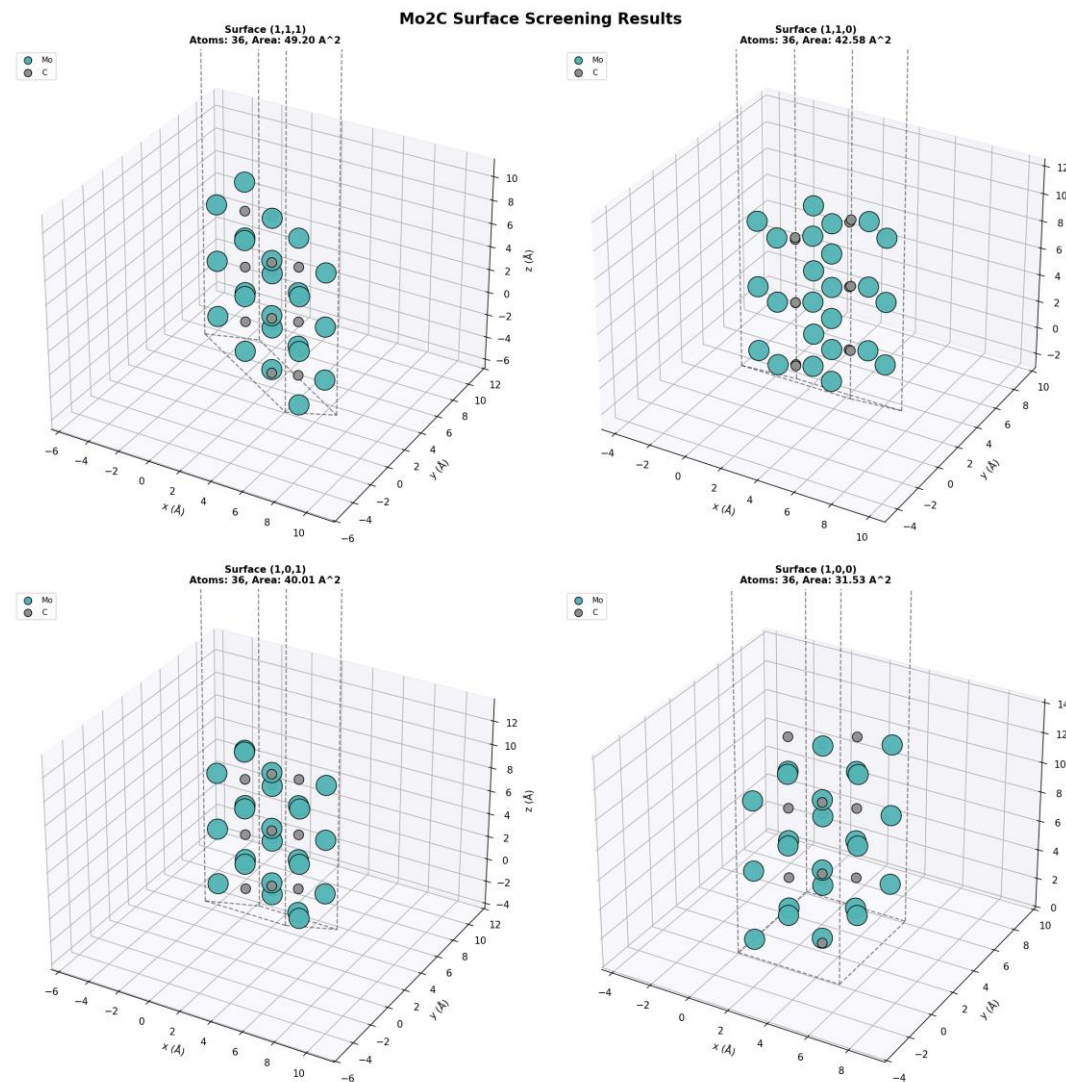
Export Options

Screening Results: Mo₂C Surface Characterization

Surface	Terminations	Area (Å ²)	Symmetric	Asymmetric
(0,0,1)	2	24.63	2	0
(0,1,0)	2	28.62	1	1
(1,0,0)	1	31.53	0	1
(0,1,1)	4	37.76	2	2
(1,0,1)	3	40.01	2	1
(1,1,0)	2	42.58	1	1
(1,1,1)	6	49.20	2	4
Total	20	--	10	10

Structure: alpha-Mo₂C (mp-1552, Pbcn, orthorhombic, 12 atoms) | Max Miller index: 1 | Z reps: 3 | Vacuum: 15 Å

Mo₂C Surface Gallery



Demo: DFT Input Generation

VASP Calculation Settings

ENCUT (eV): 400 ^ v K-point density: 50 ^ v ISIF: 2 — Relax ions only (slab) v

ISMEAR: 0 — Gaussian v SIGMA: 0.05 ^ v EDIFFG: -0.020 ^ v ☒ Auto dipole correction

☐ Selective dynamics (freeze bottom layers) Fix layers below z-fac: 0.30 ^ v

Note: Only POTCAR.spec (element list) is generated. Set PMG_VASP_PSP_DIR to enable full POTCAR generation.

INCAR Preview KPOINTS Preview

```
ALGO = Fast
DIPOL = 0.5 0.5 0.1667
EDIFF = 1e-05
EDIFFG = -0.02
ENCUT = 400.0
IBRION = 2
IDIPOL = 3
ISIF = 2
ISMEAR = 0
ISYM = 0
LCHARG = False
LDIPOL = True
LREAL = Auto
LVTOT = True
LWAVE = False
NELMIN = 6
NSW = 200
PREC = Accurate
SIGMA = 0.05
```

Generate DFT Inputs Cancel

Generated VASP Inputs

- INCAR with slab-optimized settings (ISIF=2, ISMEAR=0)
- Auto dipole correction (LDIPOL, IDIPOL=3, DIPOL from COM)
- KPOINTS with $k_z = 1$ for slab geometry
- POSCAR + POTCAR.spec
- SLURM job submission script

Advanced Options

- Selective dynamics: freeze bottom N layers
- Adjustable ENCUT, k-density, EDIFFG
- Live INCAR and KPOINTS preview tabs

Conclusions & Future Work

Conclusions

- SlabGen provides an integrated workflow from bulk crystal to DFT-ready slab models
- Systematic screening enables rapid surface exploration with symmetry classification
- Mo₂C case study: 20 terminations across 7 surfaces characterized in seconds
- Open-source, cross-platform (Python + PySide6)

Future Directions

- DFT surface energy calculations and Wulff construction
- Automated convergence testing workflows
- Adsorbate placement on generated surfaces
- Support for heterostructure interface modeling

References

[1] Ong et al. *Comp. Mater. Sci.* 68, 314 (2013)

Thank you! | Questions?