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

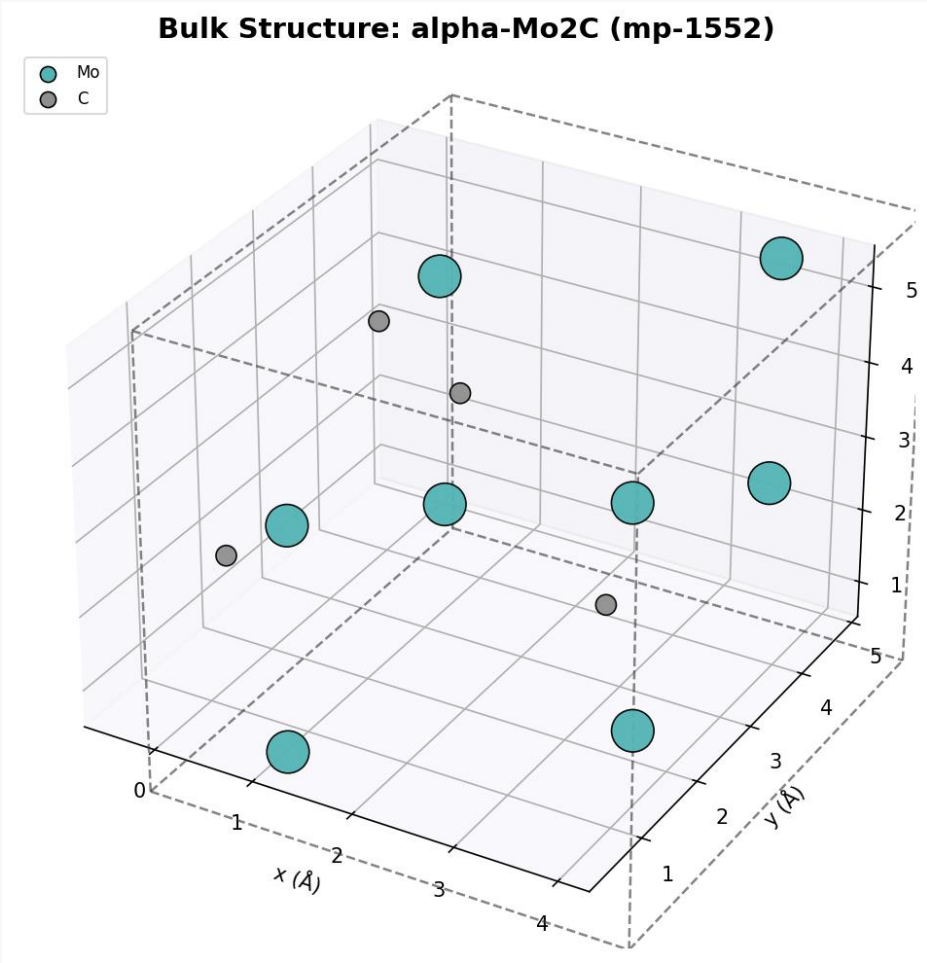
SlabGen automates the entire pipeline from bulk crystal to DFT-ready slab models.

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



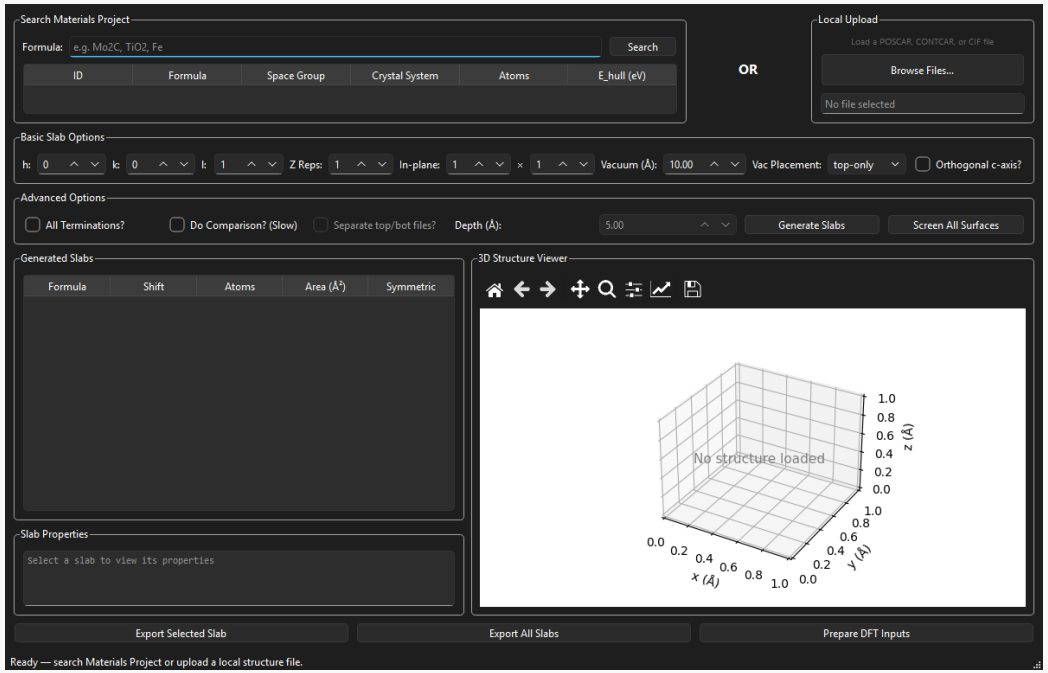
DFT for Surfaces

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

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, ...)

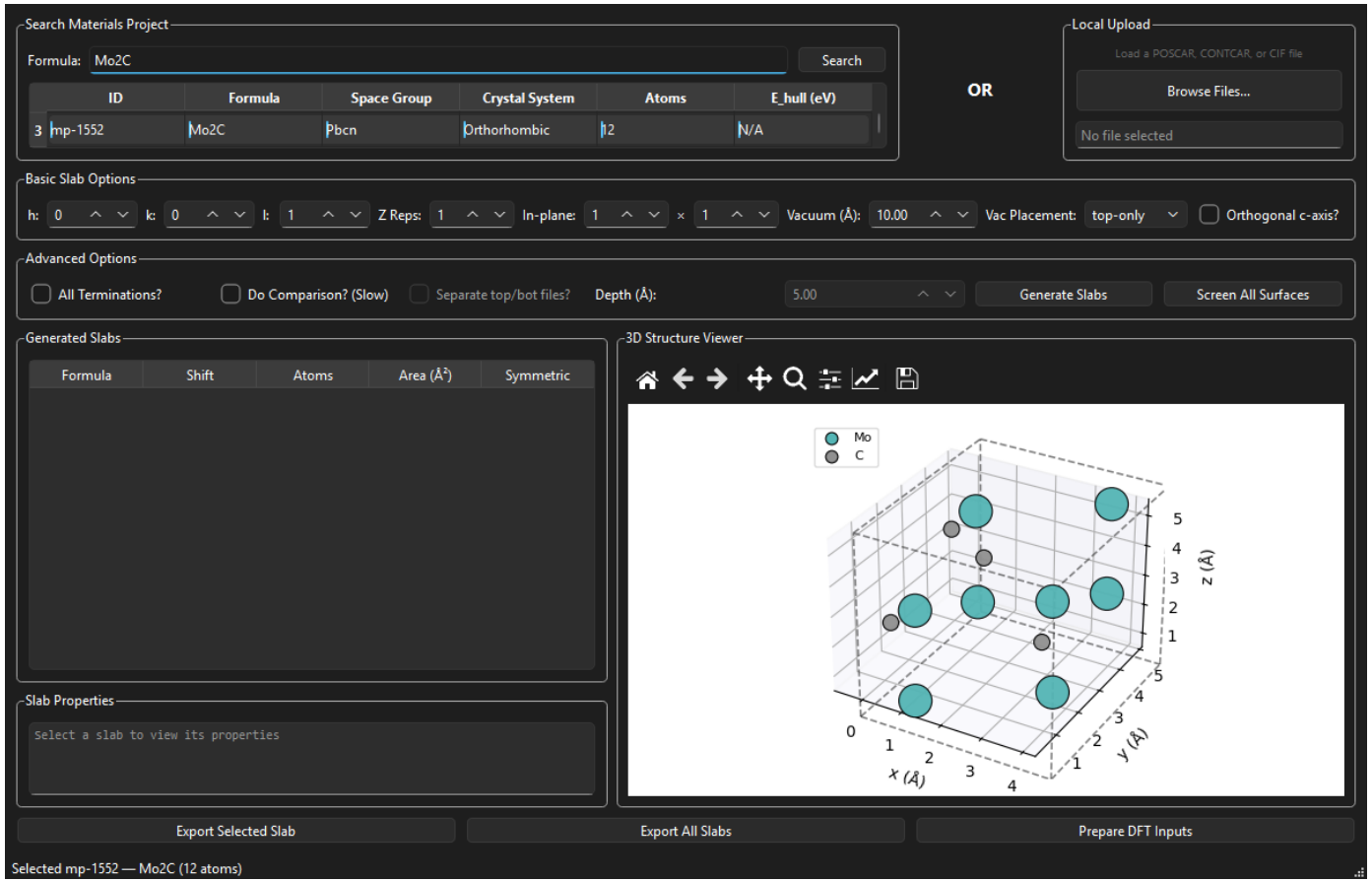
Demo: Structure Retrieval from Materials Project

Search & Select

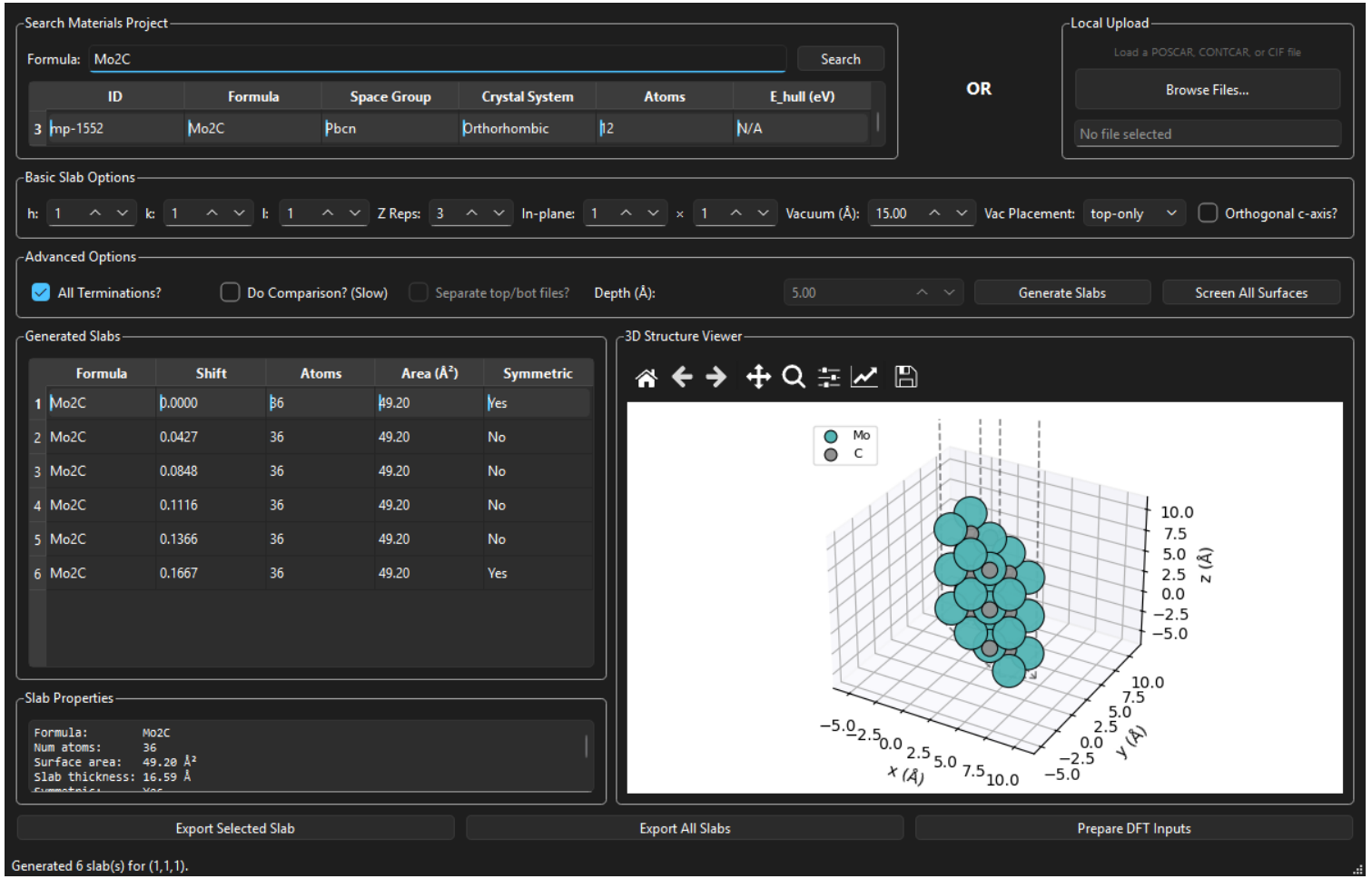
1. Enter chemical formula (Mo_2C)
2. Query Materials Project API
3. Browse results: ID, space group, crystal system, atoms
4. Select structure to load into 3D viewer

Selected: mp-1552

- Alpha-Mo_2C (Pbcn, orthorhombic)
- 12 atoms per unit cell
- Ground-state polymorph (E_hull = 0)



Demo: Slab Generation -- Mo_2C (1,1,1)



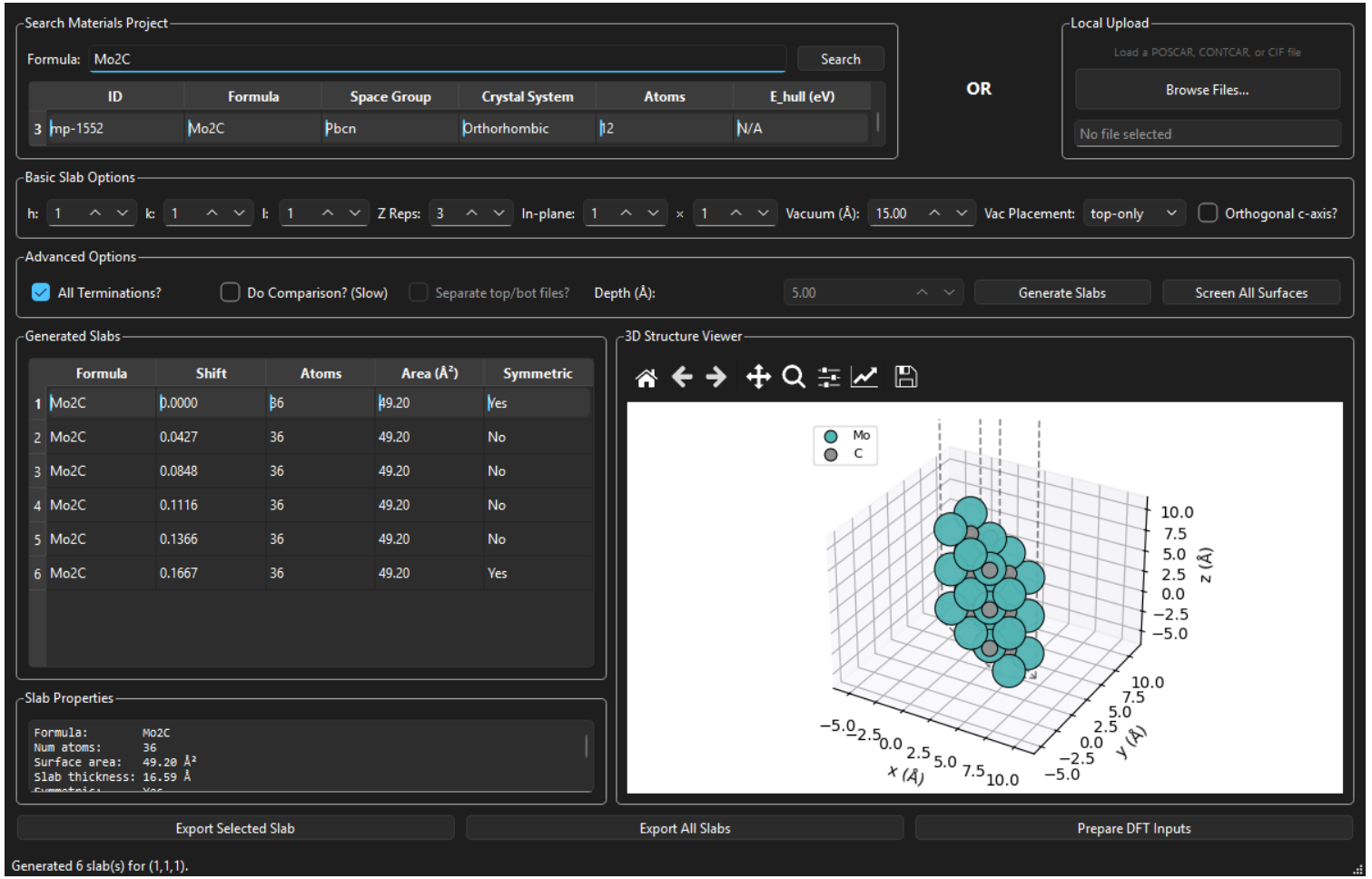
Parameters

- 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



Slab Properties

Formula: Mo_2C

Atoms: 36

Surface area: 49.20 Å²

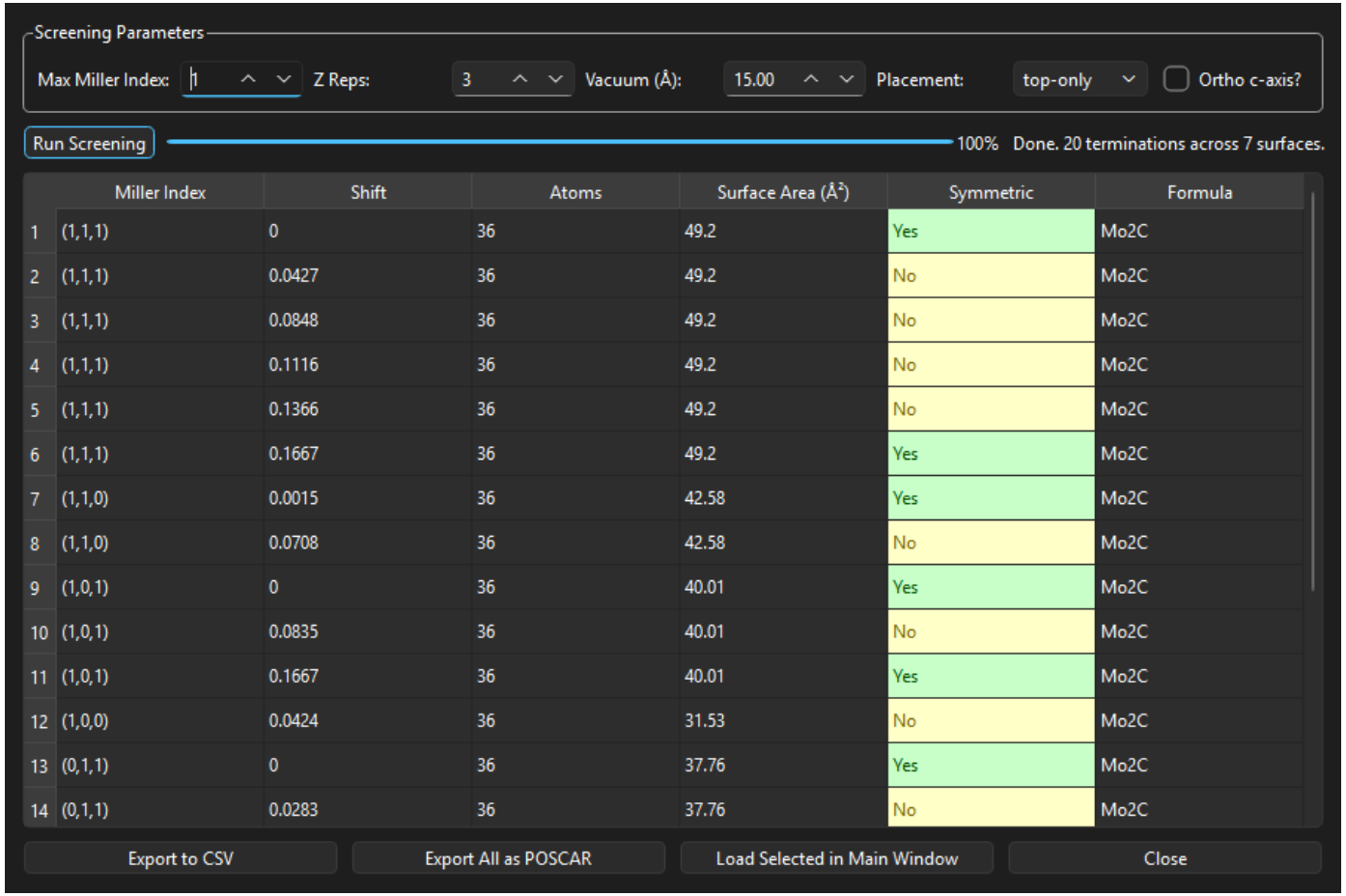
Slab thickness: 16.59 Å

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



	Miller Index	Shift	Atoms	Surface Area (Å²)	Symmetric	Formula
1	(1,1,1)	0	36	49.2	Yes	Mo2C
2	(1,1,1)	0.0427	36	49.2	No	Mo2C
3	(1,1,1)	0.0848	36	49.2	No	Mo2C
4	(1,1,1)	0.1116	36	49.2	No	Mo2C
5	(1,1,1)	0.1366	36	49.2	No	Mo2C
6	(1,1,1)	0.1667	36	49.2	Yes	Mo2C
7	(1,1,0)	0.0015	36	42.58	Yes	Mo2C
8	(1,1,0)	0.0708	36	42.58	No	Mo2C
9	(1,0,1)	0	36	40.01	Yes	Mo2C
10	(1,0,1)	0.0835	36	40.01	No	Mo2C
11	(1,0,1)	0.1667	36	40.01	Yes	Mo2C
12	(1,0,0)	0.0424	36	31.53	No	Mo2C
13	(0,1,1)	0	36	37.76	Yes	Mo2C
14	(0,1,1)	0.0283	36	37.76	No	Mo2C

Batch Screening

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

Mo_2C Results (max index 1)

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

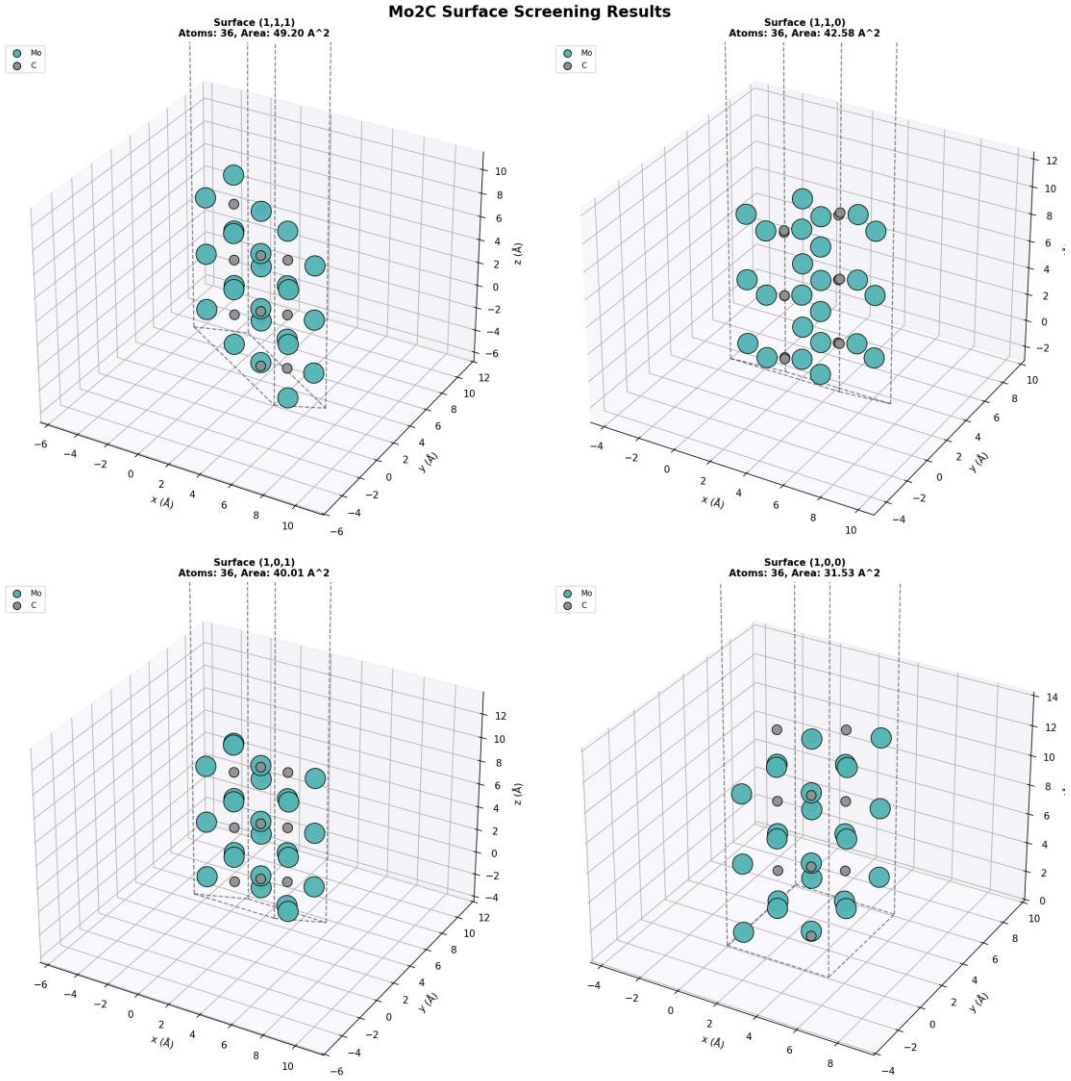
Export Options

Screening Results: Mo_2C Surface Characterization

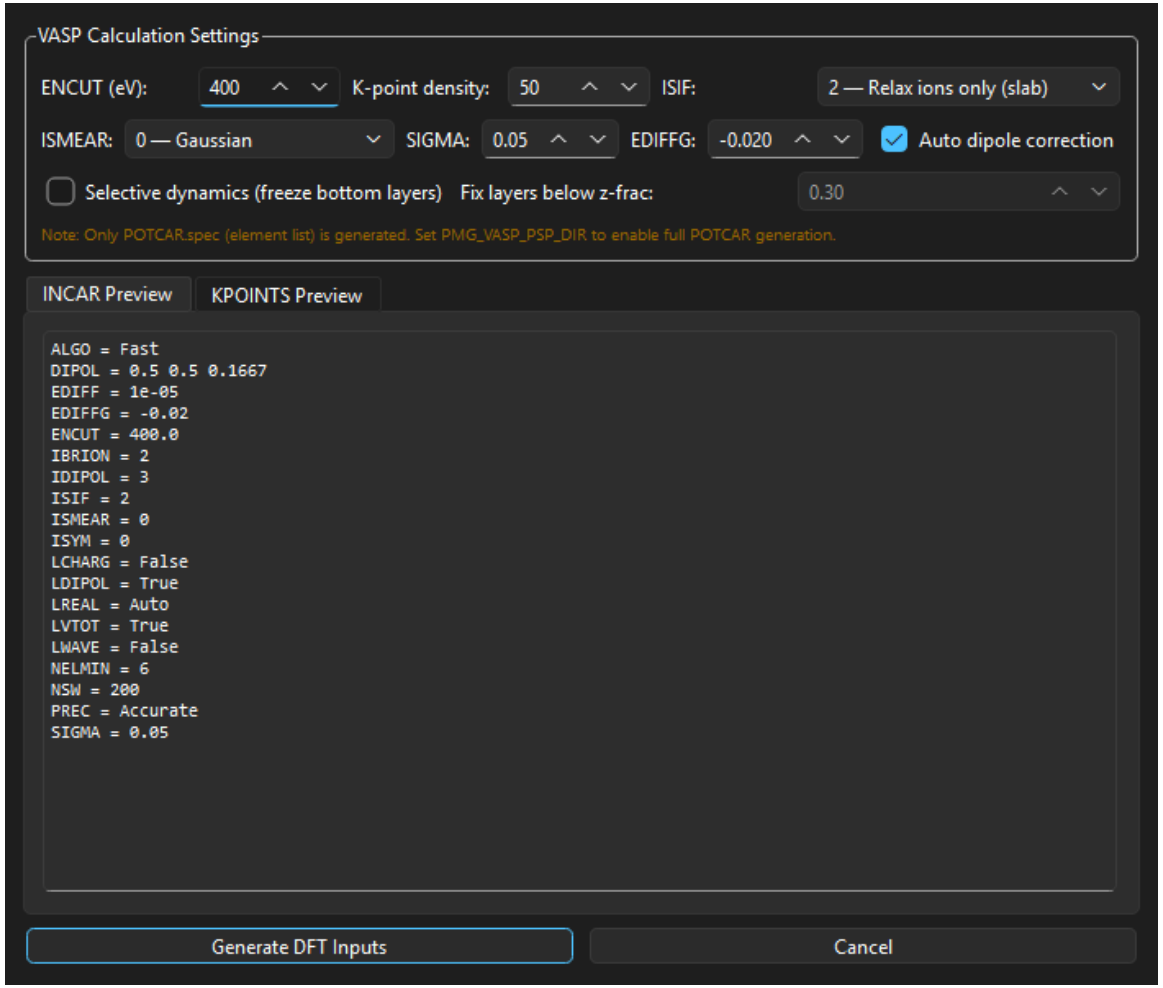
Surface	Terminations	Area (Å²)	Symmetric	Asymmetric
(0,0,1)	2	24.63	2	0
(0,1,0)	2	28.62	1	1
(1,0,0)	1	31.53	0	1
(0,1,1)	4	37.76	2	2
(1,0,1)	3	40.01	2	1
(1,1,0)	2	42.58	1	1
(1,1,1)	6	49.20	2	4
Total	**20**	**--**	**10**	**10**

Structure: alpha-Mo_2C (mp-1552, Pbcn, orthorhombic, 12 atoms) | Max Miller index: 1 | Z reps: 3 | Vacuum: 15 Å

Mo_2C Surface Gallery



Demo: DFT Input Generation



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
- Mo_2C 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?