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

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Surface properties govern how materials interact with their environment, influencing catalytic activity, corrosion resistance, coating adhesion, and crystal growth behavior. Computational studies of surfaces begin with constructing slab models — thin slices of a bulk crystal cut along specific crystallographic planes — which serve as the input for density functional theory (DFT) calculations. In practice, building these models requires writing custom scripts for each material and orientation, a workflow that demands expertise in crystallographic transformations and is vulnerable to subtle but consequential errors: incorrect surface terminations, unphysical polar surfaces, and geometric distortion of atomic positions at high-index orientations. Moreover, no existing tool connects the full pipeline from structure sourcing through surface enumeration, visualization, and DFT input preparation, forcing researchers to stitch together separate scripts and software at each stage.

We present SlabGen, an open-source graphical platform that integrates the complete surface modeling workflow into a single application. At its core, SlabGen employs a two-step orient-then-replicate algorithm: the bulk crystal is first reoriented so that the target (h,k,l) plane aligns with the slab normal and replicated to the desired thickness, then vacuum and termination enumeration are applied through a geometrically trivial (001) cut. This decomposition avoids the atom stretching and lattice distortion that arise from direct high-index slab generation. The platform supports structure input from the Materials Project database or local files in VASP and CIF formats, provides interactive 3D visualization with element-resolved Jmol coloring and unit cell rendering, and includes a batch screening engine that identifies all symmetrically distinct surfaces up to a user-specified maximum Miller index. For each surface, the screener catalogs the available terminations, flags symmetric versus asymmetric slabs, and reports structural properties. Selected surfaces can be exported directly or passed to SlabGen's DFT input generator, which produces ready-to-submit VASP file sets including POSCAR, INCAR with automatic dipole corrections for asymmetric slabs, and KPOINTS with appropriate k-mesh density.

We demonstrate SlabGen's capabilities through a systematic case study on Mo2C, a transition metal carbide of interest for heterogeneous catalysis and hard coating applications. We screen all low-index Mo2C surfaces, identify their terminations and symmetry characteristics, generate DFT inputs for selected orientations, and calculate surface energies from first-principles relaxations. The resulting surface energy landscape provides insight into the relative stability of different Mo2C facets and, through Wulff construction analysis, predicts the equilibrium crystal morphology. SlabGen reduces what typically requires days of manual scripting to minutes of guided interaction, making systematic surface studies accessible to researchers without extensive scripting experience. The platform is built with

Python, PyQt5, and pymatgen, and is freely available on GitHub under the MIT license.