SlabGen: An Integrated Platform for Surface Slab Generation and DFT Workflow Preparation

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Surfaces govern much of how materials interact with their environment, from catalytic activity and corrosion to film growth. Studying these properties from first principles typically involves constructing slab models, periodic structures obtained by cutting a bulk crystal along a chosen crystallographic plane, and relaxing them with density functional theory (DFT). While the idea is straightforward, the practical workflow is not. Each material and orientation demands its own setup, and subtle errors such as selecting an unphysical polar termination, missing a distinct surface cut, or introducing geometric distortion at high-index planes can go unnoticed and compromise results. The toolchain is also fragmented: researchers routinely move between the Materials Project or ICSD for structure sourcing, custom pymatgen or ASE scripts for slab construction, VESTA for visual inspection, and manual VASP input preparation, with no unified interface connecting these steps.

We developed SlabGen to bring this entire workflow into a single open-source desktop application. Users can query the Materials Project database or load a local structure file, generate slabs for any Miller index, and visualize them interactively in 3D. A built-in screening engine enumerates all symmetrically distinct orientations up to a chosen index, catalogs every unique termination, and flags whether each slab is symmetric or asymmetric. Selected surfaces feed directly into a DFT input generator that writes ready-to-submit VASP file sets (INCAR, KPOINTS, POSCAR, and job script) with automatic dipole corrections for asymmetric slabs. At the algorithmic level, SlabGen employs a two-step orient-then-replicate strategy: the bulk cell is first reoriented so the target (h,k,l) plane lies along the z-axis, and only then are vacuum and termination cuts applied. This separation avoids the geometric distortion artifacts that conventional single-step methods can produce for high-index surfaces.

We validate SlabGen on FCC platinum, where the predicted surface energy ordering $\gamma(111) < \gamma(100) < \gamma(110)$ is consistent with both experiment and prior computational work. We then apply it to orthorhombic Mo_2C (space group Pbcn), a transition metal carbide of growing interest for heterogeneous catalysis and hard coating applications. Screening Mo_2C up to Miller index 2 yields 19 symmetrically distinct orientations comprising 44 unique terminations, of which 34 are symmetric and 10 asymmetric. Several orientations, such as (1,1,1), present up to six distinct terminations, underscoring that the Miller index alone does not fully define a surface and that systematic enumeration is essential. SlabGen screened all 44 terminations and generated the corresponding VASP input sets in a single interactive session, a task that would conventionally require writing and adapting individual scripts for each orientation and termination. The platform is built on Python, PyQt5, and pymatgen, and is freely available on GitHub under the MIT license.