USER MANUAL

Bravais

Interactive 3D crystal-structure visualisation
and surface-slab generation

Version 1.8.0

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Contents

Chapter 1

Introduction

Bravais is a desktop application for viewing, building, and editing crystal structures. It reads CIF and VASP `POSCAR`/`CONTCAR` files, renders them in real-time 3D, and gives you a set of tools for the everyday work that surrounds a DFT calculation: cutting surface slabs, building supercells, placing adsorbates, applying strain, creating point defects, interpolating NEB paths, and exporting the result back to the formats your calculations expect.

Everything runs locally on your machine. Structures are never uploaded to a server. The one optional exception is the built-in AI assistant, which — only if you choose to use it — sends your messages to Anthropic using an API key you supply yourself.

This manual covers the application in full. It is arranged roughly in the order you meet things: loading a structure first, then moving around it, then the build and analysis tools, and finally export, sharing, and the assistant. You do not need to read it cover to cover — each section stands on its own, so feel free to jump to whatever you are trying to do.

1.1 Who this is for

Bravais is aimed at researchers and students working in computational materials science, surface science, and solid-state chemistry — anyone who routinely prepares structures for plane-wave DFT codes such as VASP. No prior experience with the app is assumed. A working familiarity with crystallographic ideas (lattices, Miller indices, fractional coordinates) will help, and the built-in learning mode covers the basics if you need them.

1.2 Conventions used in this manual

- Menu items, buttons, and tabs are written in **bold**: open the **Build** tab.
- Keyboard keys are shown like `R` or `Ctrl+Z`.
- File names and formats are shown like `POSCAR` or `structure.cif`.
- Lattice parameters use the standard symbols: edge lengths a, b, c in ångström (Å) and angles α, β, γ in degrees.

Chapter 2

Installation and first launch

Bravais is distributed as a normal desktop application for macOS, Windows, and Linux. Download the build for your platform from the Bravais page, then follow the one-time launch step below. Because the application is not yet code-signed, each operating system shows a warning the first time you open it; this is expected for a new publisher and only appears once.

2.1 System requirements

- **macOS** 11 (Big Sur) or later, Apple Silicon (M1/M2/M3/M4). Intel Macs are not currently supported.
- **Windows** 10 or later, 64-bit (x64 or ARM64).
- **Linux** a recent 64-bit distribution (x86-64), distributed as a portable AppImage.

A discrete or integrated GPU with WebGL support is recommended for smooth 3D rendering, but not required for smaller structures.

2.2 macOS

1. Open the downloaded `.dmg` and drag **Bravais** into your Applications folder.
2. In Applications, **right-click** Bravais and choose **Open** rather than double-clicking.
3. Click **Open** in the dialog. Bravais launches, and from then on you can open it normally from Launchpad, Spotlight, or the Dock.

2.3 Windows

1. Run the downloaded `.exe` installer.
2. If a *"Windows protected your PC"* dialog appears, click **More info**, then **Run anyway**.
3. Complete the installer and launch Bravais from the Start menu or the desktop shortcut.

2.4 Linux

1. Mark the AppImage executable: `chmod +x Bravais-1.8.0.AppImage` (or right-click → Properties → Permissions → "Allow executing file as program").

2. Run it: `./Bravais-1.8.0.AppImage`, or double-click it. No installation is needed.

If the AppImage does not start, install FUSE (`sudo apt install libfuse2` on Ubuntu), which some AppImages require.

Chapter 3

A quick tour

When Bravais opens you are looking at the main window. It has three regions:

- **The 3D viewport** fills most of the window. This is where the structure is drawn and where you rotate, zoom, and click on atoms.
- **The toolbar** along the top groups every tool into tabs: **File**, **View**, **Edit**, **Measure**, **Build**, **Analysis**, and **Compare**. Selecting a tab swaps the controls shown beneath it.
- **The info panel** reports details about the current structure and any atom you have selected.

The fastest way to get oriented is to load one of the built-in samples (see the next section), then drag to rotate it and click on an atom. Once something is on screen, the rest of this manual will make more sense.

Chapter 4

Loading structures

4.1 Built-in samples

The quickest way to start is the **sample dropdown** on the **File** tab. It contains a curated set of common structures grouped by type:

- **FCC metals** — Cu, Au, Al, Pt, Ni, Ag, Pd
- **BCC metals** — Fe, W, Cr, Mo
- **Diamond-cubic semiconductors** — Si, Ge, diamond
- **Zinc-blende compounds** — GaAs, ZnS
- **HCP metals** — Ti, Zn, Mg
- **Oxides** — TiO_2 (rutile), MgO (rock salt)
- **Other teaching structures** — NaCl, $CaTiO_3$ perovskite, simple-cubic Po

These are useful both for learning the app and as quick, known-good inputs for testing a workflow.

4.2 Opening your own files

Use **Open** on the **File** tab to load a structure from disk. Two formats are supported:

- **CIF** (`.cif`) — Crystallographic Information File.
- **VASP** `POSCAR` / `CONTCAR` — the structure format used by VASP.

You can also **drag a file directly onto the window** to load it.

4.2.1 How POSCAR files are read

Bravais understands the standard VASP layout: a comment line, a scale factor, three lattice-vector rows, an optional line of element symbols, the per-element atom counts, an optional Selective Dynamics line, and the coordinate-mode line followed by the atomic positions.

Both **Direct** (fractional) and **Cartesian** coordinates are accepted. If the coordinate-mode line is missing, Bravais defaults to Direct, matching VASP's own behaviour. Cartesian files are converted to fractional coordinates on load, and the scale factor is applied to both the lattice and the positions. The original coordinate mode is remembered so that exporting later reproduces the same style.

4.2.2 How CIF files are read

Bravais reads the six cell tags (`_cell_length_a/b/c` and `_cell_angle_alpha/beta/gamma`) and the `_atom_site_` loop, taking the element from `_atom_site_type_symbol` (or the label if the type symbol is absent) and the fractional coordinates from `_atom_site_fract_x/y/z`. Standard-uncertainty values in parentheses, such as `1.234(5)`, are handled correctly.

> **Important:** Bravais reads the atoms exactly as listed and does **not** expand symmetry operations. For a structure stored in space group P1 this is the complete cell. For a file that stores only the asymmetric unit, you will see fewer atoms than the full conventional cell. If a loaded structure looks sparse, convert it to P1 in your crystallography tool of choice first, or load an equivalent POSCAR.

Chapter 5

Navigating the 3D view

5.1 Mouse controls

- **Drag** anywhere in the viewport to **rotate** the structure.
- **Scroll** to **zoom** in and out.
- **Click an atom** to select it. The info panel then shows its element, its index in the structure, and its fractional coordinates.

5.2 Looking down an axis

The **a / b / c** buttons snap the camera to look straight down the corresponding crystallographic axis. This is the fastest way to check alignment, confirm a layer stacking, or line up a view before cutting a surface. Press `R` at any time to reset the camera to its default orientation if you lose your bearings.

5.3 Quad view

Press `Q`, or use the toggle on the **View** tab, to switch to **quad view**. The viewport splits into four panels showing the structure from four fixed viewpoints at once:

- **Top** — orthographic, looking down.
- **Ortho** — a second orthographic angle.
- **Left** — orthographic, from the side.
- **Perspective** — a perspective camera.

Quad view is particularly useful for slabs and interfaces, where a single viewpoint can hide what is happening along the surface normal. Press `Q` again to return to the single view.

Chapter 6

Display options (View tab)

Everything on the **View** tab changes how the structure is *drawn* — none of it alters the structure itself or what gets written when you export. Settings are applied live, so you can adjust and immediately see the result.

6.1 Display mode

Choose how atoms and bonds are represented:

- **Ball-and-stick** — atoms as spheres, bonds as cylinders. The default, and the most useful for seeing connectivity.
- **Space-filling** — atoms drawn at full (van der Waals–scale) size, packed together. Good for seeing how densely a structure fills space.
- **Wireframe** — bonds only, no atom spheres. Useful for dense structures where spheres would hide the framework.

6.2 Atom size and bonds

- **Atom scale** adjusts the rendered radius of every atom.
- **Show bonds** (`B`) turns bonds on or off.
- **Bond cut-off** sets the maximum interatomic distance, in ångström, that is drawn as a bond. There is also a tolerance based on per-element covalent radii, so chemically sensible bonds are found without manual tuning in most cases.
- **Periodic bonds** have their own toggle. These are bonds that cross the unit- cell boundary and reconnect on the opposite side. They are correct but can clutter the view, so you can hide them independently of ordinary bonds.

6.3 Colour

- **By element** uses the standard CPK-style colour scheme — the familiar colours where oxygen is red, carbon dark grey, hydrogen white, and so on.
- **By coordination** colours each atom according to how many neighbours it has. This is an excellent way to find under-coordinated atoms — surface sites, defects, edges — at a glance.

6.4 Labels

Press `L` or use the **Labels** control to annotate atoms. You can label by:

- **Element** — the chemical symbol.
- **Index** — the atom's position in the structure list, which is the number you use when measuring or editing by index.
- **Coordinates** — the fractional position.

6.5 Unit cell, boundary atoms, and lattice planes

- **Unit cell** draws the edges of the cell as a box.
- **Boundary atoms** shows atoms lying on the cell faces, repeated on the opposite face, so the cell looks visually complete. A tolerance controls how close to a face an atom must be to be duplicated.
- **Lattice plane** overlays a translucent (hkl) plane inside the cell. Enter the Miller indices and adjust the opacity and colour. This is a planning aid: you can see exactly where a plane sits before you commit to cutting a surface along it.

6.6 Theme

Bravais offers a **light** and a **dark** theme. Choose whichever is more comfortable; the theme affects only the interface and viewport background, not exported files or images.

Chapter 7

Supercells

On the **Build** tab, the **supercell** control replicates the unit cell along the a, b, and c directions, up to $5 \times 5 \times 5$. This is a viewing and export convenience: it tiles the atoms you already have into a larger periodic block, which is what you want when preparing, for example, a defect cell or an adsorption cell that needs lateral separation between repeated images.

Larger supercells contain many more atoms and are correspondingly heavier to render, so increase the size gradually and watch performance on big structures.

Chapter 8

Building surface slabs

Cutting a surface from a bulk crystal is one of the central tasks Bravais is built for. Open **Create Surface** from the **Build** tab.

8.1 The workflow

1. **Enter the Miller indices** $(h\,k\,l)$ for the surface you want to expose.
2. Bravais analyses the structure and lists the distinct **terminations** for that orientation — the symmetrically inequivalent atomic layers the surface could end on. Different terminations expose different atoms and generally have different surface energies, so this choice matters. Select the one you want.
3. **Set the number of layers.** This controls how thick the slab is. Thicker slabs converge surface properties better but cost more to compute.
4. **Set the vacuum thickness.** This is the gap of empty space added above the slab so that, under periodic boundary conditions, the slab does not interact with its own image. A typical value is 10–15 Å.
5. **Generate.** The slab is built and shown in the 3D viewport so you can inspect it — check the termination, the thickness, and the vacuum — before exporting.

8.2 How the slab is constructed

For the chosen $(h\,k\,l)$, Bravais builds the reciprocal-lattice vector to find the plane normal and the interplanar spacing, enumerates the family of parallel lattice planes, identifies the inequivalent terminations, and constructs a surface cell whose third axis is chosen to lie as close to the surface normal as possible. It then stacks the requested number of layers and adds the vacuum gap. The result is a slab with a well-defined surface on top and bottom, ready for relaxation.

8.3 Exporting surfaces

- **Export All** writes every termination of the current orientation as its own `POSCAR`, in a single step. This is a large time-saver when you are screening surfaces and want all terminations prepared at once.

- To export only the slab you are currently viewing, use the ordinary structure export on the **File** tab (see *Exporting structures*).

Chapter 9

Adsorbates

With a surface slab on screen, the adsorbate tool places molecules onto it. Open it from the **Build** tab.

9.1 The molecule library

Bravais includes a library of common adsorbates built with realistic geometry (bond lengths and angles):

- **Molecules** — H_2O (water), OH (hydroxyl), CO, CO_2, CO_3 (carbonate), NO, NO_2, NH_3 (ammonia), CH_4 (methane), OLi.
- **Single atoms** — H, O, F.

9.2 Placing and orienting

For each adsorbate you control:

- **Position** — where the molecule sits relative to the surface.
- **Tilt** and **azimuth** — the orientation, so you can set up specific binding geometries (upright, flat-lying, tilted).

Adsorbates are tracked as a separate list layered on top of the slab. You can:

- Add **several** adsorbates to the same surface.
- **Edit** or **remove** any one of them individually.
- **Clear** them all at once.
- **Export** the slab with all adsorbates included, so the combined system is written to a single structure file ready for calculation.

Chapter 10

Editing atoms

The **Edit** tab — and its keyboard shortcuts — let you change a structure directly in the viewport.

10.1 Edit modes

- **Add** (`A`) — choose an element, then place new atoms.
- **Delete** (`D`) — click atoms to remove them.
- **Move** (`M`) — reposition an atom by dragging it.

Press `Escape` to leave an editing mode and return to ordinary inspection.

10.2 Non-destructive editing and history

Editing is safe and reversible:

- The first change you make creates a **working copy** of the structure, so your originally loaded data is never overwritten in place.
- `Ctrl+Z` **undoes** the last change, stepping back through your edit history.
- **Revert** returns the structure to the state it was in when you loaded it.

The window title flags a structure as **modified** whenever it differs from what was loaded, so you always know there are unsaved changes.

Chapter 11

Measuring geometry

Bravais measures distances, angles, and dihedrals between atoms you click. Switch to the **Measure** tab, or use the number-key shortcuts directly.

11.1 Measurement modes

- **Distance** (`1`) — click **two** atoms to measure the distance between them, in ångström.
- **Angle** (`2`) — click **three** atoms; the angle is measured at the second (middle) atom, in degrees.
- **Dihedral** (`3`) — click **four** atoms to measure the torsion angle, in degrees.

Measurements accumulate in a list, so you can take several in succession and review them together. Clear the list when you are done.

11.2 Coordination number

Selecting a single atom reports its **coordination number** — the count of bonded neighbours — in the info panel. Bonds are determined using covalent radii with a tolerance, the same convention used elsewhere in the app, so the count reflects chemically reasonable nearest neighbours.

Chapter 12

Point defects and strain

Both tools are on the **Build** tab and both feed through the same undo history as manual editing, so any change can be stepped back.

12.1 Point defects

The defect builder creates:

- **Vacancy** — removes a selected atom, leaving a vacant site.
- **Substitution** — replaces an atom of one element with another element.
- **Interstitial** — adds an atom of a chosen element into a gap in the structure.

These are the building blocks for point-defect studies — dopants, vacancies, and anti-sites.

12.2 Strain

The strain tool deforms the cell by a chosen percentage:

- **Uniform (isotropic)** strain scales the cell equally in all directions.
- **Biaxial** strain scales it in-plane, the relevant case for epitaxial films and strained-layer studies.

This is the quick way to set up a lattice-parameter scan or an equation-of-state–style series of structures.

Chapter 13

NEB path builder

The **NEB** tool, on the **Build** tab, prepares an initial reaction path for a nudged-elastic-band calculation by interpolating between two endpoint structures.

13.1 Building a path

1. Provide an **initial** and a **final** structure. The two must contain the same number of atoms in the same order, since the path is built by moving each atom from its initial to its final position.
2. Choose the **number of intermediate images**.
3. Choose the **interpolation method**:
   - **Linear** moves each atom in a straight line between its endpoints. Periodic boundaries are handled with the minimum-image convention, so atoms take the shortest route rather than wrapping the long way around the cell.
   - **IDPP** (image-dependent pair potential) starts from the linear guess and relaxes the intermediate images so that interatomic distances vary smoothly along the path. This usually produces a more physical starting path with fewer atomic overlaps, and is the recommended choice for most cases.

13.2 Reviewing and exporting

The generated path can be stepped through and animated image by image in the viewport, so you can check that the interpolation is sensible before running anything. Exporting writes the path as a set of numbered folders — `00/`, `01/`, `02/`, and so on — each containing the `POSCAR` for one image, which is exactly the directory layout VASP expects for an NEB run.

Chapter 14

Analysis tools

The **Analysis** tab gathers the tools that *report on* a structure rather than change it.

14.1 Cell information

A summary of the currently loaded structure: the lattice parameters a, b, c, α, β, γ, the cell volume, the chemical formula, and the total atom count.

14.2 Radial distribution function

The **RDF** computes the radial distribution function $g(r)$ for the current structure — the distribution of interatomic separations. Peaks correspond to coordination shells, so the RDF is a quick way to inspect local structure and check nearest-neighbour distances.

14.3 Crystal morphology (Wulff construction)

The **morphology** tool predicts the equilibrium shape (crystal habit) of a crystal from its surface energies, using the Wulff construction. You provide a surface energy γ for each $(h\,k\,l)$ face you want to include, and the tool builds the polyhedron in which each face sits at a distance from the centre proportional to its energy. Lower-energy faces grow larger; higher-energy faces shrink or disappear. Because only the *relative* energies determine the shape, you can compare faces without needing absolute units — the overall scale is handled for you.

Chapter 15

Comparing structures

The **Compare** tab loads a second structure alongside the first and displays them **side by side**. This is the natural way to inspect a before-and-after pair — a relaxed structure against its unrelaxed input, two terminations of the same surface, or two candidate structures you are choosing between.

Chapter 16

Exporting structures and images

16.1 Structure files

From the **File** tab you can write the current structure to disk in three formats:

- **POSCAR** — VASP format. The coordinate mode (Direct or Cartesian) matches the mode of the file you loaded, so a load-then-save round-trips cleanly. Direct output wraps fractional coordinates into the $[0, 1)$ range for a canonical result.
- **CIF** — Crystallographic Information File, for sharing or for loading into other crystallography tools.
- **XYZ** — a simple Cartesian coordinate list, widely supported by molecular and visualization software.

Whatever modifications you have made — edits, supercell, surface, adsorbates, defects, strain — are reflected in the exported file.

16.2 Images

Export Image saves a PNG snapshot of the current viewport, at the orientation and with the display settings you have set, for use in slides, reports, and papers.

Chapter 17

Saving, loading, and sharing sessions

17.1 Sessions

A **session** captures the whole working state — the structure, your edits, and your display settings — not just the bare atoms.

- **Save Session** (`Ctrl+S`) writes the session to a file.
- **Load Session** reopens a saved session exactly as you left it.

Use sessions when you want to pause work and come back to it later with everything in place.

17.2 Share links

Share packs the current structure into a shareable link. Sending the link to a colleague lets them open the same structure in their own copy of Bravais. Nothing is uploaded to any server — the structure data is encoded directly inside the link itself, so sharing is entirely peer to peer.

Chapter 18

The AI assistant

Bravais includes an **optional** AI assistant that can both answer questions about your structure and operate the app on your behalf from a plain-language request — for example, "make a 2×2×1 supercell," "cut the (1 1 1) surface with six layers and 12 Å of vacuum," or "add a water molecule on top." The assistant carries out the actions directly rather than just describing them.

18.1 Enabling it

The assistant is disabled until you turn it on. To use it you provide your own **Anthropic API key**, obtained from the Anthropic console. The key is stored locally on your machine and is used only to send your messages to Anthropic so they can be answered. If you prefer not to use the assistant, simply leave it closed — nothing else in the application depends on it, and no data leaves your machine.

18.2 Privacy

When the assistant is active, the text of your messages and a description of the current structure are sent to Anthropic to generate a reply. Your structure files themselves are not uploaded anywhere else, and the rest of Bravais continues to work entirely offline.

Chapter 19

Learning crystallography

Under the **Analysis** tab, **Learn Crystallography** opens a set of short, guided lessons that introduce core ideas — lattices, unit cells, Miller indices, surfaces, and more — using the live 3D view to illustrate each concept. The lessons are aimed at students and at anyone new to the subject who wants to build intuition while using the same tools they will use for real work.

Chapter 20

Keyboard shortcuts

You can bring up this list inside the application at any time by pressing `?`.

Action	Shortcut
Rotate the view	Drag
Zoom	Scroll
Reset the view	`R`
Toggle quad view	`Q`
Toggle bonds	`B`
Toggle labels	`L`
Measure distance	`1`
Measure angle	`2`
Measure dihedral	`3`
Add-atom mode	`A`
Delete-atom mode	`D`
Move-atom mode	`M`
Undo last edit	`Ctrl+Z`
Save session	`Ctrl+S`
Leave current mode	`Escape`
Show shortcut list	`?`

Shortcuts are ignored while you are typing in a text field, so they will not interfere with entering values.

Chapter 21

Troubleshooting

A loaded CIF shows fewer atoms than expected. Bravais does not expand symmetry operations from CIF files. Convert the structure to space group P1 before loading, or load an equivalent POSCAR. See *Loading structures*.

Bonds look wrong or are missing. Adjust the bond cut-off on the **View** tab. Very long or very short bonds depend on the cut-off and the per-element radii; raise or lower the cut-off to match your structure. Remember that **periodic bonds** have a separate toggle.

The view is cluttered with bonds across the cell edges. Turn off **periodic bonds** on the **View** tab while keeping ordinary bonds on.

I rotated or zoomed too far and lost the structure. Press `R` to reset the camera.

Performance is slow. Large supercells multiply the atom count quickly. Reduce the supercell size, switch to wireframe display, or hide labels and periodic bonds.

The app will not open on first launch. This is the unsigned-application warning, not a fault. Follow the platform-specific steps in *Installation and first launch*.

The AI assistant does nothing. It is disabled until you open it and enter a valid Anthropic API key. It is entirely optional; the rest of the app works without it.

Chapter 22

Glossary

Adsorbate — a molecule or atom placed on a surface to study how it binds.

Cartesian coordinates — atomic positions given as absolute x, y, z distances in ångström, as opposed to fractional coordinates.

CIF — Crystallographic Information File, a standard text format for crystal structures.

Coordination number — the number of nearest-neighbour atoms bonded to a given atom.

Fractional coordinates — atomic positions expressed as fractions of the cell edges, each running from 0 to 1 within the unit cell. Bravais stores positions this way internally.

Miller indices $(h\,k\,l)$ — three integers naming a crystallographic plane or the surface exposed by cutting along it.

NEB — nudged elastic band, a method for finding the minimum-energy path of a transition between two states; Bravais prepares the initial path of images.

POSCAR / CONTCAR — VASP's input and output structure files.

RDF — radial distribution function $g(r)$, describing how interatomic separations are distributed.

Slab — a finite-thickness piece of crystal with a surface, used to model that surface under periodic boundary conditions.

Supercell — a larger cell formed by repeating the unit cell along its axes.

Termination — the particular atomic layer at which a surface is cut; a given $(h\,k\,l)$ orientation can have several inequivalent terminations.

Vacuum — the empty gap added above a slab so it does not interact with its periodic image.

Wulff construction — a geometric method for predicting a crystal's equilibrium shape from its surface energies.

Chapter 23

About

Bravais is developed by Ali Abbasi. It is built with Electron, React, and Three.js, and runs entirely on your own machine.

Bravais is proprietary software. The bundled End-User Licence Agreement permits free personal, academic, and internal-evaluation use; redistribution, modification, reverse engineering, and commercial use require written permission.

For support, feedback, feature requests, or commercial licensing, please use the contact details on the Bravais website.

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