Atomic Simulation Environment Component manual

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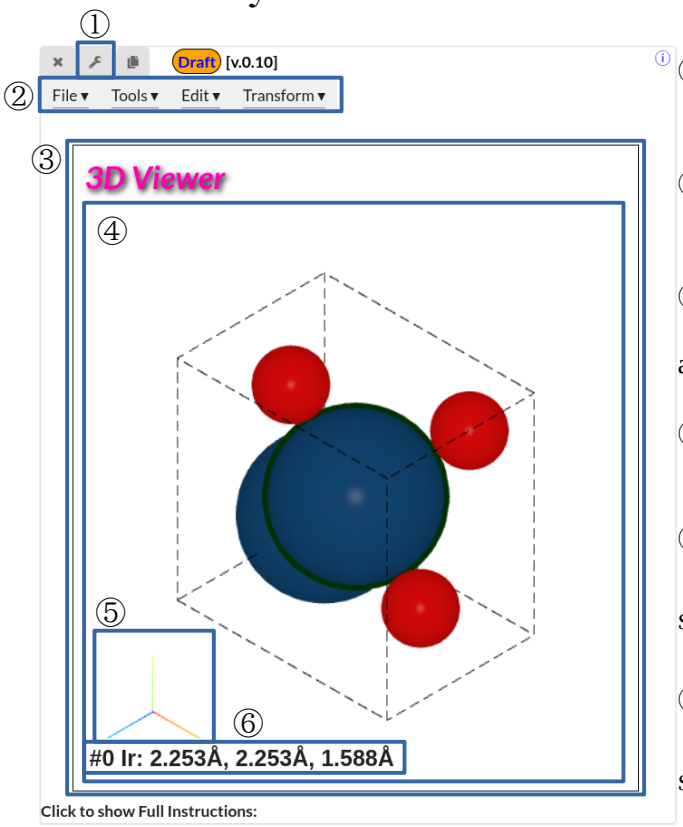
1 Introduction

The Atomic Simulation Environment (ASE) is a widely used Python library for creating, manipulating, and analyzing atomic structures.
This component reproduces part of ASE's graphical user interface (GUI) in a web-based environment, enabling interactive visualization and geometry inspection directly in the browser.

2 UI components description

2.1 Viewer layout



① Configure
Upload your structure files from this section.

② Menu bar
Contains the *File*, *Tools*, *Edit*, and *Transform* menus.

③ 3D Viewer
The main workspace for visualizing and editing the atomic structure.

④ 3D structure
Displays the atomic structure currently being edited.

⑤ Axes Helper
Shows the orientation of the coordinate system using X, Y, and Z axes.

⑥ Atoms information
Displays detailed information about the selected atom(s).

2.2 Atoms information

- **One atom selected** — atom index , atomic symbol and 3D coordinates

  #0 Ir: 2.253Å, 2.253Å, 1.588Å

- **Two atoms selected** — atomic symbols and distance between them

  Ir-Ir: 3.560Å

- **Three atoms selected** — atomic symbols and the angle defined by the three atoms

  Ir-Ir-O: 90.0°, 28.9°, 61.1°

- **More Atoms selected** — number of selected atoms

  4 atoms

3 Basic Viewer Operations

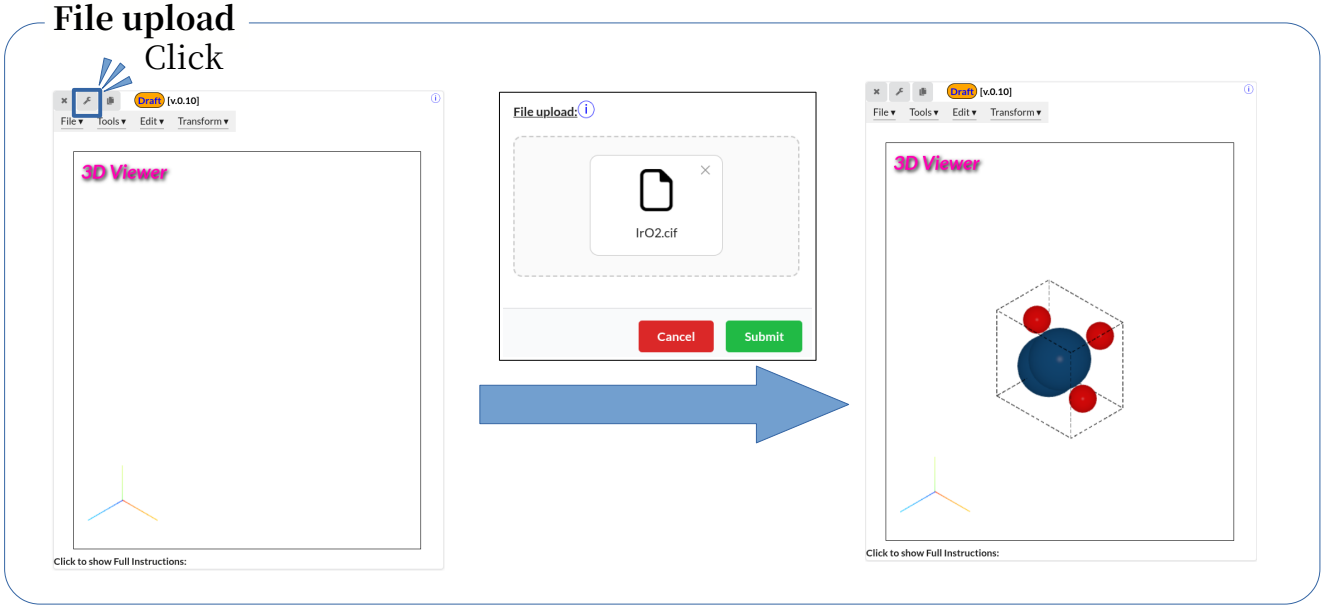
3.1 Camera Contols

- **Rotate** — Right-click and drag to rotate the camera around the structure.
- **Pan** — Hold Ctrl or Shift, then right-click and drag to move the view horizontally or vertically.
- **Zoom** — Scroll the mouse wheel to zoom in or out.

3.2 Atom selection

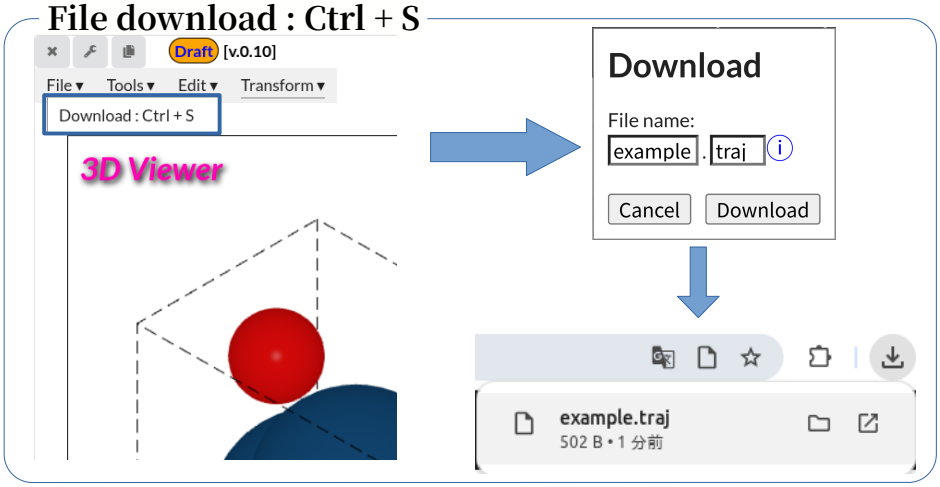
- **Select a single atom** —Hover over an atom and left-click.
- **Select multiple atoms** — Left-click and drag to draw rectangle; all atoms within the region will be selected.
- **Deselect atoms** — Left-click on an empty area.
- **Add atoms to the selection** — Holed the **Ctrl** key and left-click or drag to keep the current selection and add more atoms.

4 Configure



5 Menu

5.1 File



Available format :
traj, cif, xyz, etc.

See the ASE documentation for the full list.

https://ase-lib.org/ase/io/io.html

5.2 Tools

Copy — Ctrl + C

Copies the selected atoms' information to the clipboard, including atomic symbols and coordinates, and the unit cell and periodic boundary settings.

Cut — Ctrl + X

Copies the selected atoms and then removes them from the structure.

Paste — Ctrl + V

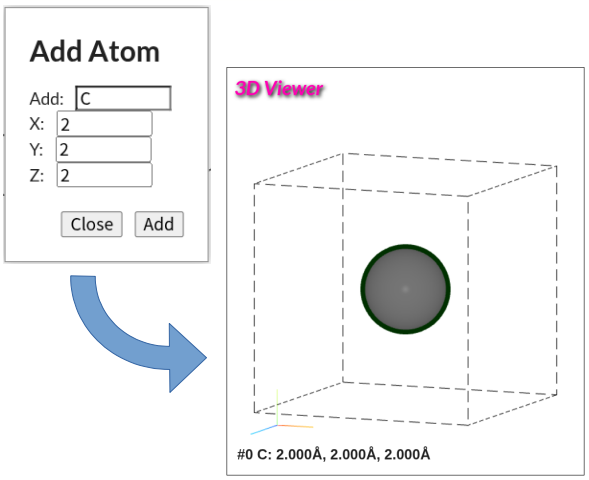
Inserts atoms stored in the clipboard into the current structure at a specified position.

Delete — Backspace

Removes the selected atoms from the structure.

5.3 Edit

Add atoms : Ctrl + A

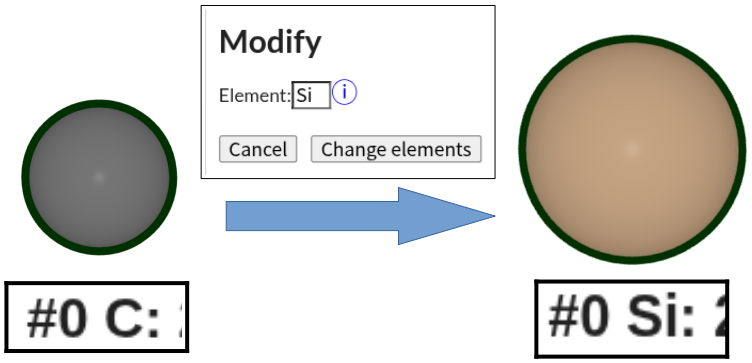


Edit Cell : Ctrl + E

Modify the unit-cell parameters in two ways:

- **Lattice vectors (3×3)**: Enter the three lattice vectors.
- **Lengths and angles**: Enter a, b, c and α, β, γ.

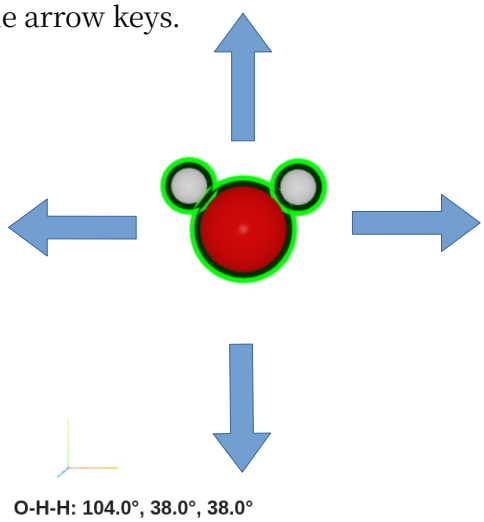
Change : Ctrl + Y



5.4 Transform

Move : Ctrl + M

Enable translation of selected atoms with the arrow keys.



Rotate : Ctrl + R

Enable rotation of selected atoms with the arrow keys.