

Motivation and vision for GUI

- To lower the entry barrier for people with little DFT experience
- To hide and abstract away the inner bits
- To give the people the freedom of calculating (almost) everything they want, but to guide them to avoid common mistakes
- Overall, to make the user's life easier



GIMS – Graphical Interface for Materials Simulations



Graphical Interface for Materials Simulations

- (as of now) Input generator and output parser
 - Soon, much more than that
- Free and open source:
 - Repository: <https://gitlab.com/gims-developers/gims/>
 - Feel free to contribute 😊
- Available as a web-based (and standalone) application
 - <https://gims.ms1p.org> - current stable version
 - <https://gims-dev.ms1p.org> – the HEAD of the master branch
- As of now, FHI-aims and Exciting codes are supported

GIMS main features

- Easy structure manipulations and visualization

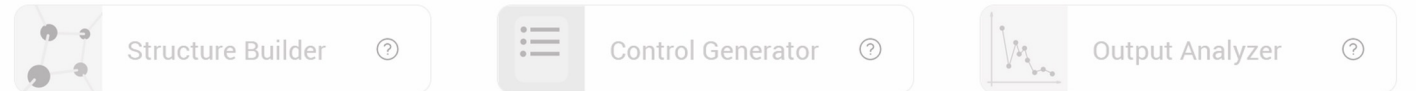


- Guided input file generation and easy output visualization

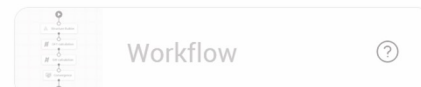


- Seamless switching between versions: stable, development and fallback

user menu
feedback



- Standalone desktop app built for main operating systems





Code and GIMS version chooser;
Settings button

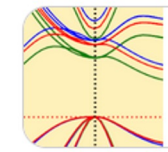

Choose your code   |  SETTINGS

Choose GIMS version

Calculation Apps



 Simple Calculation 



 Band Structure 

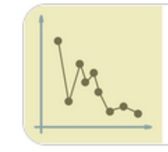

 GW Calculation 

Apps producing inputs for specific calculation modes

Elemental Apps

 Structure Builder 

 Control Generator 

 Output Analyzer 

“Elemental” apps with elemental functions

user manual

feedback



Features: Structure Builder

The screenshot displays the Structure Builder interface. On the left, a legend identifies the atomic species: Cd (orange), Sr (green), and Ta (blue). The central 3D model shows a crystal structure with axes labeled *a*, *b*, and *c*. The *a*-axis is red, *b* is green, and *c* is blue. The structure consists of Sr atoms (green) at the corners and Cd atoms (orange) at the midpoints of the *a* and *b* axes. Ta atoms (blue) are located at the centers of the edges along the *c*-axis. The interface includes a file browser at the top left showing 'CdSrTa.in', a 'View options' button, a camera icon, and an 'Edit structure' toggle set to 'OFF'. A '0/0' counter is also visible. On the right, a control panel with 'Import' and 'Export' buttons contains the following sections:

- Lattice Vectors**: A table of lattice vectors in units of Å.

	<i>a</i>	<i>b</i>	<i>c</i>
<i>a</i> :	7.550000	0.000000	0.000000
<i>b</i> :	0.000000	7.550000	0.000000
<i>c</i> :	0.000000	0.000000	7.550000

Options: Scale atom positions with lattice vectors, Remove Lattice Vectors
- Structure Info**: A dropdown menu.
- Supercell**: A dropdown menu.
- Standardized Cells**: A dropdown menu.
- Surface (Slab) Construction**: A dropdown menu.
- Basis Atoms**: A section with a '1/2' indicator, a 'New atom' button, and a 'Constrain all atoms' button. It includes a checkbox for 'Fractional coordinates' and a note: 'Click on the species color to specify more atomic properties (e.g. initial moment)'. Below this is a table of basis atoms:

	<i>x</i>	<i>y</i>	<i>z</i>	Species
1.	0.000000	3.775000	3.775000	Cd

- Import structure from ASE supported formats (e.g. CIF) and export to geometry.in
- Edit / Remove lattice vectors
- Simply create supercell / primitive cell
- Create and terminate slabs in a straightforward way
- Add / remove atoms, change atomic species, constraint atomic relaxation
- Get information about structure
- Visualize Brillouin zone with high symmetry points and paths

Features: Control Generator

Basic Settings ^

Geometry species

XC functional

Species Default Settings

Spin

K-grid ▾

Post-processing ▾

Structure Optimization, Forces, and Stress ▾

Numerical Accuracy (optional) ▾

Extra keywords ^

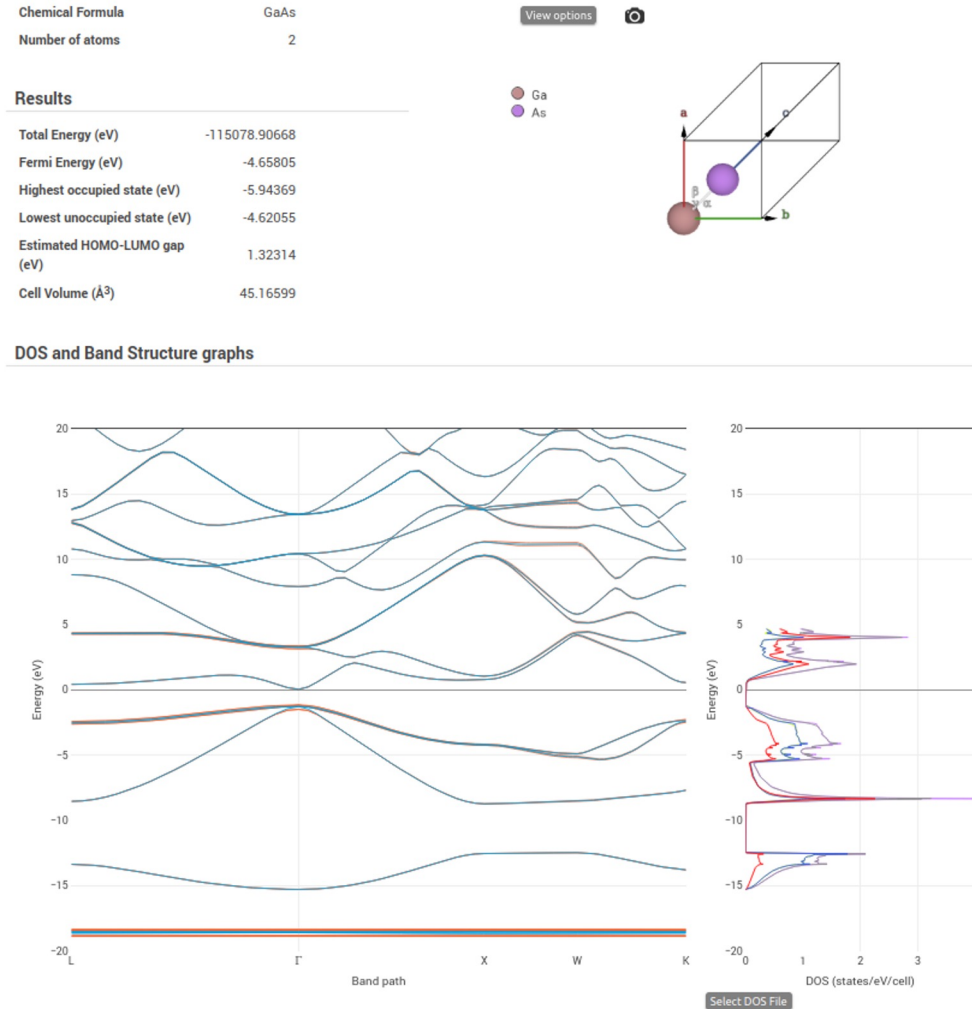
Here any non-essential keywords can be added to control.in. Please beware that there are no sanity checks for these and use with discretion.

Key	Value
<input type="text" value="output"/>	<input type="text" value="json_log"/>

Specifies whether or not a spin-polarized calculation is run. If you choose 'collinear', please assign initial moments in the Structure Builder to at least one atom. Choosing the right initial spin density can be performance-critical, and critical for the resulting physics.

- A set of mostly used input file keywords with explanation
- A simple mechanism of visibility constraints (certain keyword inputs may not be visible based on other inputs' values) and sanity checks of inputs' values based on other inputs and structure
- Extra keywords table allows building complicated input files

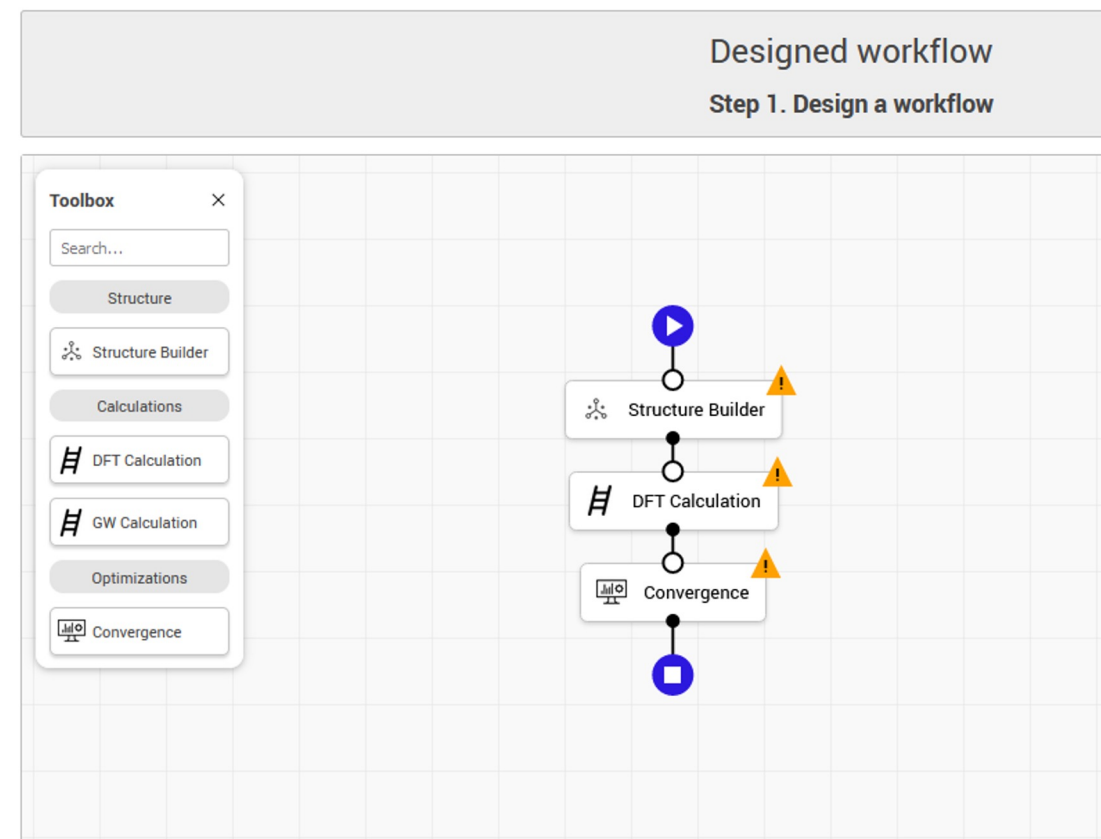
Features: Output Analyzer



- Numerical and graphical representation of the output file
- Graphs: convergence (energy, eigenvalues, density for each ionic step; forces), band structure, DOS, dielectric function
- Graphical representation of charge analysis results
- Graceful error handling

Development plans for GIMS 2.0

- “Designed” workflows with *Jobflow* package as middleware
- Decoupling of code-specific and common parts and offering code-specific parts as plugins



Choose your code



A longer road ahead...

- Jupyter notebook integration

- ChatGPT integration?

- *Stay tuned; feature requests are more than welcome!*

