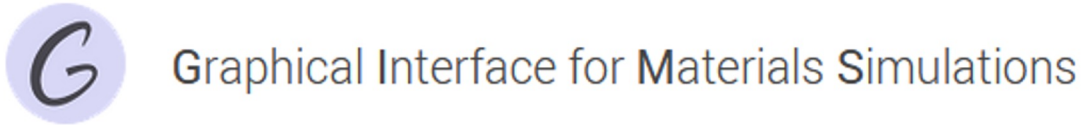
Motivation and vision for GUI

- 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

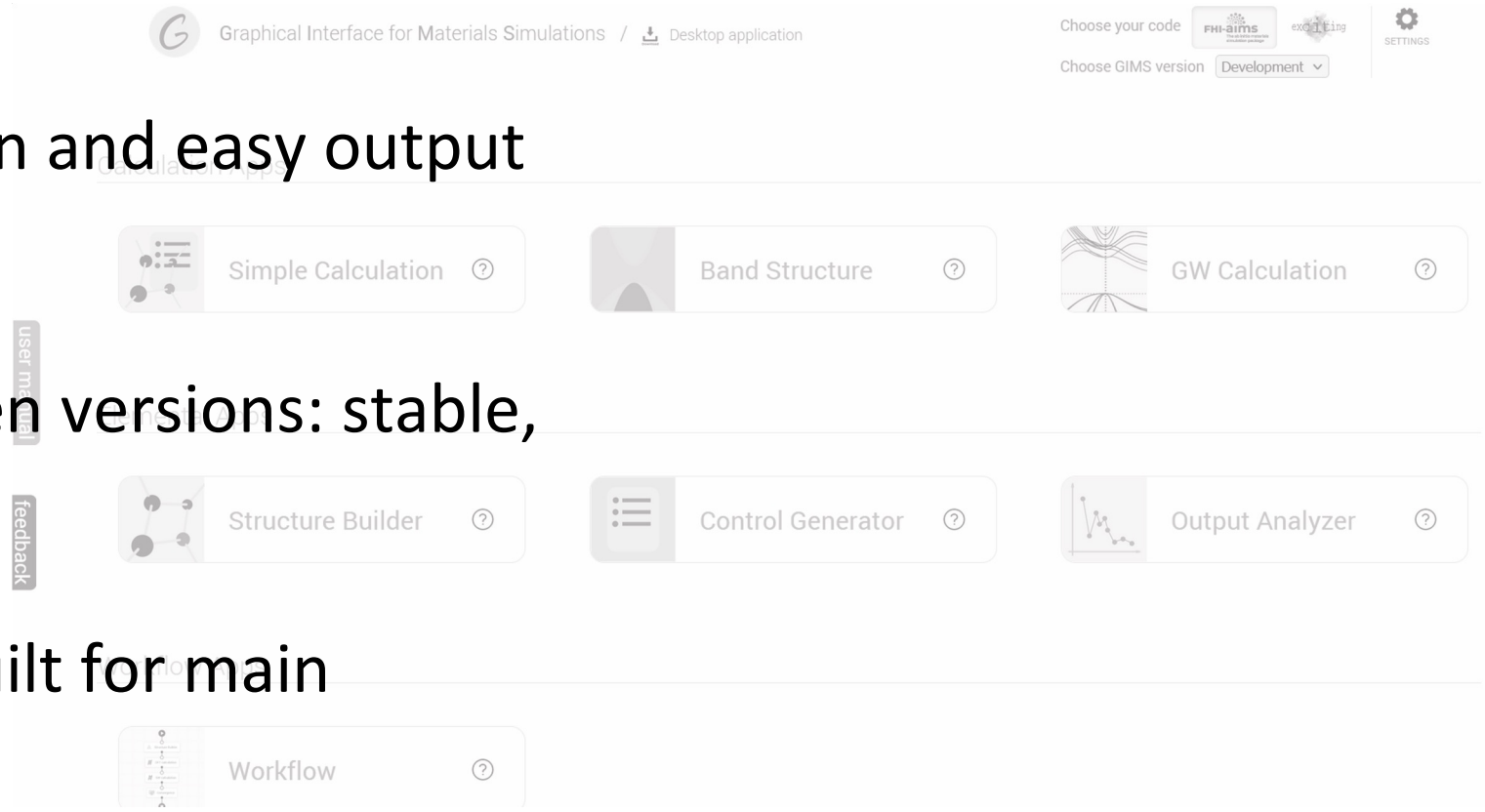
GIMS – Graphical Interface for Materials Simulations



- (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
- Standalone desktop app built for main operating systems



Code and GIMS version chooser;
Settings button

Graphical Interface for Materials Simulations / Desktop application

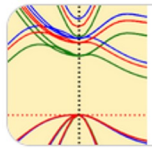
Choose your code FHI-aims exciting SETTINGS

Choose GIMS version Development

Calculation Apps


Simple Calculation


Band Structure

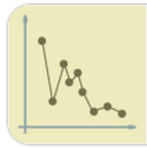

GW Calculation

Apps producing inputs for specific calculation modes

Elemental Apps


Structure Builder


Control Generator

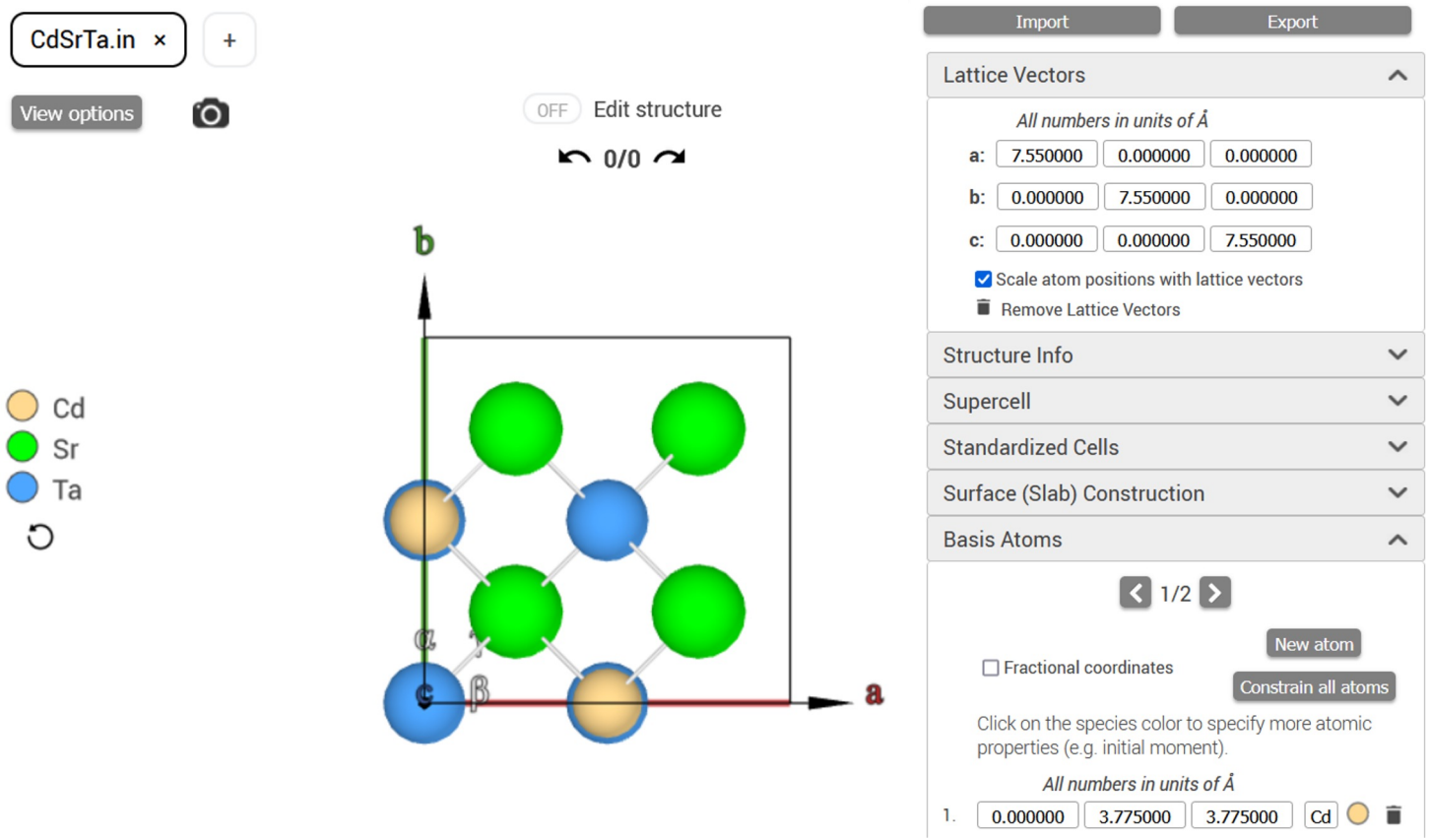

Output Analyzer

"Elemental" apps
with elemental functions

user manual

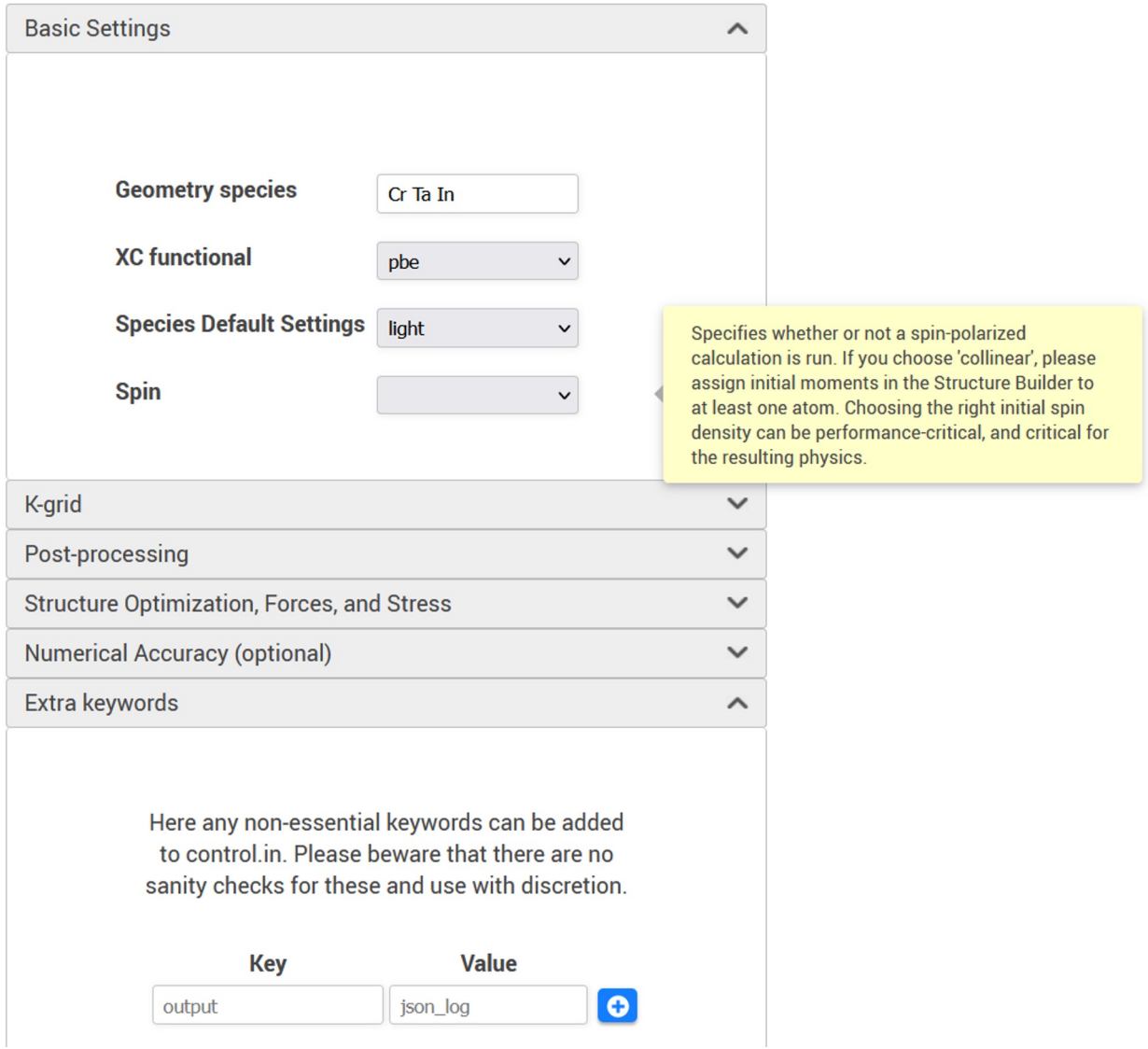
feedback

Features: Structure Builder



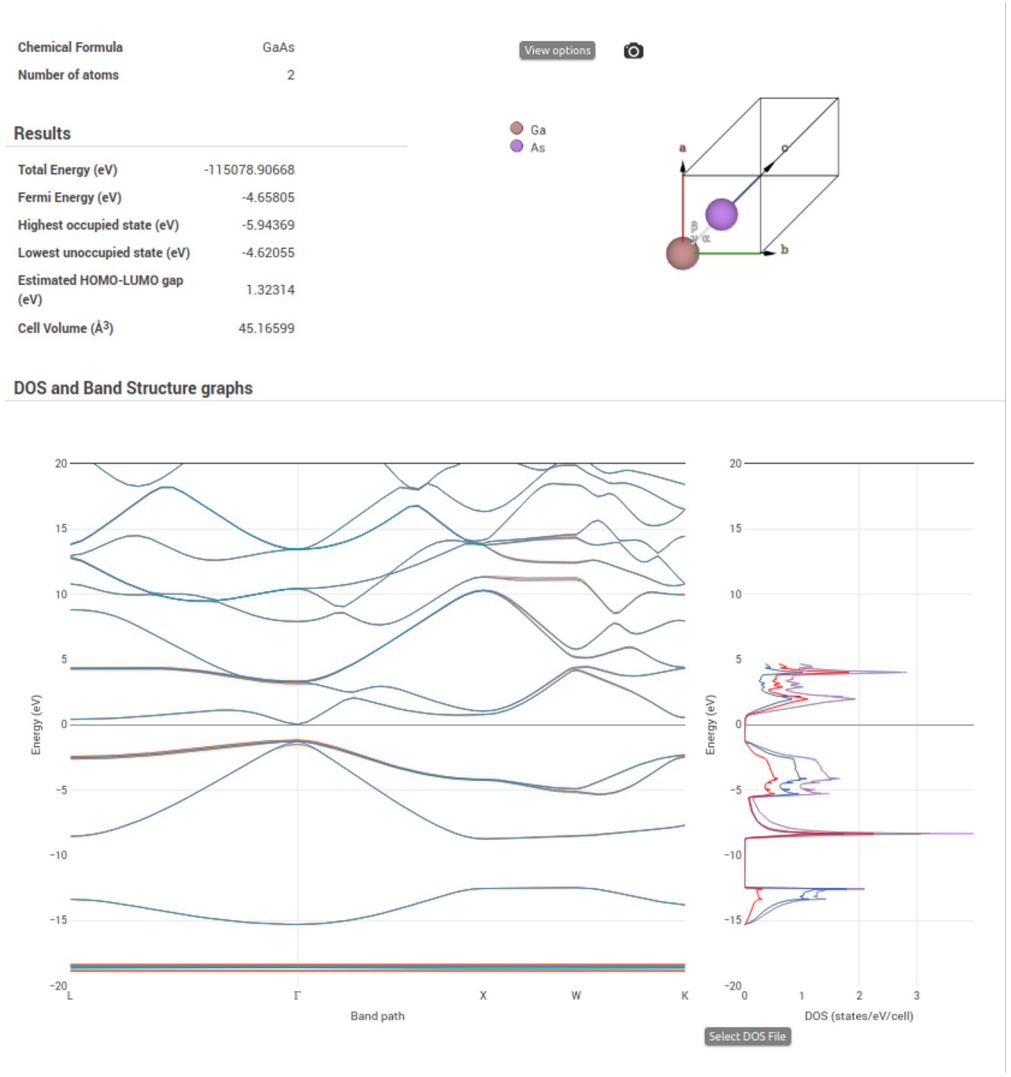
- Import structure from ASE supported formats (e.g. CIF) and export to geometry.in
- Edit / Remove lattice vectors
- Simply create supercell / primitive cell
- Create and terminate slabs in a straightforward way
- Add / remove atoms, change atomic species, constraint atomic relaxation
- Get information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

Features: Control Generator



- 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

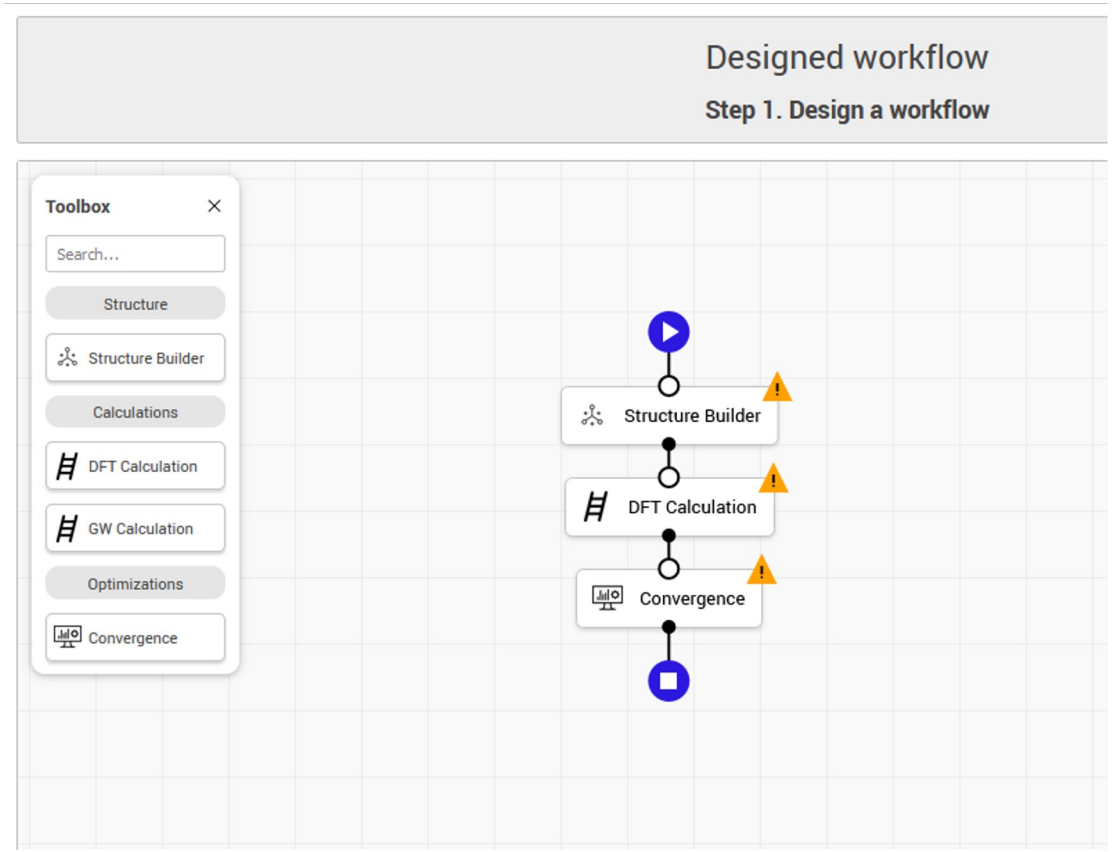


- Numerical and graphical representation of the output file
- Graphs: convergence (energy, eigenvalues, density for each ionic step; forces), band structure, DOS, dielectric function
- Graphical representation of charge analysis results
- Graceful error handling

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

FHI-aims

exciting

A longer road ahead…

- Jupyter notebook integration
- ChatGPT integration?
- *Stay tuned; feature requests are more than welcome!*