
Atomsciflow Docs

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Contents:

1	The Python interface	3
2	Indices and tables	5

The AtomSciFlow project is a workflow manager for scientific research involving atoms.

The Python interface

Using of atomsciflow in python is like:

```
>>> from atomsciflow.gamessus import Gamessus
>>> task = Gamessus()
>>> task.get_xyz("CH4.xyz")
>>> task.run("job-running")
```


Indices and tables

- `genindex`
- `modindex`
- `search`