

Relevant topics in Atomic Simulation Environment

- ASE [mainpage](#)
 - Modules relevant to our discussion
 - Atoms, db, formula, ...
 - build, geometry, atom
 - Important attributes of Atoms object
 - How to 'set' and 'get' those
 - Database formats: different back-ends
 - SQLite3 server-less database: .db files
- `$ ase db -h` ! Help about the command; available keys.

Computational Materials Repository

- CMR mainpage
 - Available databases
 - Browsing databases
 - How to filter materials

```
# Connect to database
From ase.db import connect
db = connect('c2db.db')
.....
rows = db.select('hform<0, is_magnetic=True, magstate=FM', sort='gap')
```

- Key-value pairs