Developments in the Atomic Simulation Environment

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The Atomic Simulation Environment — introduction

- Python library for working with atoms
- Use Python scripts to run calculations with many different codes
- Atoms object represents structure
- Calculator provides interface to computational code
- Algorithms can work on top of atoms and calculators: Geometry optimisation, molecular dynamics, vibration analysis, ...
- Additional tools: structure builders, read/write formats, database, GUI, command-line interface, ...

Reference: Larsen *et al.* 2017 J. Phys.: Condens. Matter 29 273002

Running ASE calculations

```
from ase.build import molecule
from ase.optimize import BFGS
from ase.calculators.siesta import Siesta

atoms = molecule('CH3CH2OH')
atoms.calc = Siesta()
opt = BFGS(atoms, trajectory='opt.traj')
opt.run(fmax=0.01)
```

- 30+ calculators available: Abinit, FHI-Aims, Quantum Espresso, GPAW, NWChem, ...
- Communication with external code takes place via files, sockets, pipes, or direct Python interface

ASE ecosystem, decentralization, and "librarization"

- AMP: Parametrize force fields using machine learning `https://pypi.org/project/amp-atomistics/`
- ASR: Atomic Simulation Recipes `https://pypi.org/project/asr/`
- atomicrex: construct interatomic potentials `https://www.atomicrex.org/`
- CLEASE: Cluster expansion code `https://pypi.org/project/clease/`
- COGEF: Analyse bond-breaking `https://pypi.org/project/ase-cogef/`
- elastic: Elastic constants `https://pypi.org/project/elastic/`
- evgraf: Crystal analysis package `https://pypi.org/project/evgraf/`
- FHI-vibes: Lattice dynamics (talk by F. Knoop) `https://pypi.org/project/fhi-vibes/`
- hiphive: High-order force constants `https://hiphive.materialsmodeling.org/`
- icet: Cluster expansion code `https://icet.materialsmodeling.org/`
- Sella: Saddle-point search `https://pypi.org/project/Sella/`

Band structures in ASE

- New(-ish) functionality to determine Bravais lattices, band paths
- Simple objects for representing band paths and band structures
- Related: On-going work on DOS, Vibrations (Adam Jackson)
- Follows AFlow conventions

W. Setyawan, S. Curtarolo.
Comp Mater Sci, Volume 49, Issue 2, August 2010, 299–312

Band structures

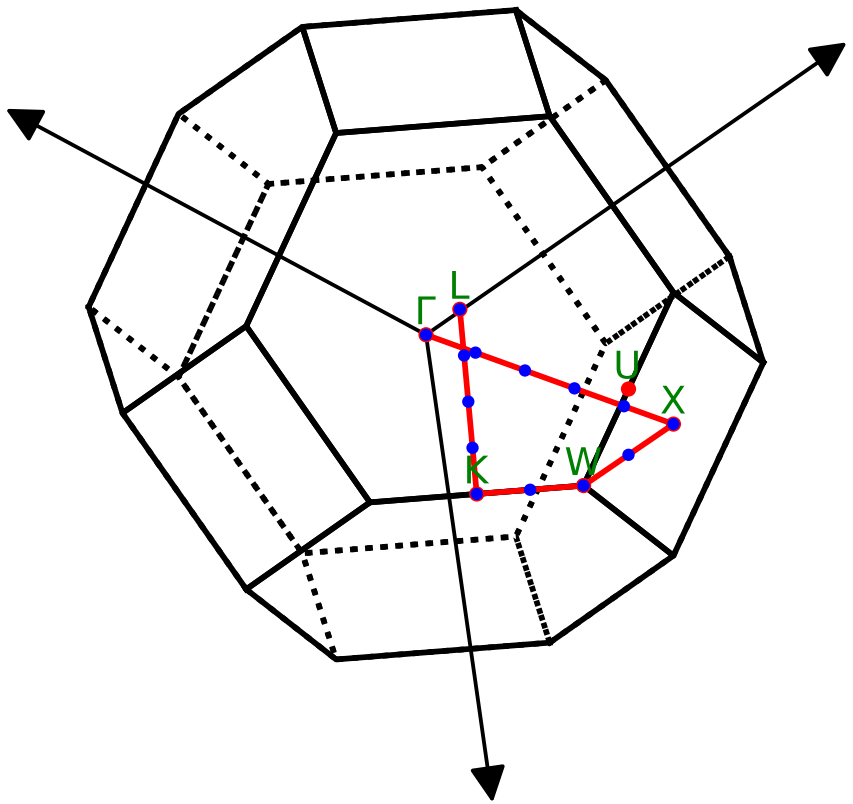
```
>>> print(atoms.cell.get_bravais_lattice().description())
FCC(a=5.43)
  Variant name: FCC
  Special point names: GKLUWX
  Default path: GXWKGLUWLK,UX

  Special point coordinates:
    G    0.0000   0.0000   0.0000
    K    0.3750   0.3750   0.7500
    L    0.5000   0.5000   0.5000
    U    0.6250   0.2500   0.6250
    W    0.5000   0.2500   0.7500
    X    0.5000   0.0000   0.5000

>>> print(atoms.cell.bandpath('GXWKL'))
BandPath(path='GXWKL', cell=[3x3], special_points={GKLUWX},
>>> bs = calculate_band_structure(atoms, path)
>>> bs.write('bs.json')
```

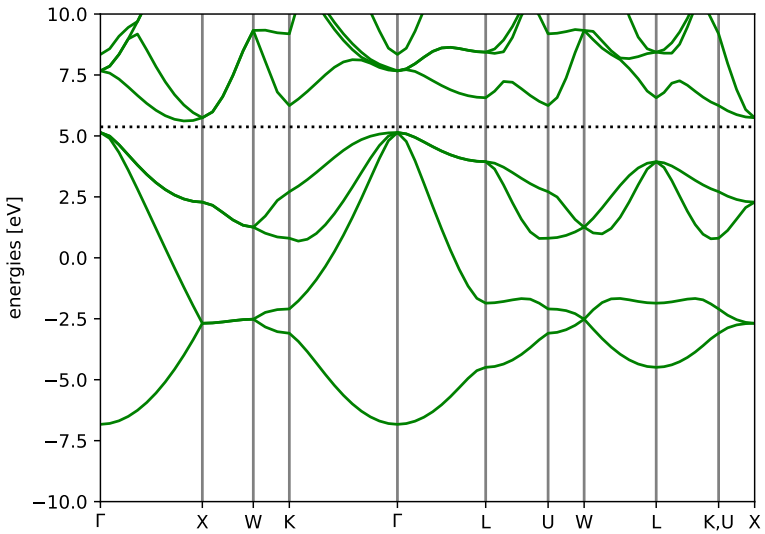
Plotting band paths

- `>>> bandpath.plot(show=True)`
- JSON storage: `bandpath.write('bandpath.json')`
- `$ ase reciprocal bandpath.json`



Band-structure plotting and I/O

- `>>> bs.plot(show=True)`
- `>>> bs.write('bandstructure.json')`
- `$ ase band-structure bandstructure.json`



A `BandStructure` object consists of a `BandPath`, an array of energies, and a reference energy.

On Bravais lattice recognition

- How do we recognize this lattice to propose a band path?

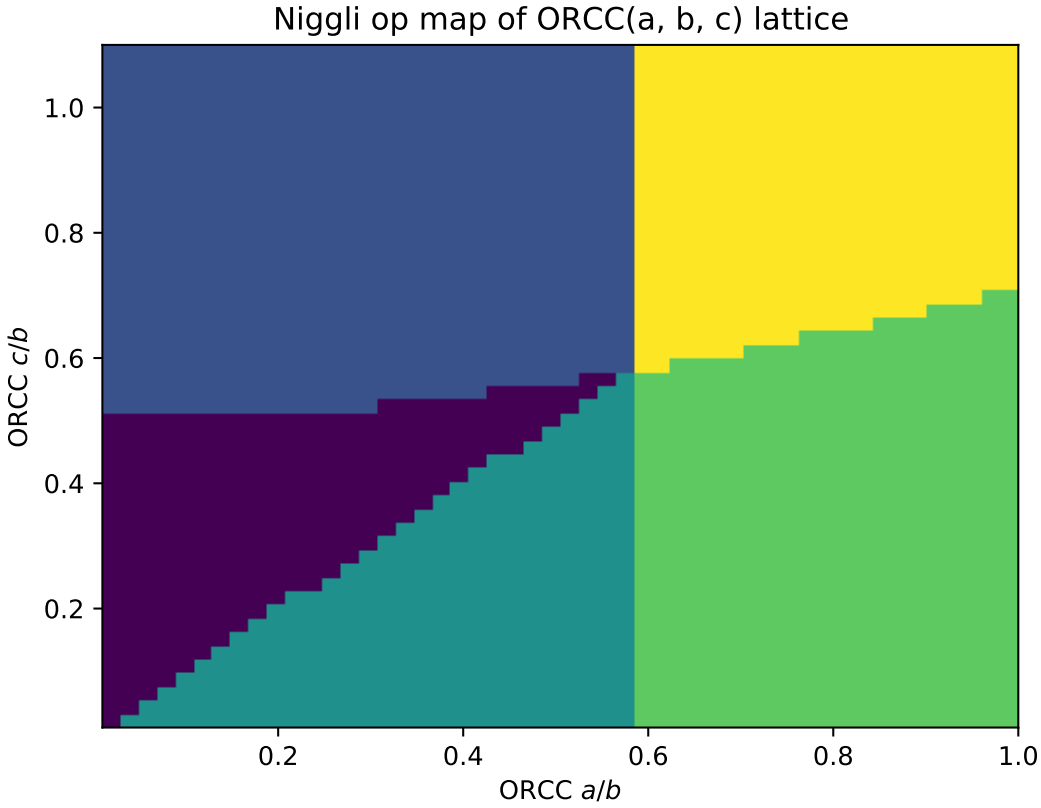
$$\begin{aligned} \mathrm{a}_1 &= (4.4, 0, 0) \\ \mathrm{a}_2 &= (-3.27, 2.96, 0) \\ \mathrm{a}_3 &= (-0.57, -1.48, 4.11) \end{aligned}$$

- Equivalent lattice in normalized form — body-centred tetragonal (BCT):

$$\begin{aligned} \mathrm{a}_1 &= (-a, a, c)/2 \\ \mathrm{a}_2 &= (a, -a, c)/2 \\ \mathrm{a}_3 &= (a, a, -c)/2 \end{aligned}$$

- Both these lattices reduce to the same unique Niggli form.

- Different Niggli-reduced forms of all ORCC(a, b, c) lattices.



- Each colour is an equivalence class of lattices that Niggli-reduce in the same way
- Any ORCC lattice (whether in standard form or not) reduces to a Niggli cell represented by one of these colours

Brute-force Bravais lattice determination

- Tabulate Niggli-reduction operations of all normalized-form lattices
- Niggli-reduce the unknown input lattice
- Check which inverse Niggli-operation recuperates normalized form
- Create band path in normalized form
- Transform band path k-points back to original cell

Conclusion

- Many projects in ASE ecosystem (new and old)
- Work to decentralize codebase, “librarization”
- Focus on workflows and representations of band paths, band structures, DOS, vibrational spectra, ...
- Thanks to Simune Atomistics S.L. for support