The Atomic Simulation Environment (ASE) for quantum chemical calculations

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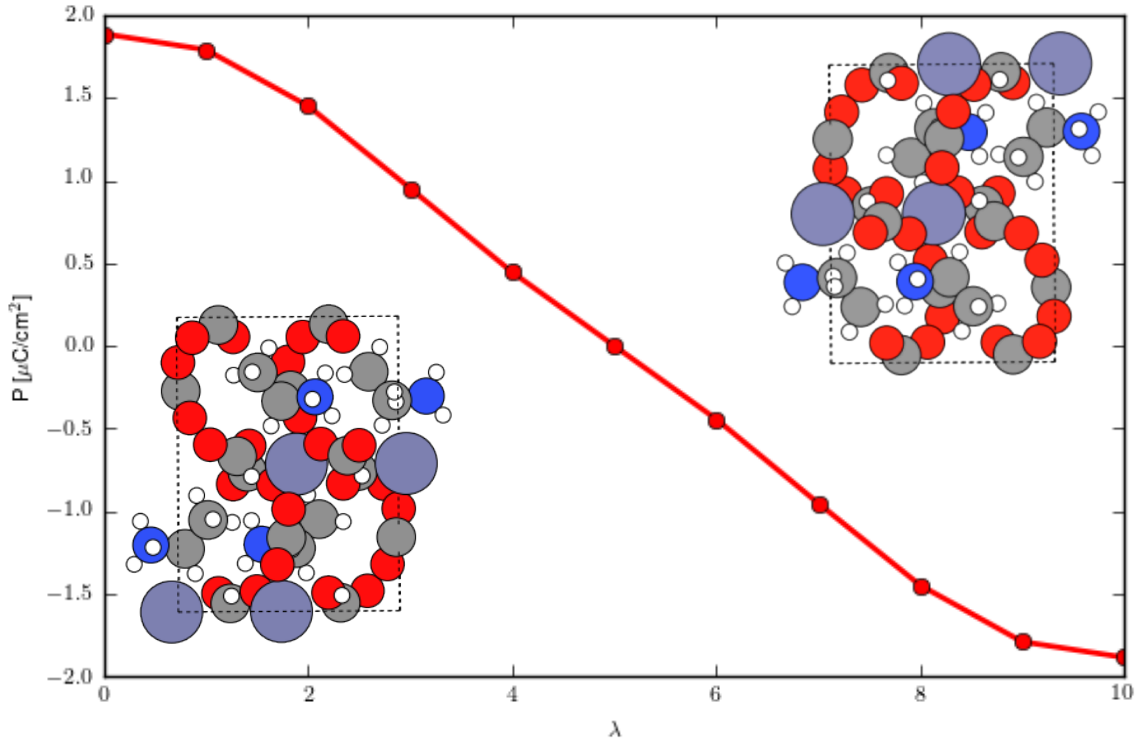
A little about research

- The examples in this talk are taken from my own research – mostly related to ferroelectric hybrid materials.



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What is ASE?

- The Atomic Simulation Environment (ASE) is a python-based package for:
  - Setting up structures
  - Steering calculations
  - Analysing output

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What is ASE?

- Developed at the Danish Technical University in Copenhagen, which also develops the Grid-based Projector Augmented Wave (GPAW) software for DFT-calculations, however the code can be used with other DFT packages as well.
- The code is open-source and developed by the users

Input and output file formats

format	description	capabilities
abinit	ABINIT input file	RW
aims	FHI-aims geometry file	RW
aims-output	FHI-aims output	R+
bundletrajectory	ASE bundle trajectory	RW
castep-castep	CASTEP output file	R+
castep-cell	CASTEP geom file	RW
castep-geom	CASTEP trajectory file	R+
castep-md	CASTEP molecular dynamics file	R+
castep-phonon	CASTEP phonon file	R
cfg	AtomEye configuration	RW
cif	CIF-file	RW+
cmdft	CMDFT-file	R
cube	CUBE file	RW
dacapo	Dacapo netCDF output file	R
dacapo-text	Dacapo text output	R
db	ASE SQLite database file	RW+
dftb	DftbPlus input file	RW
elk	ELK atoms definition	R
eon	EON reactant.con file	RW
eps	Encapsulated Postscript	W
espresso-in	Quantum espresso in file	R
espresso-out	Quantum espresso out file	R
etsf	ETSF format	RW
exciting	exciting input	RW
extxyz	Extended XYZ file	RW+
findsym	FINDSYM-format	W+
gaussian	Gaussian com (input) file	RW
gaussian-out	Gaussian output file	R
gen	DFTBPlus GEN format	RW
gpaw-out	GPAW text output	R+
gpw	GPAW restart-file	R
gromacs	Gromacs coordinates	RW
gromos	Gromos96 geometry file	RW
html	X3DOM HTML	W
iwm	?	R
json	ASE JSON database file	RW+
jsv	JSV file format	RW
lammps-dump	LAMMPS dump file	R
mol	MDL Molfile	R
nwchem	NWChem input file	RW
octopus	Octopus input file	R
pdb	Protein Data Bank	RW+
png	Portable Network Graphics	W
postgresql	ASE PostgreSQL database file	RW+
pov	Persistance of Vision	W
py	Python file	W+
res	SHELX format	RW
sdf	SDF format	R
struct	WIEN2k structure file	RW
struct-out	SIESTA STRUCT file	R
traj	ASE trajectory	RW+
trj	Old ASE pickle trajectory	RW+
turbomole	TURBOMOLE coord file	RW
turbomole-gradient	TURBOMOLE gradient file	R+
v-sim	V_Sim ascii file	RW
vasp	VASP POSCAR/CONTCAR file	RW
vasp-out	VASP OUTCAR file	R+
vasp-xdatcar	VASP XDATCAR file	R+
vasp-xml	VASP vasprun.xml file	R+
vti	VTK XML Image Data	W
vtu	VTK XML Unstructured Grid	W
x3d	X3D	W
xsd	Materials Studio file	R
xsf	XCrySDen Structure File	RW+
xyz	XYZ-file	RW+

Example 1:
Convert one format to another

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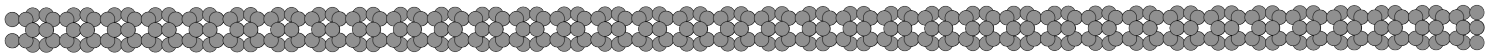
Visualising structures



- Not always easy to install, but very powerful!

- Examples:
- Visualising MD simulation
  - This just looks nice! But be careful with large files…
- View structure relaxation
  - If something is wrong, this will often give you an idea where to look.
- Compare energies of a set of structures
  - Nice graphical way to compare energies and geometries simultaneously

Setting up structures

- Spacegroup package
- Surface package
- Python scripts for structure generation

- Example – making a path for a Berry Phase calculation
  - The aim here is to make a continuous path between the structure with Ps and –Ps with sensible geometries.

Running calculations

- Run your favorite calculator through ASE
- Genetic algorithm
- Nudged Elastic band
- Rich choice of constraints – or make your own!
  - Constraints
    - The FixAtoms class
    - The FixBondLength class
    - The FixBondLengths class
    - The FixedLine class
    - The FixedPlane class
    - The FixedMode class
    - The Hookean class
    - The FixInternals class
    - Combining constraints
    - Making your own constraint class
    - The Filter class
    - The UnitCellFilter class
    - The StrainFilter class

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Analysing output

- Python scripts for structure analysis
- Database
- Minimum image convention

- Example – Are structure 1 and structure 2 different?
  - In this case we calculate and sort all inter-atomic distances for structure 1 and 2 and, and compare the two arrays.

Useful resources

- The ase homepage contains installation guides, documentaion and tutorials: https://wiki.fysik.dtu.dk/ase/index.html
- Mailing lists for users and developers: https://wiki.fysik.dtu.dk/ase/mailinglists.html
- Talk and some of the examples can be found at: https://github.com/WMD-group/ASE-Tutorials
- Reference: *An object-oriented scripting interface to a legacy electronic structure code*, S. R. Bahn and K. W. Jacobsen, Comput. Sci. Eng., Vol. **4**, 56-66, 2002