Atomic Simulation Environment - a Python library

Modern Tools for Spectroscopy on Advanced Materials
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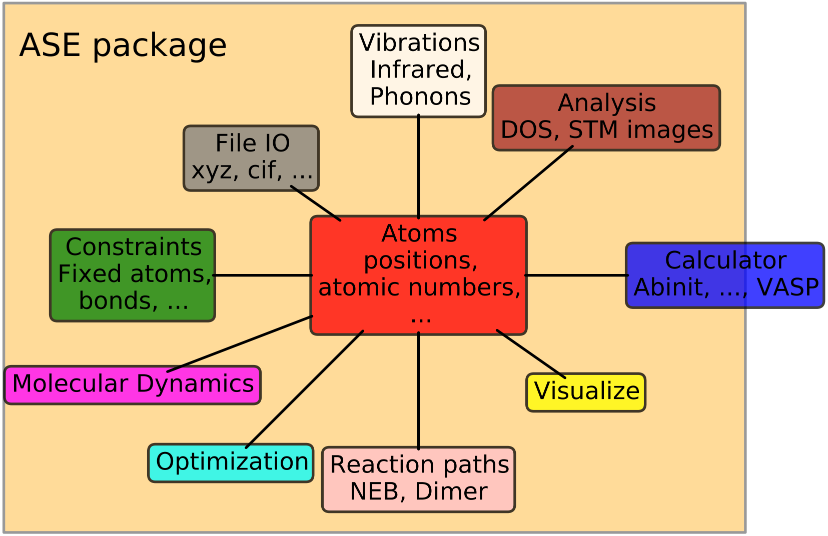
- Overview of ASE
- The Python language
- The `Atoms` object
- Building stuff (molecules, surfaces, ...)
- Doing stuff with atoms (MD, optimization, ...)
- Databases
- Installing ASE
- Development of ASE

What is ASE?

ASE is a Python library for working with atoms:


ASE package
Vibrations Infrared, Phonons
Analysis DOS, STM images
File IO xyz, cif, ...
Atoms positions, atomic numbers, ...
Constraints Fixed atoms, bonds, ...
Calculator Abinit, ..., VASP
Molecular Dynamics
Visualize
Optimization
Reaction paths NEB, Dimer

`http://wiki.fysik.dtu.dk/ase`

A recipe for your atoms

```python
from ase import Atoms
from ase.optimize import BFGS
from ase.calculators.nwchem import NWChem
from ase.io import write
h2 = Atoms('H2',
           positions=[(0, 0, 0),
                      (0, 0, 0.7)])
h2.calc = NWChem(xc='PBE')
opt = BFGS(h2)
opt.run(fmax=0.02)
write('H2.xyz', h2)
```

Units: eV and Å.

An interactive recipe for your atoms

```
>>> from ase import Atoms
>>> from ase.optimize import BFGS
>>> from ase.calculators.nwchem import NWChem
>>> from ase.io import write
>>> h2 = Atoms('H2',
               positions=[(0, 0, 0),
                          (0, 0, 0.7)])
>>> h2.calc = NWChem(xc='PBE')
>>> opt = BFGS(h2)
>>> opt.run(fmax=0.02)
BFGS:   0  19:10:49    -31.435229     2.2691
BFGS:   1  19:10:50    -31.490773     0.3740
BFGS:   2  19:10:50    -31.492791     0.0630
BFGS:   3  19:10:51    -31.492848     0.0023
>>> write('H2.xyz', h2)
>>> h2.get_potential_energy()
-31.492847800329216
```

What is Python?

`http://www.python.org`

- Interpreted language
- Dynamically typed
- Easy to read and write, and very expressive
- Great for scripting a calculation
- Great for small and large programs
- Optimized for programmer productivity
- Can be extended in C/C++/Fortran
- General purpose language

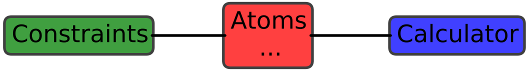
Numpy:	Base N-dimensional array package
Scipy:	Fundamental library for scientific computing
Matplotlib:	Comprehensive 2D Plotting
Sympy:	Symbolic mathematics.

Structure of ASE

- Python modules and sub-modules: `constraint`, `data`, `db`, `dft`, `dimer`, `ga`, `infrared`, `io`, `md`, `neb`, `optimize`, `phonons`, `structure`, `thermochemistry`, `transport`, `units`, `vibrations` and `visualize`.
- Command-line tools:

ase-gui:	Graphical user interface
ase-db:	Manipulate ASE-database
ase-build:	Build molecules or crystals
ase-run:	Run simple calculation

The Atoms object



What's inside?

- Positions, atomic numbers, velocities, masses, initial magnetic moments, charges, tags
- Unit cell
- Boundary conditions
- (Calculator)
- (Constraints)

Methods and attributes of the Atoms object

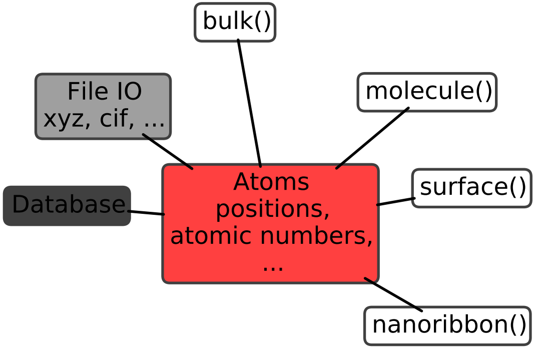
List methods:

```
a.pop()  # remove last atom
a.append('Xe')  # append xenon atom
a.extend(Atoms('H2'))  # append 2 hydrogens
a[1]  # second atom
del a[-3:]  # delete three last atoms
```

Other methods: `repeat()`, `translate()`, `center()`, `rotate()`, `get_distance()`, `get_angle()`, `get_moments of_inertia()`, ...
Special attributes: `positions`, `numbers`, `cell`, `pbc` (Numpy n-d arrays)

```
x1, x2 = a.positions[-2:, 0]  # x-coords of
                              # last two atoms
a.positions[-2:, 0] += 0.1  # translate atoms
a.positions[:, 2].max()  # maximum z-coord
```

Building the Atoms object



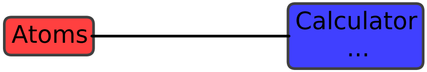
Building the Atoms object ...

```
from ase import Atoms
h2 = Atoms('H2', [(0, 0, 0), (0, 0, 0.74)])
from ase.structure import molecule
water = molecule('H2O')
from ase.lattice import bulk
si2 = bulk('Si')
from ase.lattice.spacegroup import crystal
rutile = crystal(['Ti', 'O'],
                 basis=[(0, 0, 0), (u, u, 0)],
                 spacegroup=136,
                 cellpar=[a, a, c,
                          90, 90, 90])
from ase.lattice.surface import fcc110
slab = fcc110('Pt', (2, 1, 7), a=4.0,
              vacuum=6.0)
from ase.lattice.surface import add_adsorbate
add_adsorbate(slab, 'H', site='hollow')
```

Building the Atoms object, continued ...

```python
from ase.lattice.surface import surface
nasty_cut = surface(rutile, (1, 1, 0),
                    layers=5)
from ase.io import read
q = read('quarts.cif')
import ase.db
con = ase.db.con('mystuff.db')
atoms = con.get_atoms(foo='bar', H=0)
# same as this:
atoms = read('mystuff.db@foo=bar,H=0')
```

ASE's calculators



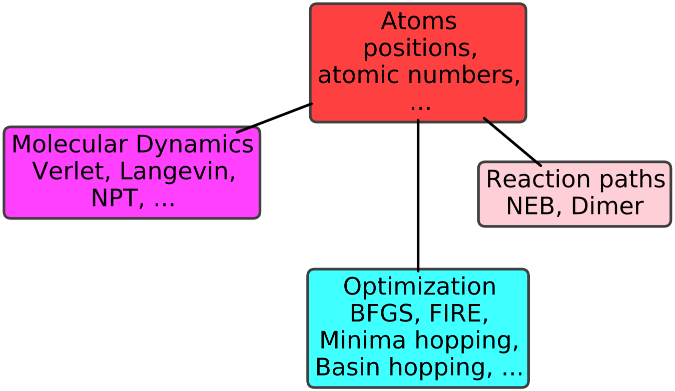
DFT, *ab initio*:

Abinit, Castep, ELK, Exciting, FHI-Aims, Fleur, Gaussian, GPAW, Jacapo, JDFTx, NWChem, QuantumEspresso, SIESTA, Turbomole, VASP

(Semi-)empirical potentials:

ASAP, DFTB+, EAM, EMT, Gromacs, Hotbit, LAMMPS, Lennard-Jones, MOPAC, Morse

Optimization, MD and minimum energy paths



ASE-database

In each row we have:

Taxonomy:

- `Atoms` object (positions, atomic numbers, ...)
- ID, user-name, creation and modified time
- Constraints
- Calculator name and parameters
- Energy, Forces, Stress tensor, dipole moment, magnetic moments

Folksonomy:

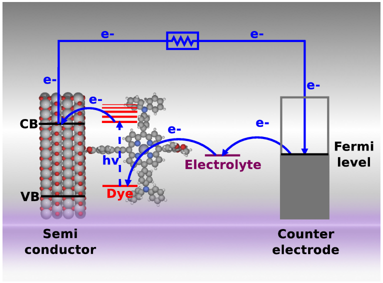
- Key-value pairs
- Keywords

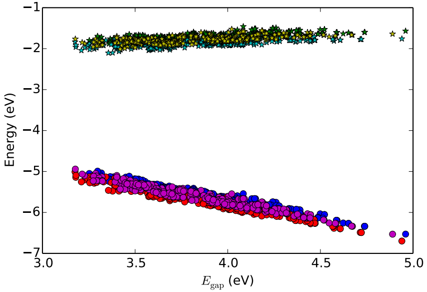
Additional stuff:

- extra data (band structure, ...)

Back-ends: JSON, SQLite3 and PostgreSQL.

Dye sensitized solar cells





[1]Kristian B. Ørnsø, Christian S. Pedersen, Juan M. Garca-Lastra and Kristian S. Thygesen *Optimizing porphyrins for dye sensitized solar cells using large-scale ab initio calculations* Phys. Chem. Chem. Phys., 2014, 16, 16246-16254

A figure from Ørnsø *et al.* (almost)

```
import matplotlib.pyplot as plt
import ase.db
con = ase.db.connect('dssc.db')
for M in ['Zn', 'TiO', 'H2']:
    gap = []
    homo = []
    lumo = []
    for dct in con.select(metal=M,
                          anchor='EthynPhA'):
        gap.append(dct.E_gap)
        homo.append(dct.E_HOMO)
        lumo.append(dct.E_LUMO)
    plt.plot(gap, homo, 'o')
    plt.plot(gap, lumo, '*')
plt.ylabel(r'Energy (eV)')
plt.xlabel(r'$E_{\mathrm{gap}}$ (eV)')
plt.savefig('homolumo.svg')
```

Three types of calculators

1)
   a) ASE writes input file
   b) ASE starts Fortran/C/C++ code (maybe in parallel)
   c) ASE waits for Fortran/C/C++ code to finish
   d) ASE reads output file
2) Same as above, except that the Fortran code doesn't stop - it waits for a new input file with new coordinates (QuantumEspresso, Dacapo).
3) Python solution (EMT, EAM, ...). For parallel calculations, the Python interpreter runs on all processes (GPAW, ASAP)

Installing ASE

Requirements: Python and NumPy (`ase-gui`: PyGTK and Matplotlib)

```
$ SVN=https://svn.fysik.dtu.dk/projects
$ svn co $SVN/ase/trunk ase
$ cd ase
$ python setup.py install --user
$ python setup.py test  # takes 1 min.
```

Where is what?

`ase/`:

Source code.

`tools/`:

Command-line tools

`ase/doc/`:

Documentation (source for web-page)

Questions

How to get started?

- *`http://wiki.fysik.dtu.dk/ase`*
- *`http://docs.scipy.org/doc/numpy`*
- *`http://www.python.org`*

How to get help?

Write to the `ase-users` mailing list.

How is ASE developed?

Mostly by volunteers. Coordination and discussions on the `ase-developers` mailing list.

How to contribute?

Please send us bug-reports, patches, code and ideas.

License?

LGPLv2.1+

Thanks

Andrew Peterson, Anthony Goodrow, Ask Hjorth Larsen, Carsten Rostgaard, Christian Glinsvad, David Landis, Elvar Örn Jónsson, Eric Hermes, Felix Hanke, Gaël Donval, George Tritsaris, Glen Jenness, Heine Anton Hansen, Ivano Eligio Castelli, Jakob Blomquist, Jakob Schiøtz, Janne Blomqvist, Janosch Michael Rauba, Jens Jørgen Mortensen, Jesper Friis, Jesper Kleis, Jess Wellendorff Pedersen, Jingzhe Chen, John Kitchin, Jon Bergmann Maronsson, Jonas Bjork, Jussi Enkovaara, Karsten Wedel Jacobsen, Kristen Kaasbjerg, Kristian Baruel Ørnsø, Lars Grabow, Lars Pastewka, Lasse Vilhelmsen, Marcin Dulak, Marco Vanin, Markus Kaukonen, Mattias Slabanja, Michael Walter, Mikkel Strange, Poul Georg Moses, Rolf Würdemann, Steen Lysgaard, Stephan Schenk, Tao Jiang, Thomas Olsen, Tristan Maxson, Troels Kofoed Jacobsen, ...

Extra material

How to use `sys.argv`, other ASE functions, for-loops and string interpolation:

```python
import sys
from ase.lattice.surface import fcc111
from gpaw import GPAW, PW
a = float(sys.argv[1])
k = int(sys.argv[2])
for n in range(1, 5):
    slab = fcc111('Cu', size=(1, 1, n),
                  a=a, vacuum=5.0)
    slab.calc = GPAW(mode=PW(ecut=400),
                     kpts=(k, k, 1),
                     txt='Cu%d.txt' % n)
    slab.get_potential_energy()
```