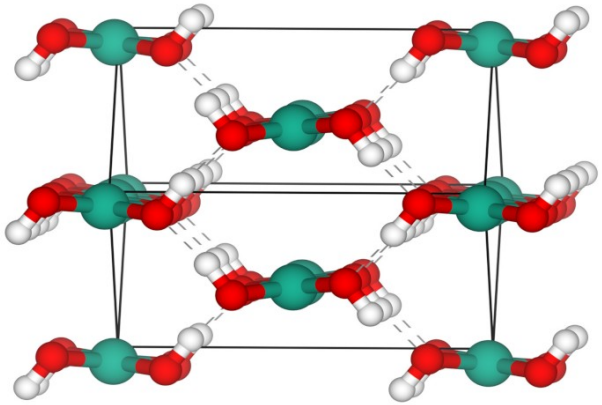
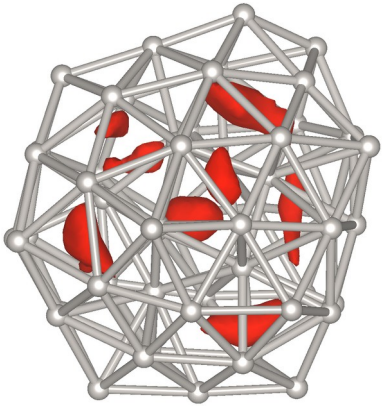
Global crystal structure optimization with ASE

(and with a little help from DFTB)





Maxime Van den Bossche

Overview

1. Functionality for crystal structure prediction (`ase.ga`)

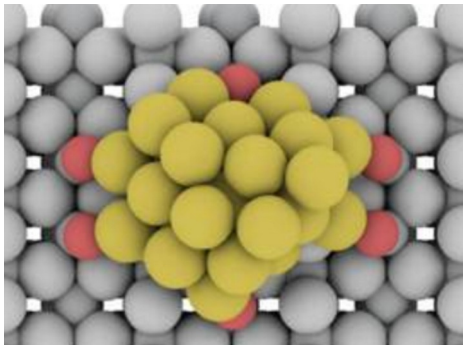
2. Calculators: DFTB+ and QuantumEspresso

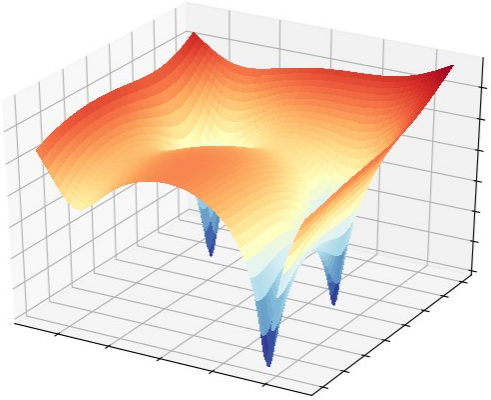
3. Miscellaneous

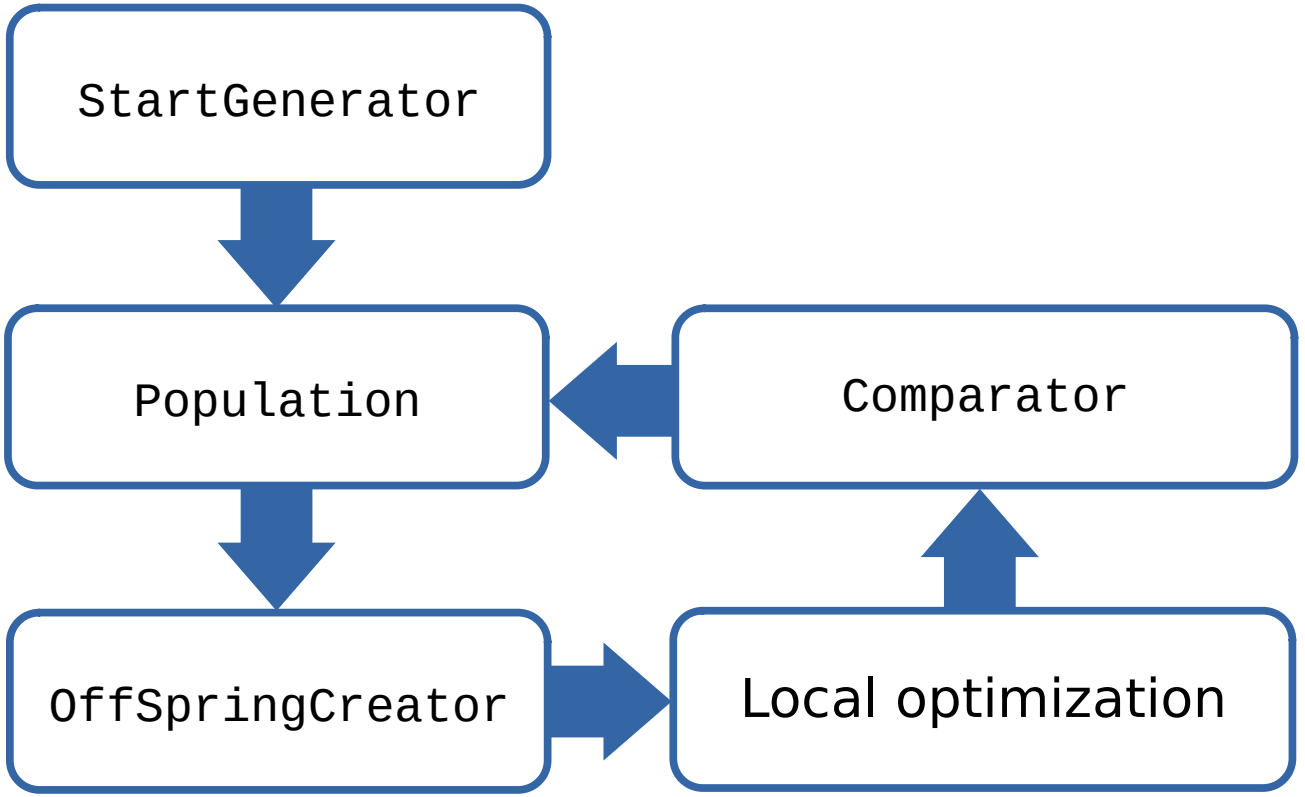
4. Wrap-up

ASE-GA crystal structure prediction

Genetic algorithm workflow with `ase.ga`:

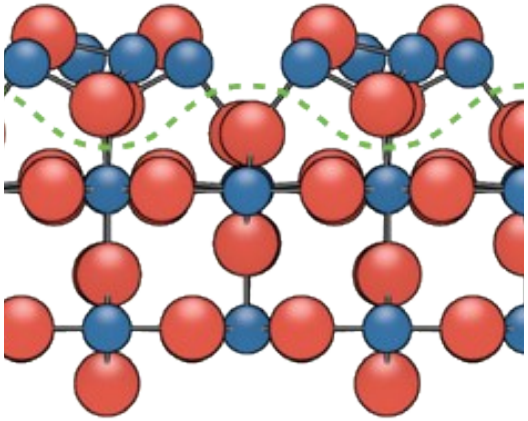






ASE-GA crystal structure prediction

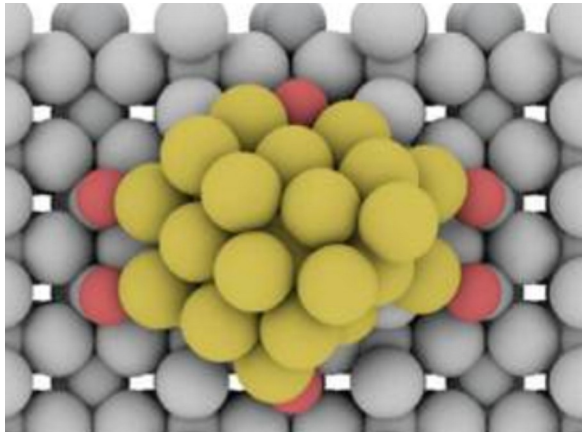
$SnO_2(110)$-(4x1)



Merte et al.,

PRL 119 (2017)

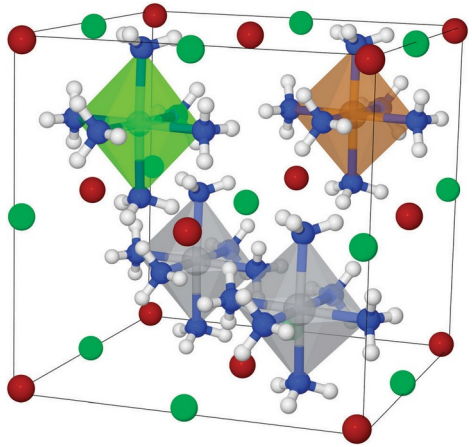
Au/TiO_2



Vilhelmsen, Hammer,

ACS Catal. (2014)

$M_aX_b(NH_3)_c$



Jensen et al.,

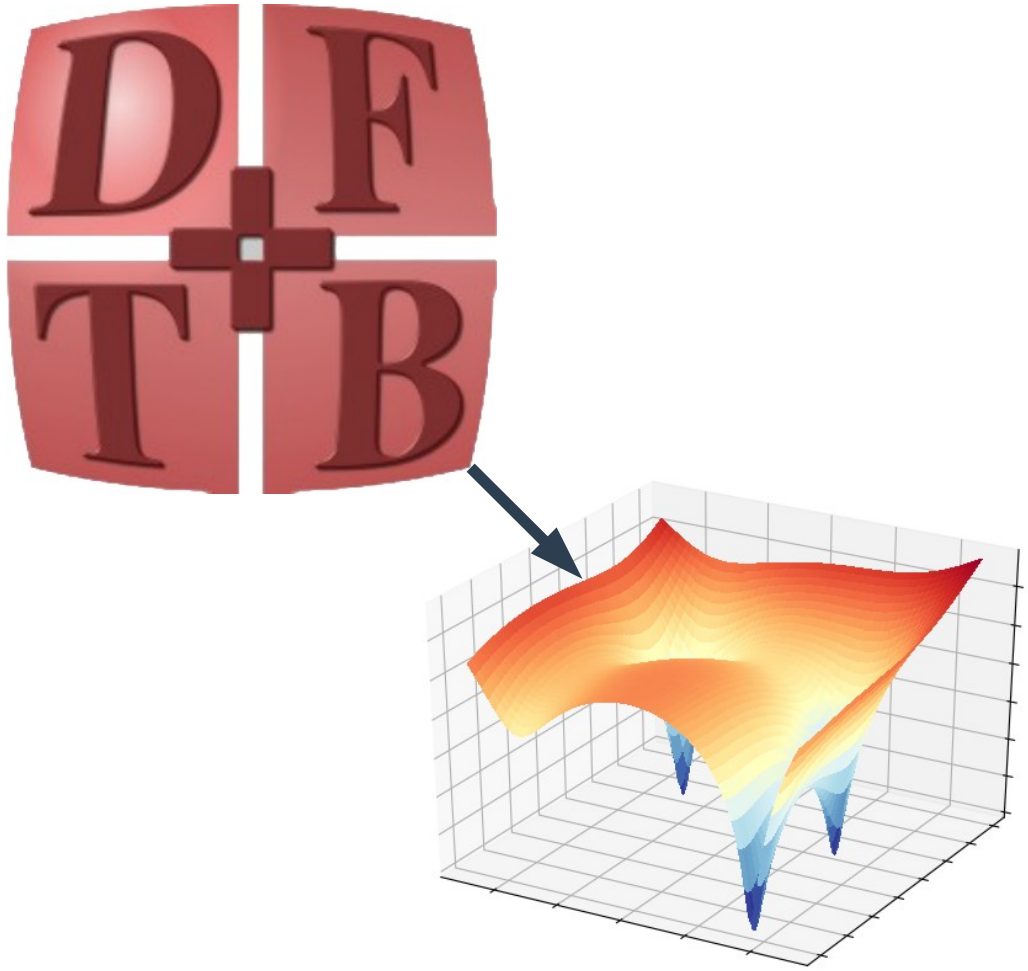
PCCP (2014)

Previous implementation = without ‘global’ cell vector optimization

ASE-GA crystal structure prediction

Motivation:

Development of
- **T**ight-binding
- **A**pproximation
- e**N**hanced
- **G**lobal
- **O**ptimization



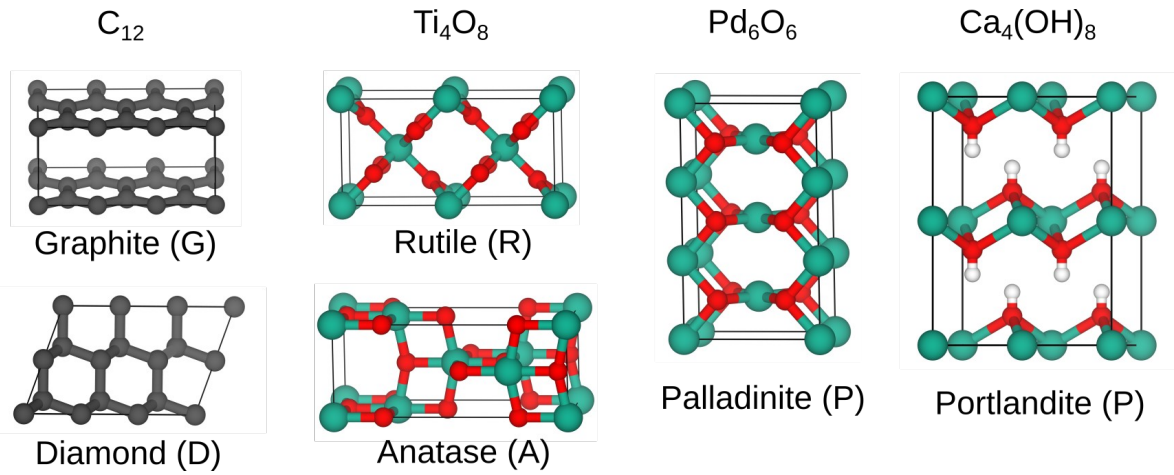
[MVdB, Grönbeck, Hammer, *JCTC* 14 (2018)]

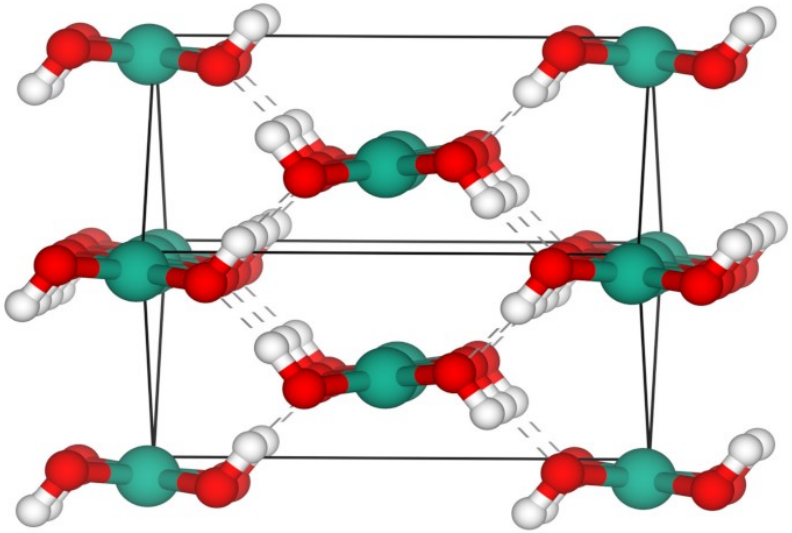
[www.dftbplus.org]

ASE-GA crystal structure prediction

Motivation:

Development of
Tight-binding
Approximation
e**N**hanced
Global
Optimization



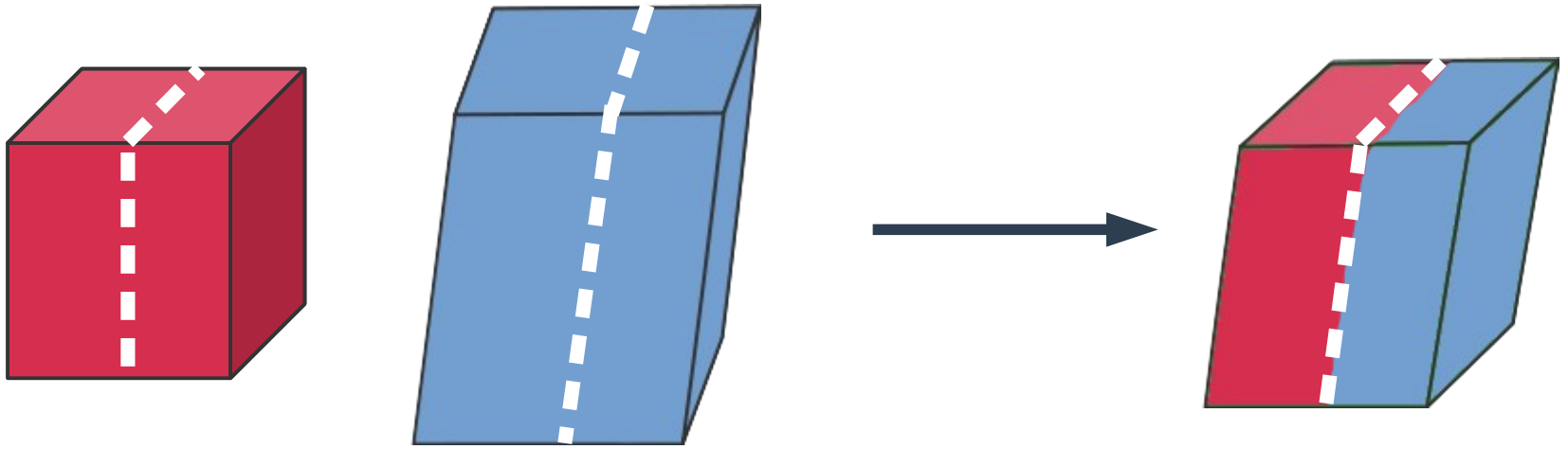


$Pd(OH)_2$

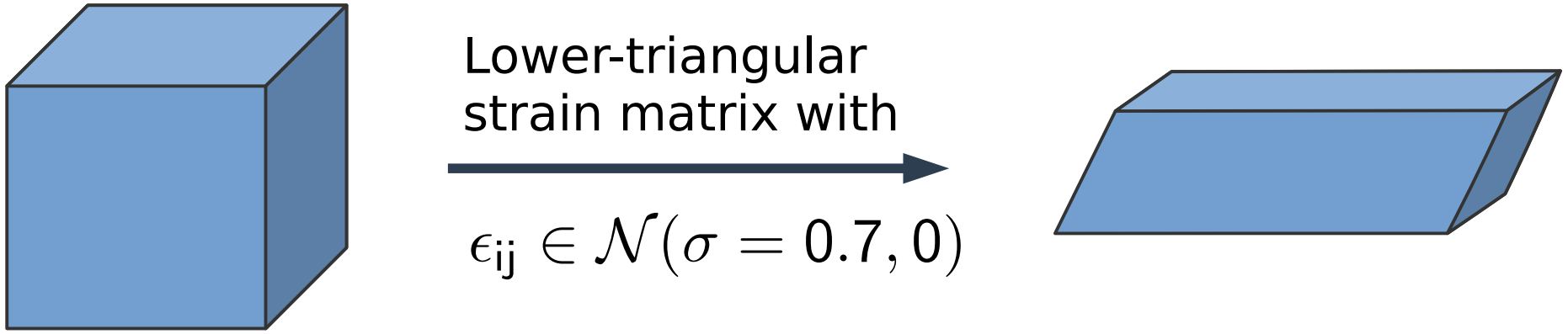
[MVdB, Grönbeck, Hammer, *JCTC* 14 (2018)]

ASE-GA crystal structure prediction

* “*cut-and-splice*” crossover:



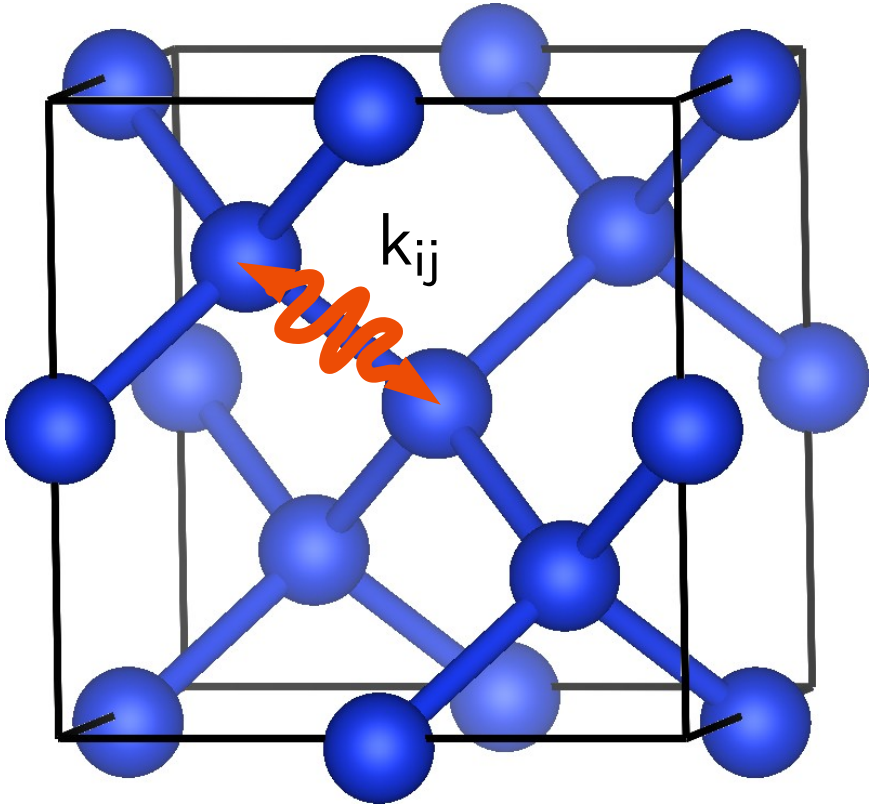
* “*strain*” mutation:



[Glass et al.. *Comp. Phys. Comm.* 175 (2006), Lonie et al., *Comp. Phys. Comm.* 182 (2011)]

ASE-GA crystal structure prediction

* *"soft"* mutation:



Displacement along softest non-zero vibrational mode

Model hessian inspired by bond valence method

[Oganov and Valle, *J. Chem. Phys.* 130 (2009)] [Lyakhov and Oganov, *PRB* 84 (2011)]

ASE-GA crystal structure prediction

GA-operator-related code in `ase.ga`:

```
cutandsplicepairing.py
element_crossovers.py
element_mutations.py
particle_comparator.py
particle_crossovers.py
particle_mutations.py
slab_operators.py
standard_comparators.py
standardmutations.py
startgenerator.py
utilities.py
```

New:

```
bulk_crossovers.py
bulk_mutations.py
bulk_startgenerator.py
bulk_utilities.py
ofp_comparator.py
```

Future work (I):

Generalization
⇒ less redundancy
⇒ also 1D and 2D-vc-opt

ASE-GA crystal structure prediction

GA-operator-related code in `ase.ga`:

```
cutandsplicepairing.py
element_crossovers.py
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```
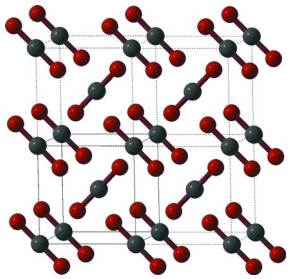

New:

```
bulk_crossovers.py
bulk_mutations.py
bulk_startgenerator.py
bulk_utilities.py
ofp_comparator.py
```

Future work (II):

Tutorial for global optimization of molecular crystals



[Zhu et al., *Acta Cryst. B* 64 (2012)]

Overview

1. Functionality for crystal structure prediction (`ase.ga`)

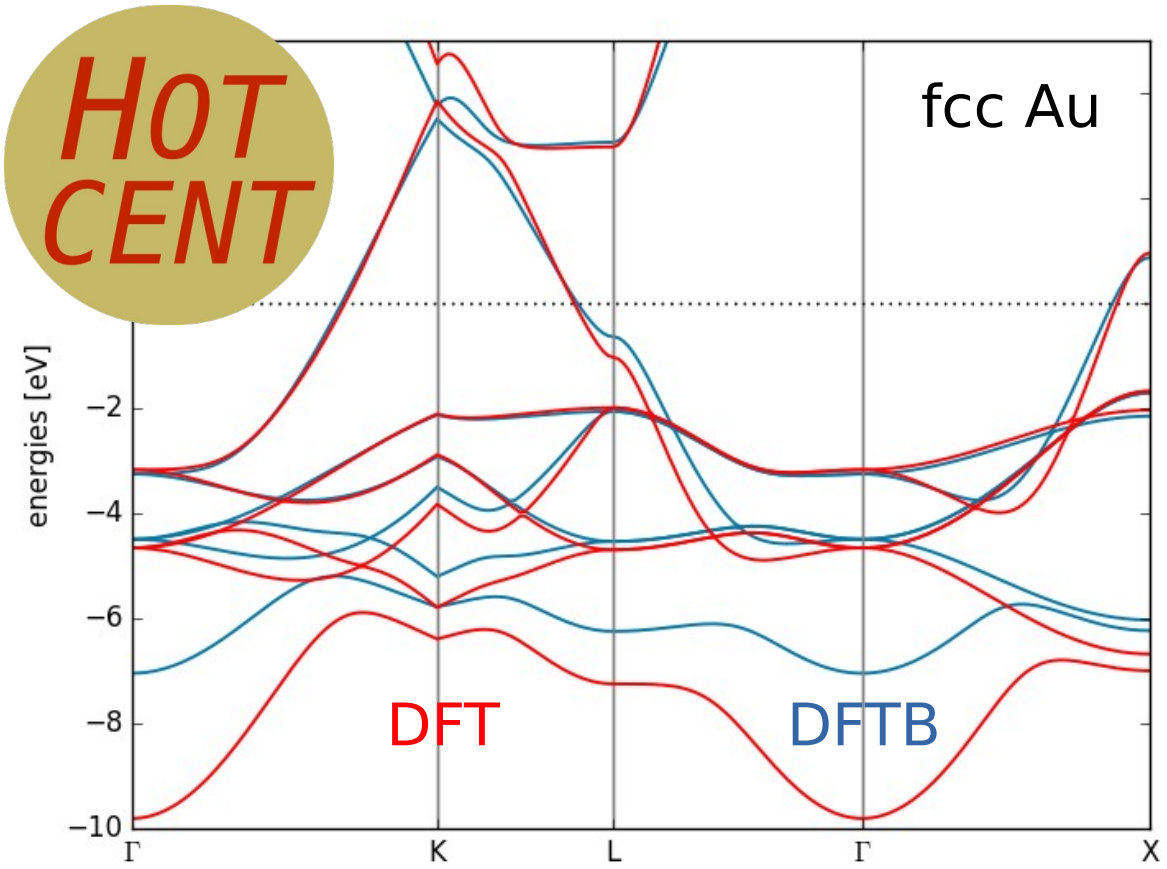
2. Calculators: DFTB+ and QuantumEspresso

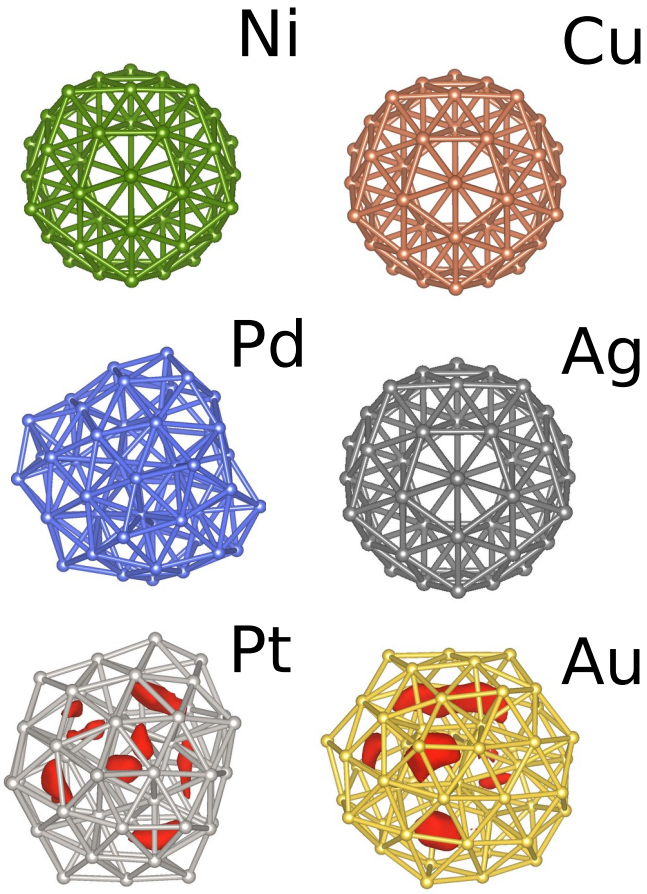
3. Miscellaneous

4. Wrap-up

Calculators: DFTB+ and QuantumEspresso

Motivation: calculating and plotting the band structure
e.g. for tight-binding parameter optimization





[MVdB, *J. Phys. Chem. A* 123 (2019)]

Calculators: DFTB+ and QuantumEspresso

Changes in both calculators:

1. “Advanced” k-point input

2. Parsing the eigenvalues, Fermi energy

   & irreducible BZ k-points

Calculators: DFTB+ and QuantumEspresso

```
calc = Espresso/DftbPlus(...)
atoms.set_calculator(calc)
atoms.get_potential_energy()
efermi = calc.get_fermi_level()

<change settings for non-self-consistent run>
calc.set(kpts={‘path’:’GKLGX’, npoints=100})
calc.calculate(atoms)

bs = calc.band_structure()
bs.reference = fermi_energy
bs.plot()
```

Calculators: DFTB+ and QuantumEspresso

Future work:

→ More extensive and easy-to-run test suite

→ Deal with changes in newest DFTB+ release (19.2)

(Fermi energy, eigenvalues, … no longer in `results.tag`)

Overview

1. Functionality for crystal structure prediction (`ase.ga`)

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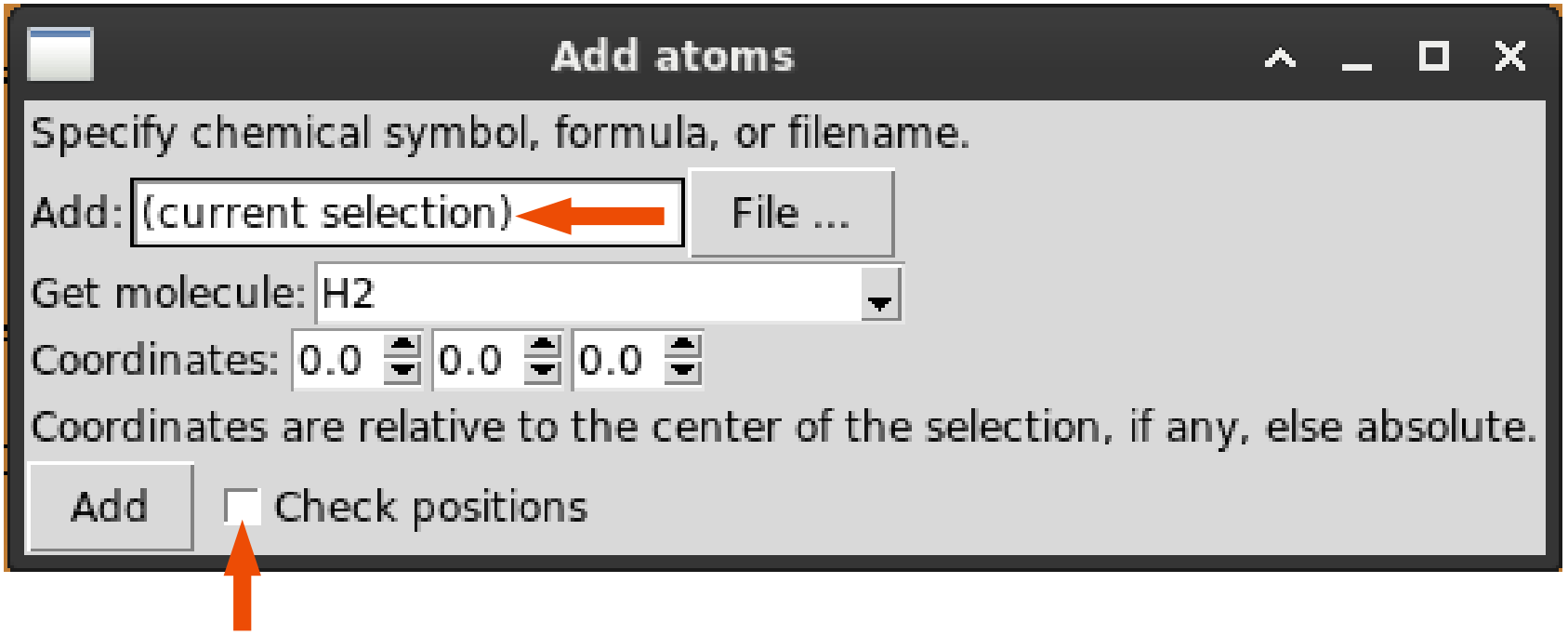
Miscellaneous

Copy-pasting back in the GUI



Miscellaneous

Tutorial

DFTB with ASE:
From Zero to Hero

Friday at 9:00

FT4011

Overview

1. Functionality for crystal structure prediction (`ase.ga`)
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Conclusions

1. Functionality for crystal structure prediction (`ase.ga`)

2. Calculators: DFTB+ and QuantumEspresso

gitlab.com/mvdb

Acknowledgements

CHALMERS UNIVERSITY OF TECHNOLOGY

Henrik Grönbeck

Paul Erhart

DTU

Steen Lysgaard

Bjørk Hammer group

AARHUS UNIVERSITY

SIMUNE

Ask Hjorth Larsen