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koopmans

an open-source package for accurately and efficiently predicting spectral properties with Koopmans functionals

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Summary

`koopmans` contains everything you need to run a Koopmans functional calculation without expert knowledge, including implementations of Koopmans functionals in QUANTUM ESPRESSO as well as automated workflows.

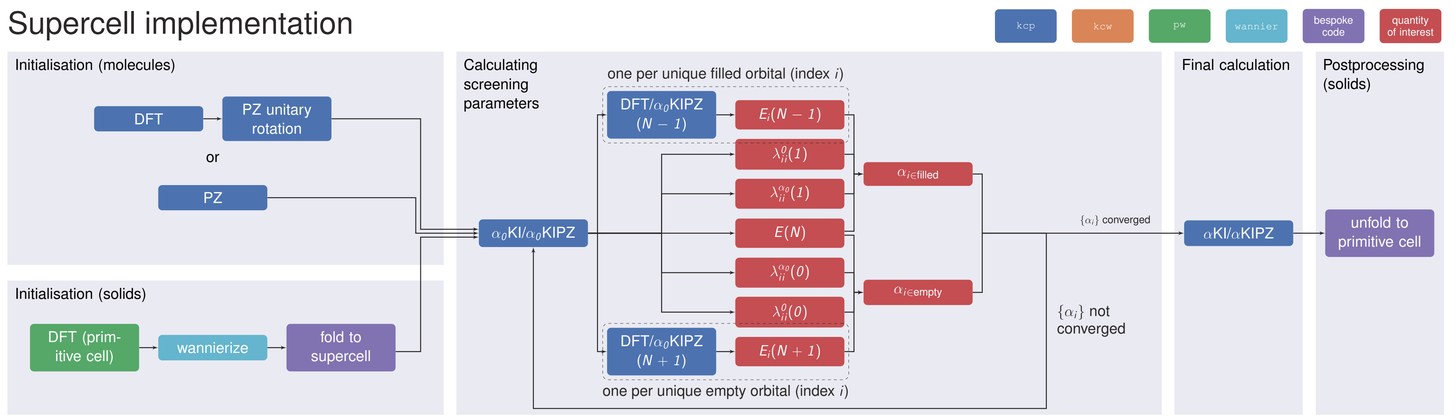
1. What are Koopmans functionals?

Koopmans functionals are a class of functionals that aim to reproduce spectral properties (charged excitations) and total energies on the same footing, enforcing a generalised piecewise linearity condition:

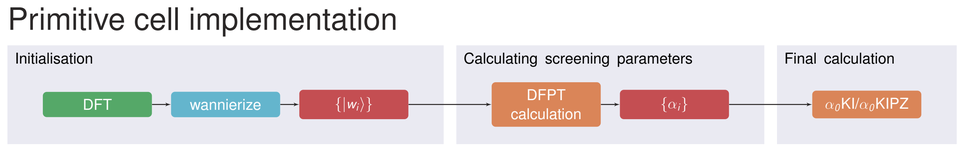
$$E_{\text{Koopmans}} = E_{\text{DFT}} + \sum_i \alpha_i \Big[\underbrace{-\left(E_{\text{DFT}} - E_{\text{DFT}}|_{f_i=0}\right)}_{\text{removes the erroneous curvature}} \underbrace{+f_i\eta_i}_{\text{restores the correct linearity}} \Big]$$

2. Workflows

Supercell implementation



Primitive cell implementation

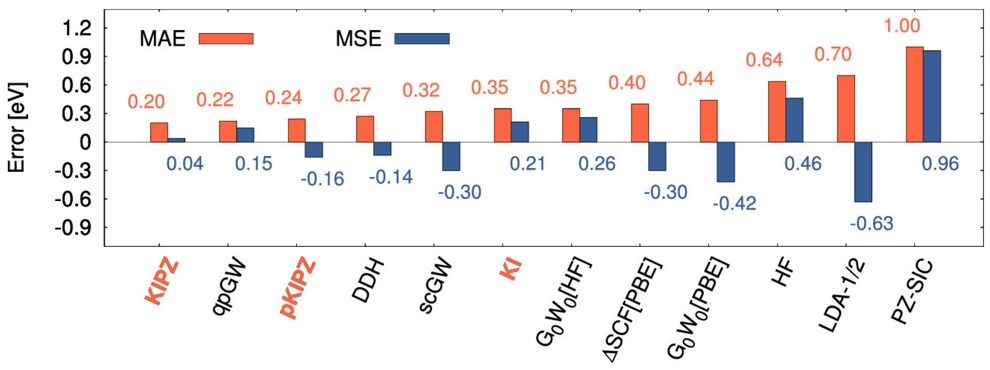


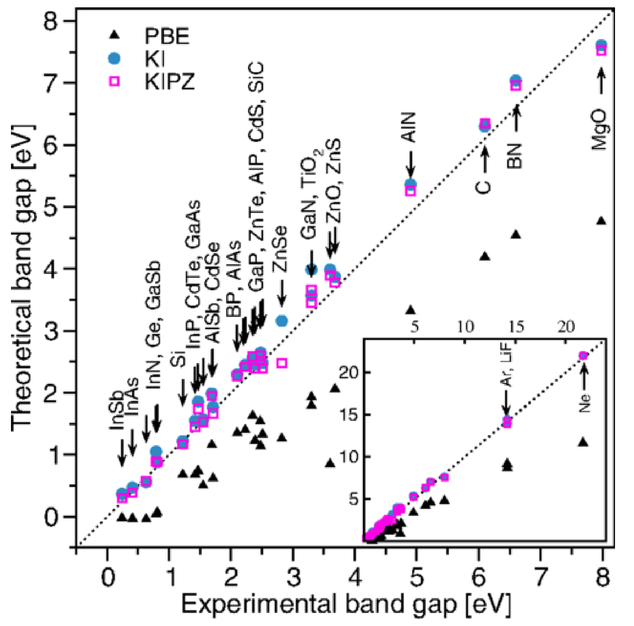
3. Example results

Koopmans functionals give band structures and orbital energies as accurate as state-of-the-art GW, at a fraction of the computational cost.

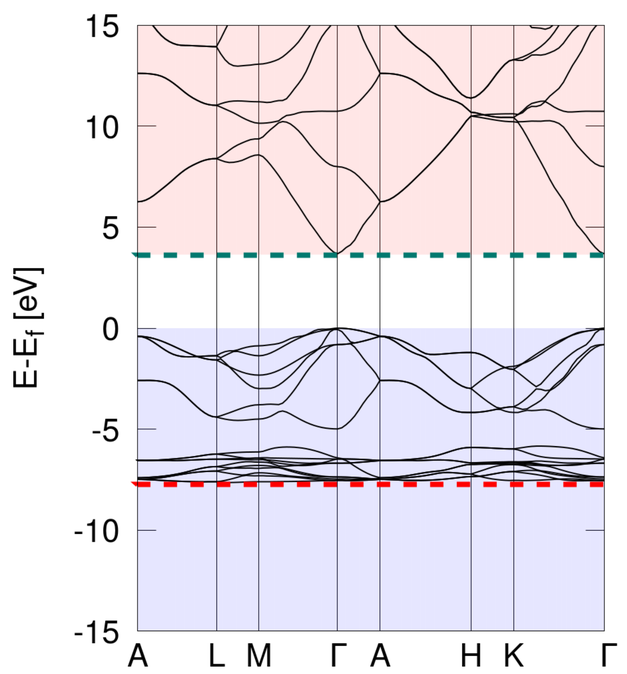
Semiconductors and insulators (right) Band gap and ionisation potential of semiconductors and insulators compared to experiment Nguyen *et al.* 2018

Molecules (below) The KI, pKIPZ, and KIPZ Koopmans functionals give ionization potentials comparable to qpGW across the GW100 dataset Colonna *et al.* 2019





		PBE	G_0W_0	KI	KIPZ	QSGŴ
E_{gap}	MAE (eV)	2.54	0.56	0.27	0.22	0.18
	MAPE (%)	48.28	12.10	7.09	5.37	4.46
IP	MAE (eV)	1.09	0.39	0.19	0.21	0.49
	MAPE (%)	15.58	5.71	2.99	3.14	7.41



The KI band structure of ZnO compared to the experimental band gap and *d*-band position Colonna *et al.* 2022

4. What does running `koopmans` look like?

Koopmans takes a single `JSON` file as input e.g. for bulk silicon

```
{
  "workflow": {
    "functional": "ki",
    "base_functional": "lda",
    "method": "dscf",
    "init_orbitals": "mlwfs",
    "pseudo_library": "pseudo_dojo_standard"
  },
  "atoms": {
    "cell_parameters": {
      "periodic": true,
      "ibrav": 2,
      "celldms": {"1": 10.2622}
    },
    "atomic_positions": {
      "units": "crystal",
      "positions": [["Si", 0.00, 0.00, 0.00],
                    ["Si", 0.25, 0.25, 0.25]]
    }
  },
  "kpoints": {"grid": [4, 4, 4], "path": "LGXKG"},
  "calculator_parameters": {
    "pw": {"system": {"nbnd": 20}},
    "w90": {"auto_projections": true}
  }
}
```

Running from the command line looks like this:

```
$ koopmans si.json
  _
 | | _____   ___   _ __   _ __ ___    __ _ _ __  ___
 | |/ / _ \ / _ \ | '_ \ | '_ ` _ \  / _` | '_ \/ __|
 |   < (_) | (_) || |_) || | | | | || (_| | | | \__ \
 |_|\_\___/ \___/ | .__/ |_| |_| |_| \__,_|_| |_|___/
                  |_|

 Koopmans spectral functional calculations with Quantum ESPRESSO

 Written by Edward Linscott, Riccardo De Gennaro, and Nicola
↪  Colonna

  Initialisation of density and variational orbitals
  ==================================================

   Wannierisation
   ==============
    Running wannier/scf... done
    Running wannier/nscf... done
    Running wannier/occ_emp/wann_preproc... done

...

Workflow complete
```

or run with `python`:

```
from ase.build import bulk
from koopmans.kpoints import Kpoints
from koopmans.workflows import SinglepointWorkflow

# Use ASE to create bulk silicon
atoms = bulk('Si')

# Create the workflow
workflow = SinglepointWorkflow(atoms=atoms,
        parameters={'pseudo_library': 'pseudo_dojo_standard', 'base_functional': 'lda', 'init_orbitals': 'mlwfs'}
        kpoints = Kpoints(grid=[4, 4, 4], path='LGXKG', cell=atoms.cell),
        calculator_parameters = {'pw': {'nbnd': 20}, 'w90': {'auto_projections': True}}

# Run the workflow
workflow.run()
```

References, affiliations, and acknowledgements

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... go to `koopmans-functionals.org` to find out more!