



British Society for
Ecological Modelling
and Enviroinfo

Making Koopmans functionals accessible

10

Outline



koopmans

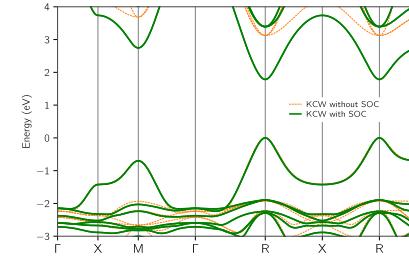
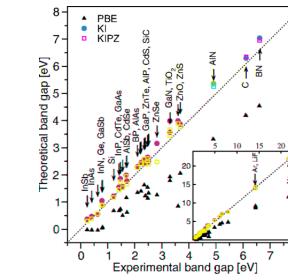
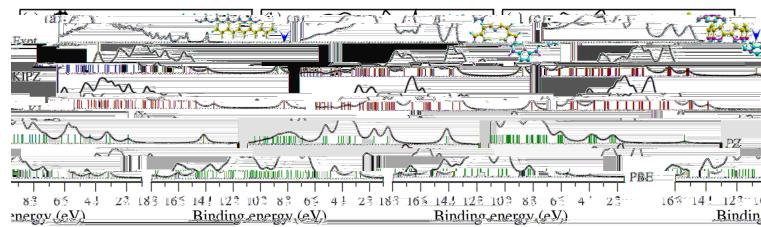
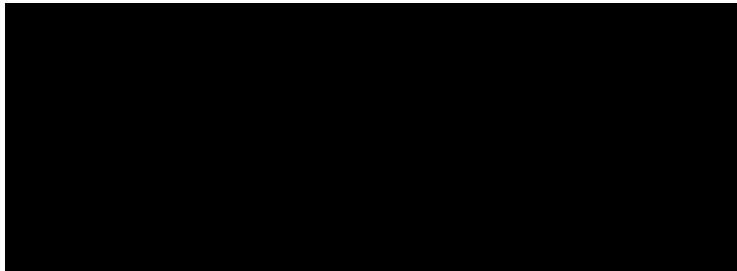
koopmans

- ▶
- ▶
- ▶

AiiDA

Koopmans functionals

A powerful tool for computational spectroscopy



15,

8,

114,

Koopmans functional theory



$$K^I[\{ \cdot \}] = DFT[\cdot] + \left\{ \begin{array}{l} - (DFT[\cdot] - [\cdot \quad 0]) + (DFT[\cdot^1] - DFT[\cdot^0]) \\ \{ \quad \text{remove non-linear dependence} \quad \text{restore linear dependence} \end{array} \right\}$$

Koopmans functional theory

$$K^I[\cdot, \{\cdot\}] = DFT[\cdot]$$

$$+ \begin{cases} - (DFT[\cdot] - [\cdot - 0]) \\ \{ \} \end{cases}$$

Koopmans functional theory



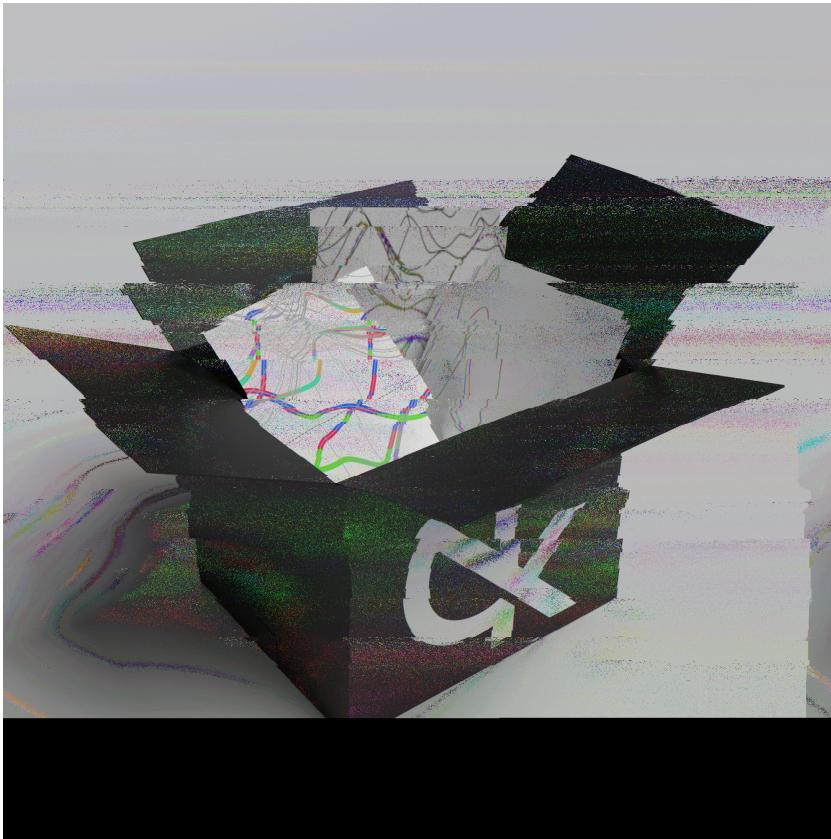
$$K^I[\{ \cdot \}] = DFT[\cdot] + \left\{ \begin{array}{l} - (DFT[\cdot] - [\cdot \quad 0]) + (DFT[\cdot^1] - DFT[\cdot \quad 0]) \\ \{ \quad \text{remove non-linear dependence} \quad \text{restore linear dependence} \end{array} \right\}$$

Koopmans

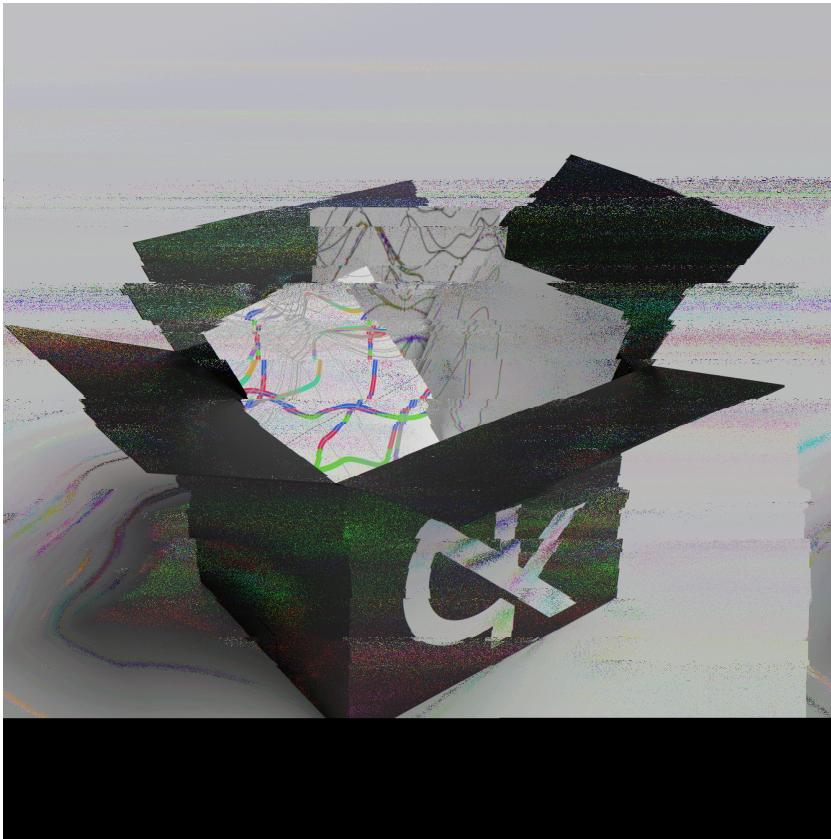
koopmans

koopmans-functionals.org

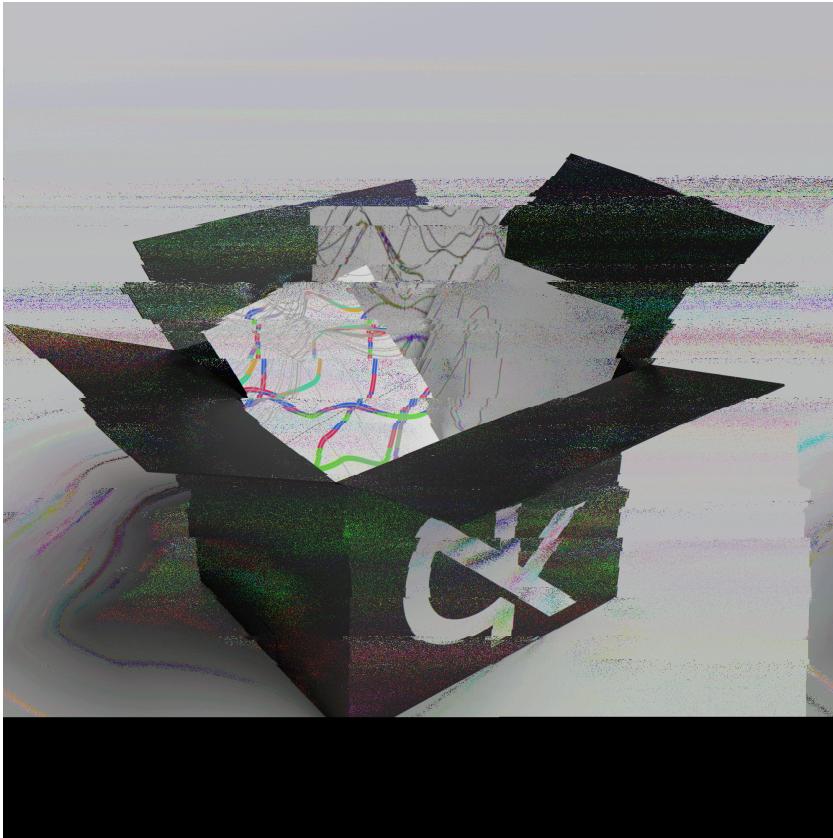
Making Koopmans functionals accessible



Making Koopmans functionals accessible



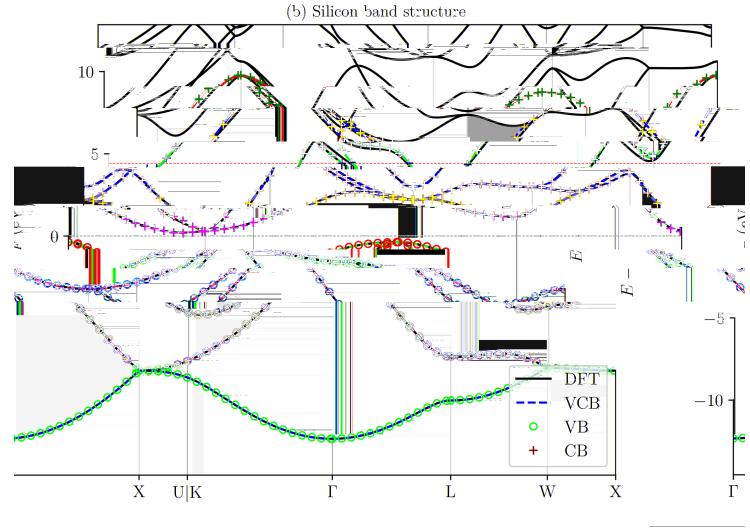
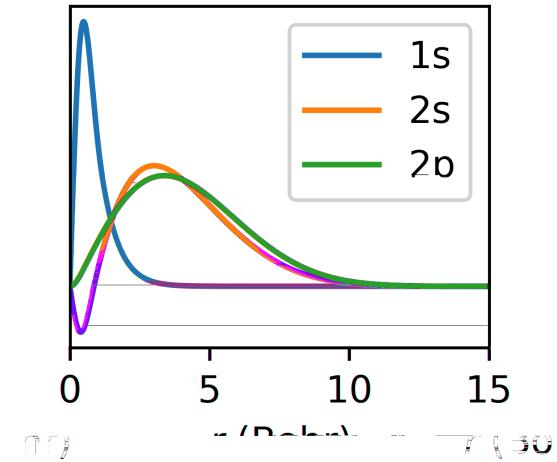
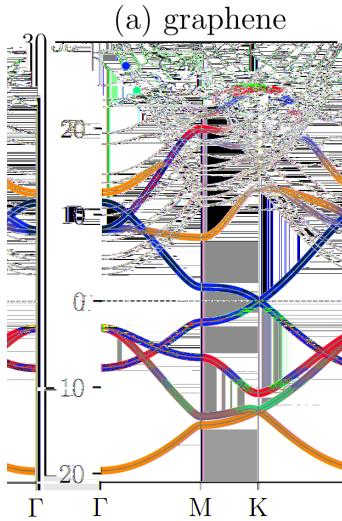
Making Koopmans functionals accessible



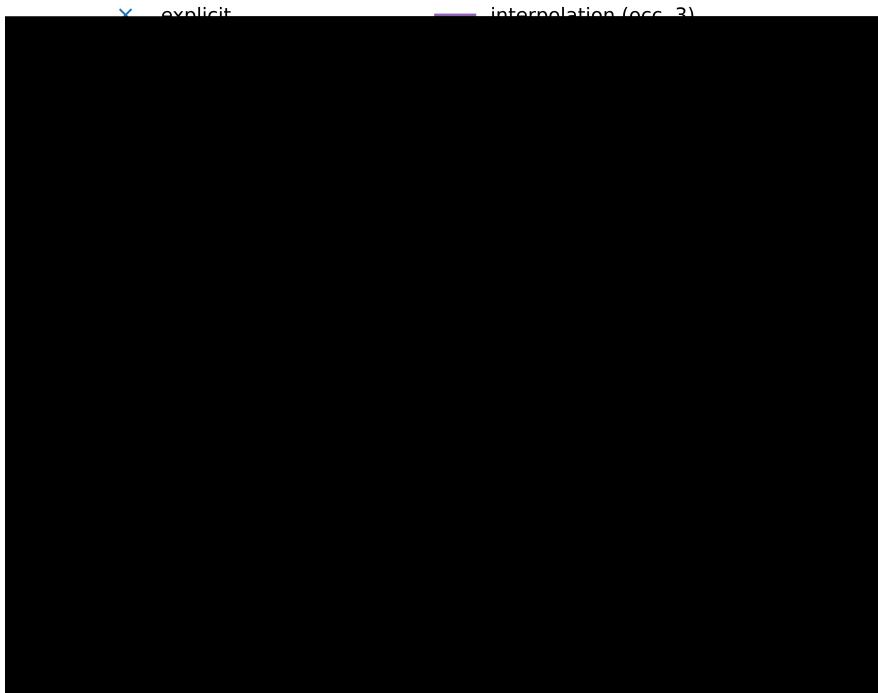
AiiDA

Automated Wannierisation

The three pillars of automated Wannierisation

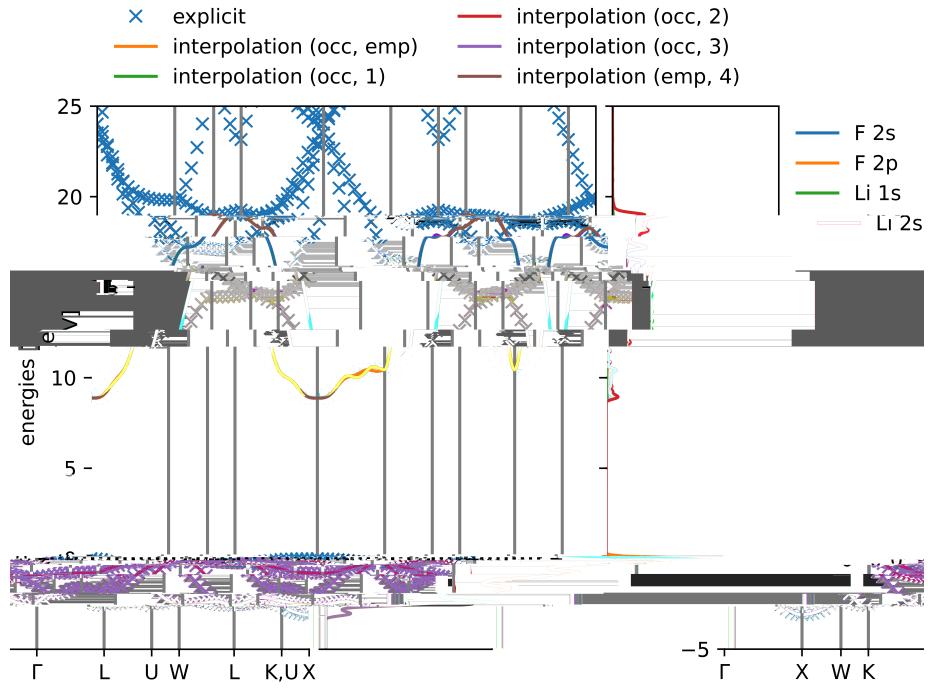


Example 1: TiO₂

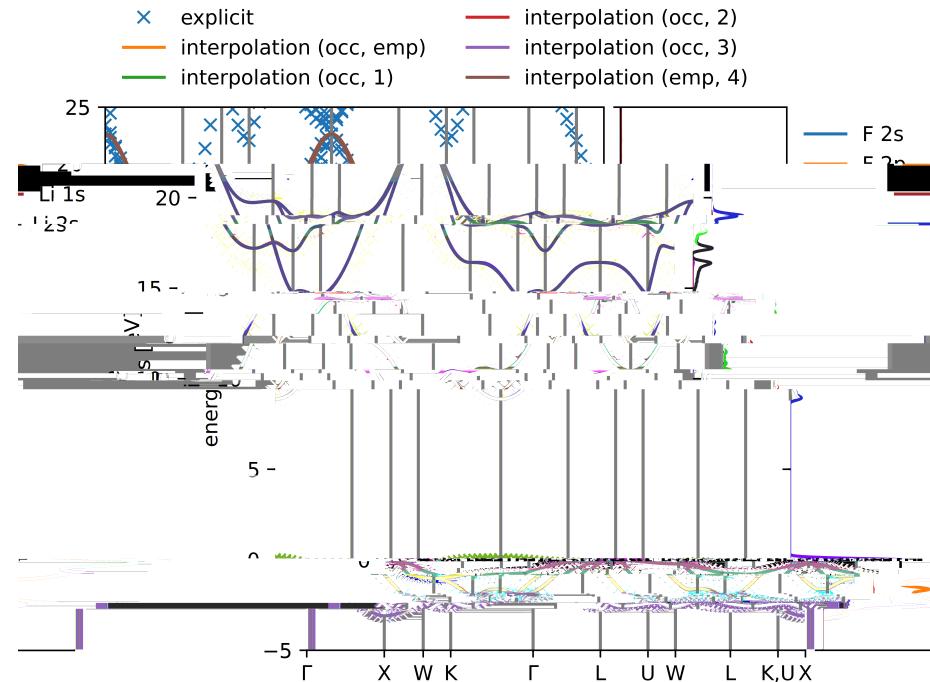
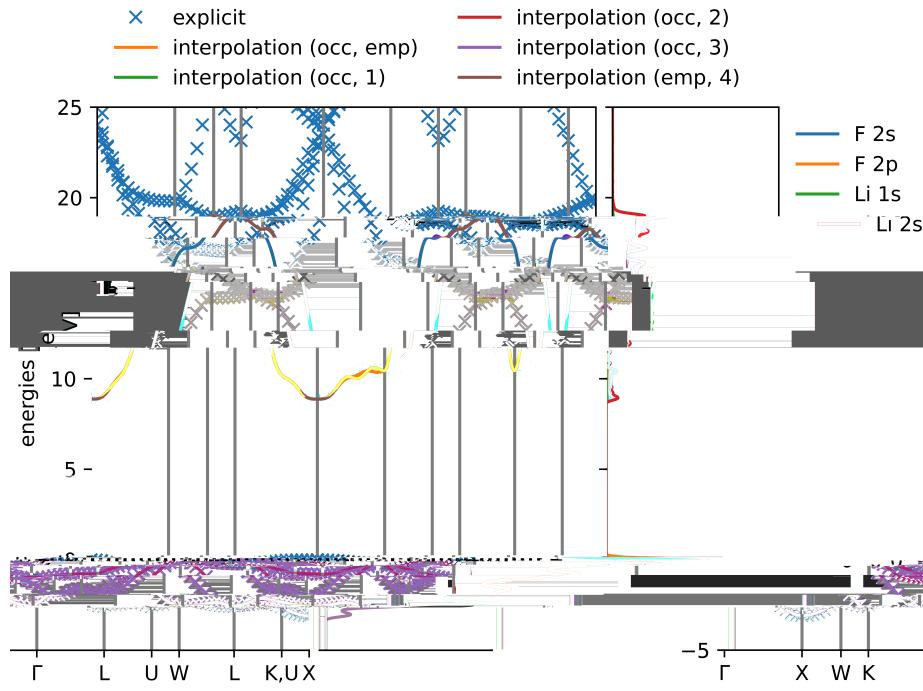


```
{  
  "workflow": {  
    "task": "wannierize",  
    "init_orbitals": "mlwfs",  
    "pseudo_library": "pseudo_dojo_standard_v0.4.1"},  
  "atoms": {  
    "cell_parameters": {  
      "ibrav": 6,  
      "celldms": {"1": 8.675923, "3": 0.645248},  
      "periodic": true},  
    "atomic_positions": {  
      "positions": [  
        ["Ti", 0.5, 0.5, 0.5],  
        ["Ti", 0.0, 0.0, 0.0],  
        ["O", 0.1814, 0.8186, 0.5],  
        ["O", 0.8186, 0.1814, 0.5],  
        ["O", 0.3186, 0.3186, 0.0],  
        ["O", 0.6814, 0.6814, 0.0]  
      ],  
      "units": "crystal"}},  
  "kpoints": {"grid": [3, 3, 4]},  
  "calculator_parameters": {  
    "w90": {"auto_projections": true}}}
```

Example 2: LiF



Example 2: LiF



Electronic screening via machine learning

Electronic screening via machine learning



$$= \frac{| -1_{Hxc} |}{| Hxc |}$$

8,

14,

106,

18,

Electronic screening via machine learning



$$= \frac{| -1_{Hxc} |}{| Hxc |}$$

8,

14,

106,

18,

Electronic screening via machine learning



$$= \frac{| -1_{Hxc} |}{| Hxc |}$$

8,

14,

106,

18,

Electronic screening via machine learning



$$= \frac{| -1_{Hxc} |}{| Hxc |}$$

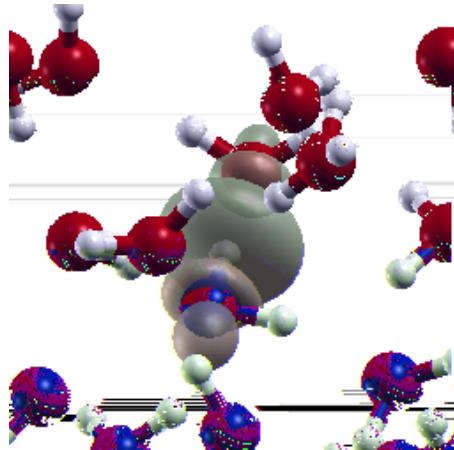
8,

14,

106,

18,

The machine-learning framework



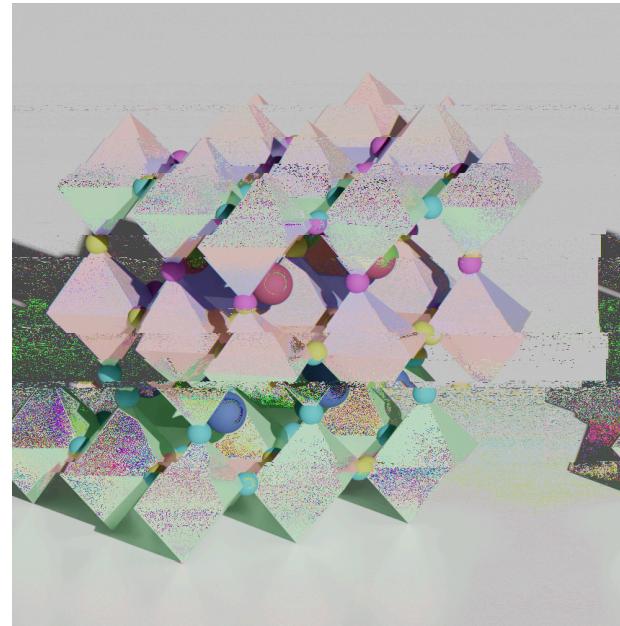
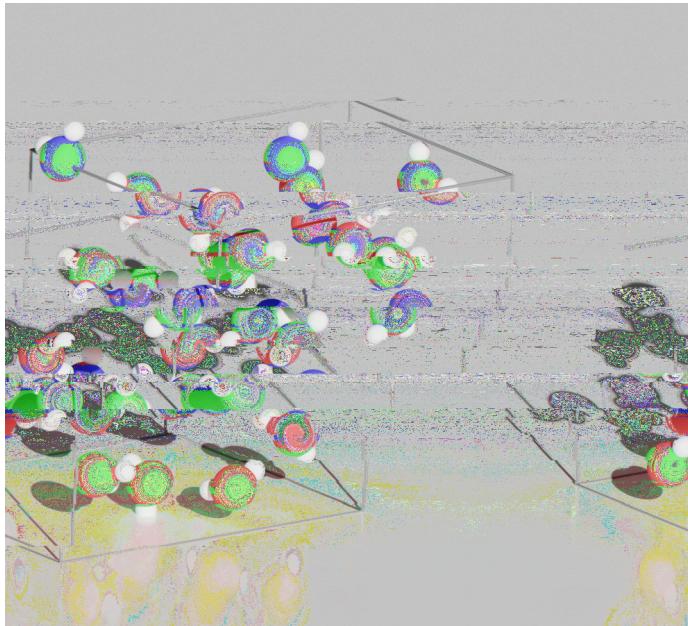
power spectrum decomposition

0 ridge regression
1
2

$$, = d () (,) (-)$$

$$\begin{matrix} 1 & 2 & \cdot & 1 & 2 \end{matrix} = \frac{\overline{8}}{\overline{2 + 1}} \begin{matrix} 1 & \cdot & 1 & 2 & \cdot & 2 \end{matrix}$$

Two test systems



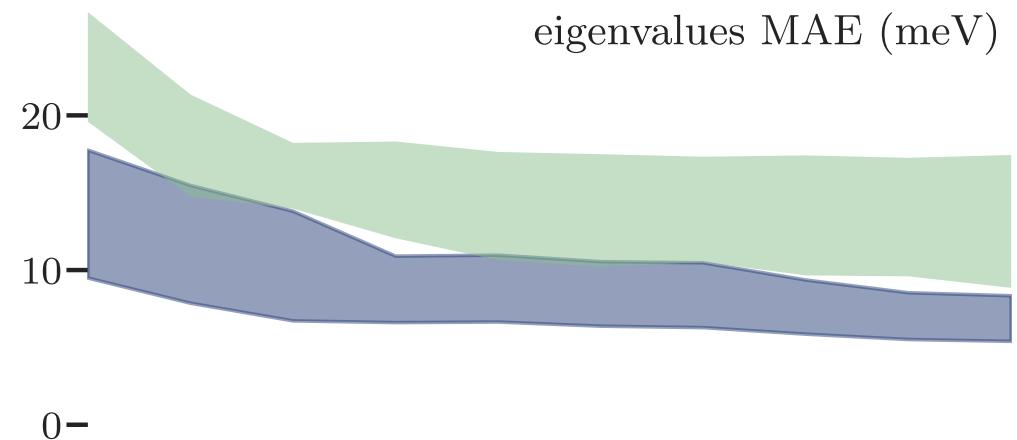
Results



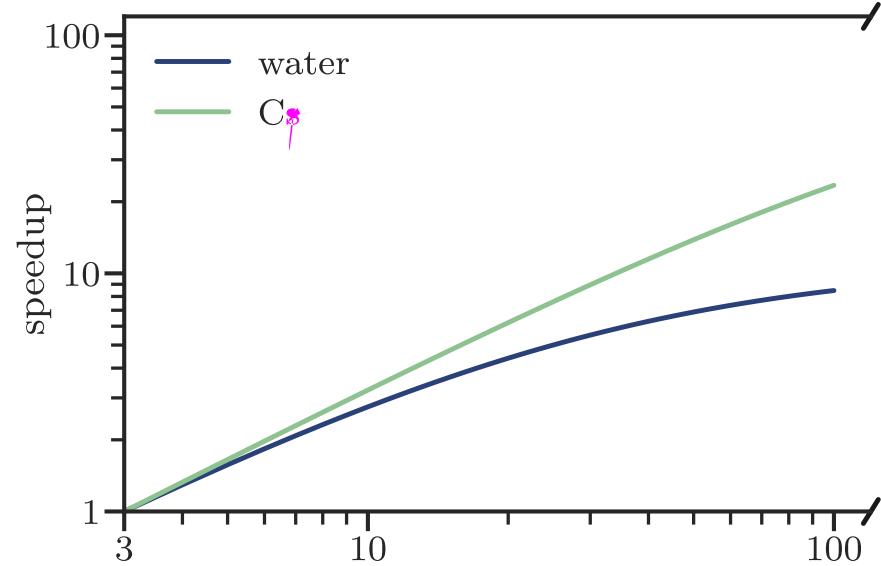
Results



Results



Results



Integration with AiiDA

Integration with

Integration with AiiDA



koopmans AiiDA

Integration with AiiDA



koopmans AiiDA

AiiDA

Integration with AiiDA



koopmans AiiDA

AiiDA

Integration with AiiDA



koopmans AiiDA

AiiDA

Integration with AiiDA



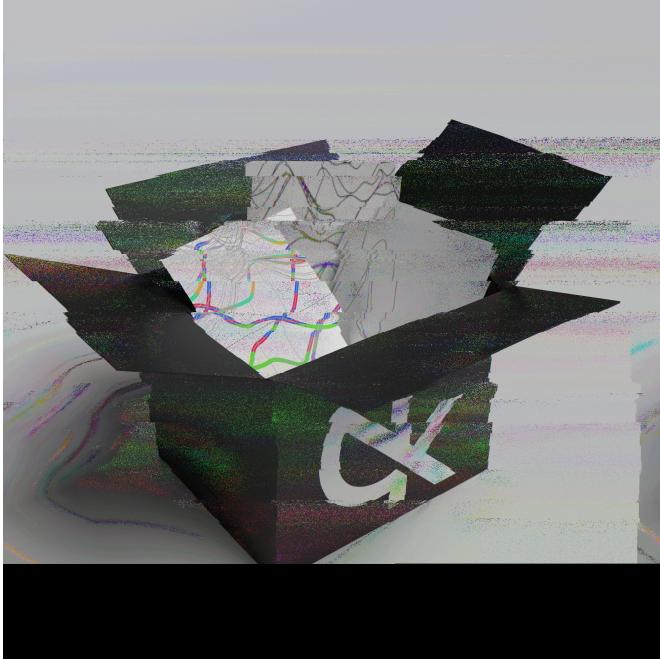
koopmans AiiDA

AiiDA

koopmans

Summary

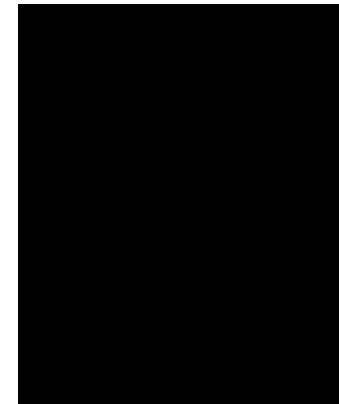
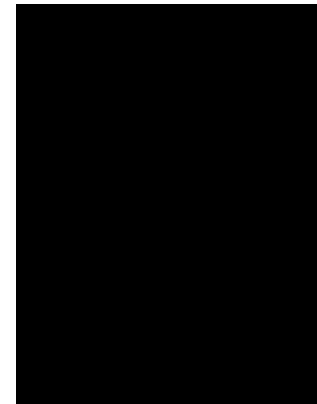
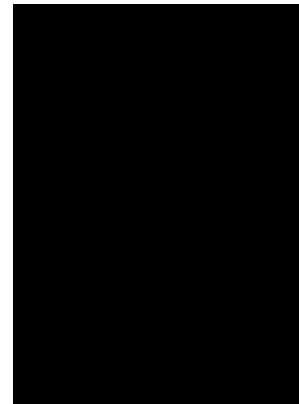
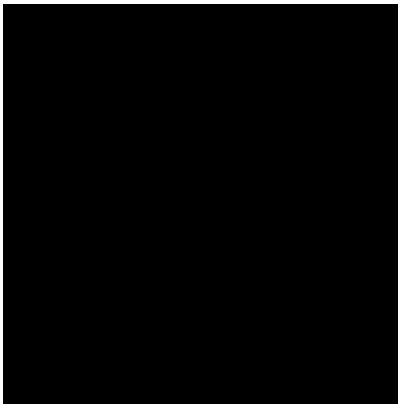
Summary



- ▶
- ▶
- ▶
- ▶

AiiDA

Acknowledgements



**Swiss National
Science Foundation**

WATER-E₂
XYLLOE₂

Spare slides

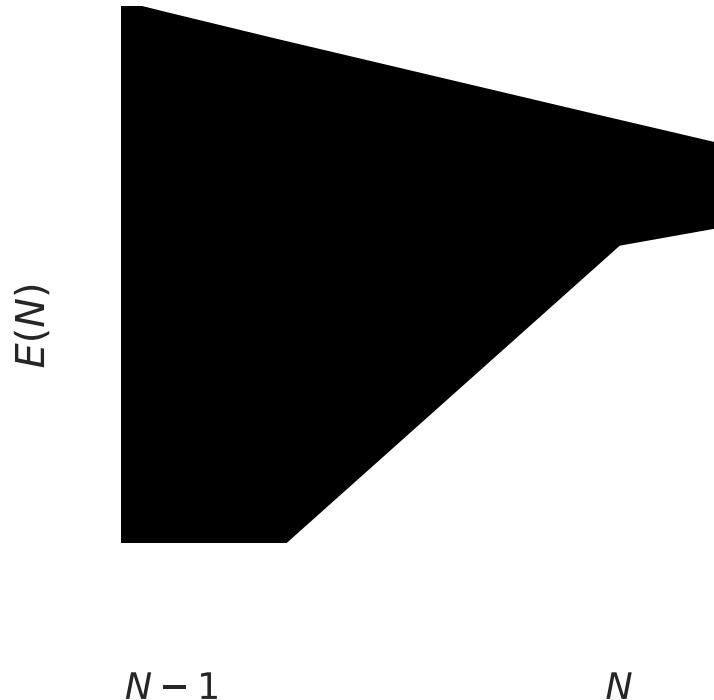
Koopmans functional basics



$$= \begin{cases} (\) - (\ - 1) & \text{if occ} \\ (\ + 1) - (\) & \text{if emp} \end{cases}$$

Spare slides

$$\text{Koopmans} = | - | = \frac{d}{d}$$



References



- 15,
- 8,
- 114,
- 19,
- 9,
- 9,
- 106,
- 14,
- 18,

References

