

Band structure calculations that are accurate, efficient, accessible, and scalable

Edward Linscott

Paul Scherrer Institute

MARVEL Review & Retreat | Grindelwald | 14 January 2025

This talk

Our progress on Koopmans functionals over the past year: how are we making them...

- accurate
- efficient
- accessible
- scalable

This talk

Our progress on Koopmans functionals over the past year: how are we making them...

- accurate
- efficient
- accessible
- scalable



Nicola Colonna



Giovanni Cistaro



Yannick Schubert



Miki Bonacci



Nicola Marzari

Accurate

Koopmans functionals

- screening parameters

Results: molecules

Text

Results: bulk materials

Text

Efficient

Taking advantage of symmetries

Text

Accessible

The koopmans package

Text

Scalable

AiiDA integration

Text

Machine-learning

Text

Introduction

Subsection

Lorem ipsum dolor sit amet, consectetur adipiscing elit, sed do eiusmod tempor incididunt ut labore et dolore magnam aliquam quaerat voluptatem. Ut enim aequale doleamus animo, cum corpore dolemus, fieri tamen permagna accessio potest, si aliquod aeternum et infinitum impendere malum nobis opinemur. Quod idem licet transferre in voluptatem, ut postea variari voluptas distinguere possit, augeri amplificarique non possit. At etiam Athenis, ut e patre audiebam facete et urbane Stoicos irridente, statua est in quo a nobis philosophia defensa et collaudata est, cum id, quod maxime placeat, facere possimus, omnis voluptas assumenda est, omnis dolor repellendus. Temporibus autem quibusdam et aut officiis debitis aut rerum necessitatibus saepe eveniet, ut et voluptates repudiandae sint et molestiae non recusandae. Itaque earum rerum defuturum, quas natura non depravata desiderat. Et quem ad me accedis, saluto: 'chaere,' inquam, 'Tite!' lictores, turma omnis chorusque: 'chaere, Tite!' hinc hostis mi Albucius, hinc inimicus. Sed iure Mucius. Ego autem mirari satis non queo unde hoc sit tam insolens domesticarum rerum fastidium. Non est omnino hic docendi locus; sed ita prorsus existimo, neque eum Torquatum, qui hoc primus cognomen invenerit, aut torquem illum hosti detraxisse, ut aliquam ex eo est consecutus? – Laudem et caritatem, quae sunt vitae.¹

¹E. B. Linscott et al. J. Chem. Theory Comput. (2020)



Here is a focus slide presenting a key idea

This is a matrix slide

You can use it to present
information side-by-side

with an arbitrary number of rows
and columns

Subsection

More text appears under the same subsection title as earlier

New Subsection

But a new subsection starts a new page.

Now, let's cite a nice paper.¹

¹E. B. Linscott et al. J. Chem. Theory Comput. **19**, 7097–7111 (2023)



Thank you!

References

E. B. Linscott, D. J. Cole, N. D. M. Hine, M. C. Payne & C. Weber. Onetep + toscam: uniting dynamical mean field theory and linear-scaling density functional theory. J. Chem. Theory Comput. (2020)

E. B. Linscott et al. koopmans: An open-source package for accurately and efficiently predicting spectral properties with Koopmans functionals. J. Chem. Theory Comput. **19**, 7097–7111 (2023)