http://exciting-code.org

exciting in a nutshell

Pasquale Pavone and the exciting team

Humboldt-Universität zu Berlin, Germany

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exciting in a coconutshell

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Outline

- **Following the 5W rule**
- **DFT/MBPT** from an **exciting** perspective
- **exciting** functionalities
- Subsidiary tools
- **XML** input format
- **exciting *neon***

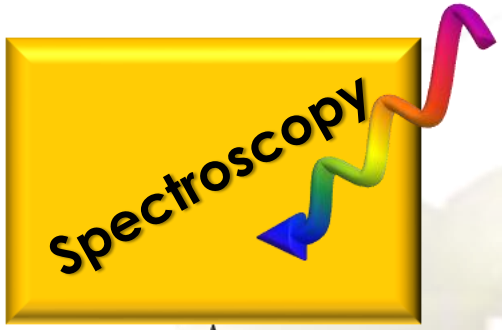
The 5W Rule

- What?
- Why?
- Who?
- Where?
- When?

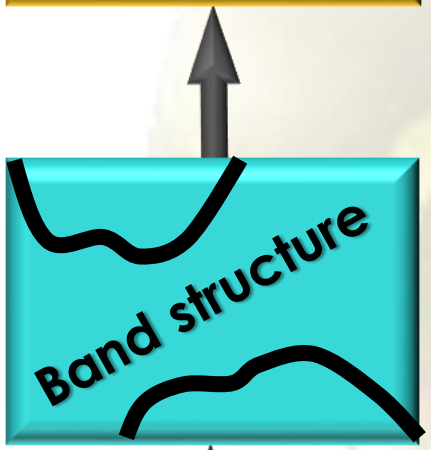
What is exciting ?

- Computation package based on
  - Density-functional theory
  - Many-body perturbation theory

What is exciting ?



Optical spectroscopy
Core excitations
Raman spectra



Many-body perturbation theory

Electronic band structure
Energy gaps
Effective masses

Density-functional theory

Equilibrium geometries
Phonon frequencies
Phase diagrams

What is exciting ?

- Computation package based on
  - Density-functional theory
  - Many-body perturbation theory

- Basis functions
  - Augmented plane waves (L)APW + lo

Why is exciting special?

- All-electron
  - Core + valence electrons
- Full-potential
  - Non spherical potentials inside MT
- Open source
- High standard of accuracy
  - Golden standard of DFT

Who is exciting ?

You!

Where is exciting?

When?

Where is exciting?

Main hub:

Leoben (Austria)

Up to 2011

Where is exciting?

November 2011

Where is exciting?

Main hub:

Berlin (Germany)

Since 2012

Where is exciting?

Main hub:

Berlin (Germany)

Riga

Stockholm / Oslo

Linköping

Leoben

Where is exciting?

DFT in exciting

- Solution of Kohn-Sham (KS) equations:

$$\left[-\nabla^2 + V_{eff}(\mathbf{r})\right]\psi(\mathbf{r}) = \varepsilon\psi(\mathbf{r})$$

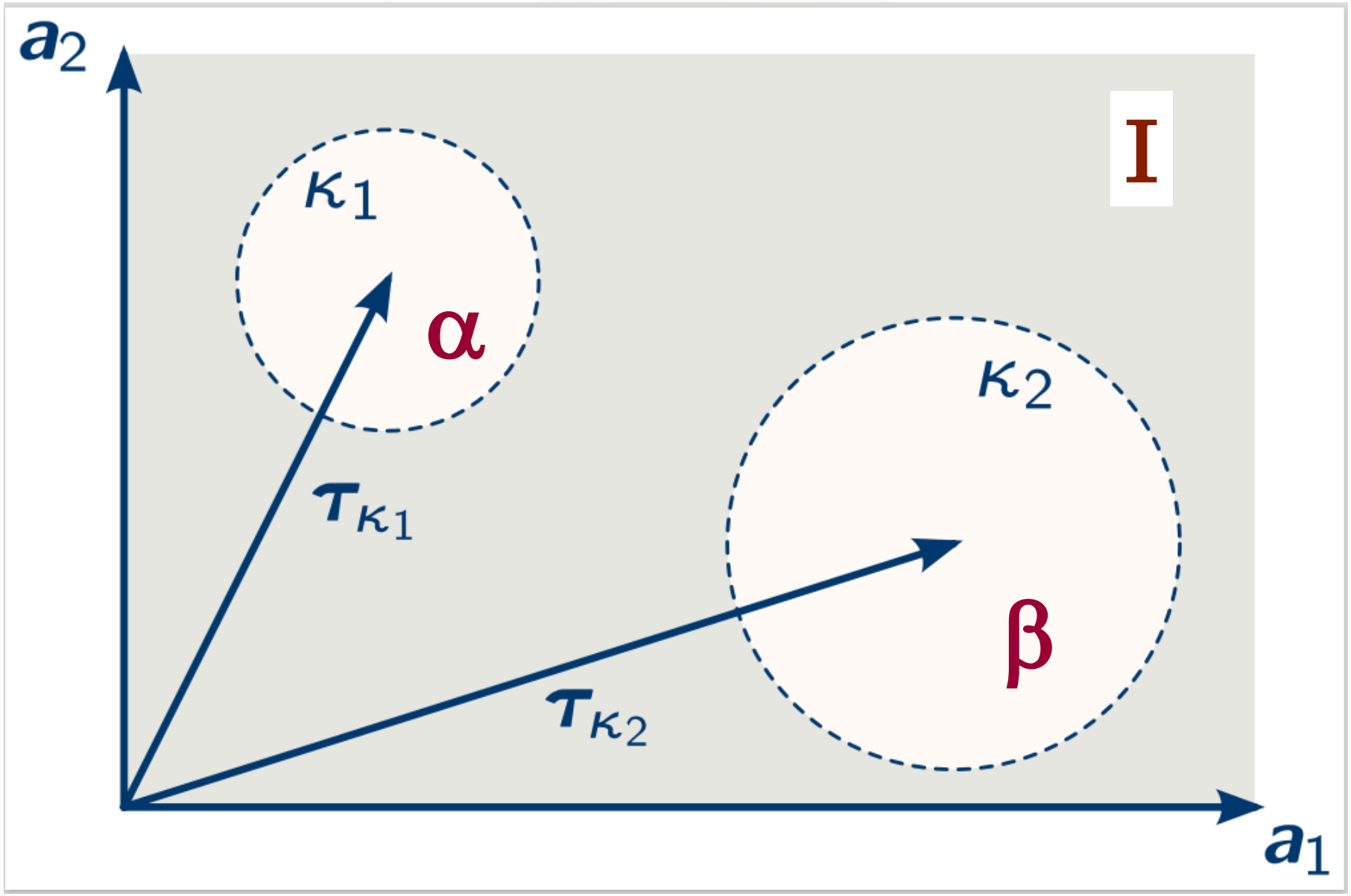
- Expansion in basis functions (APW+LO)

$$\psi(\mathbf{r}) = \sum_n c_n \phi_n(\mathbf{r})$$

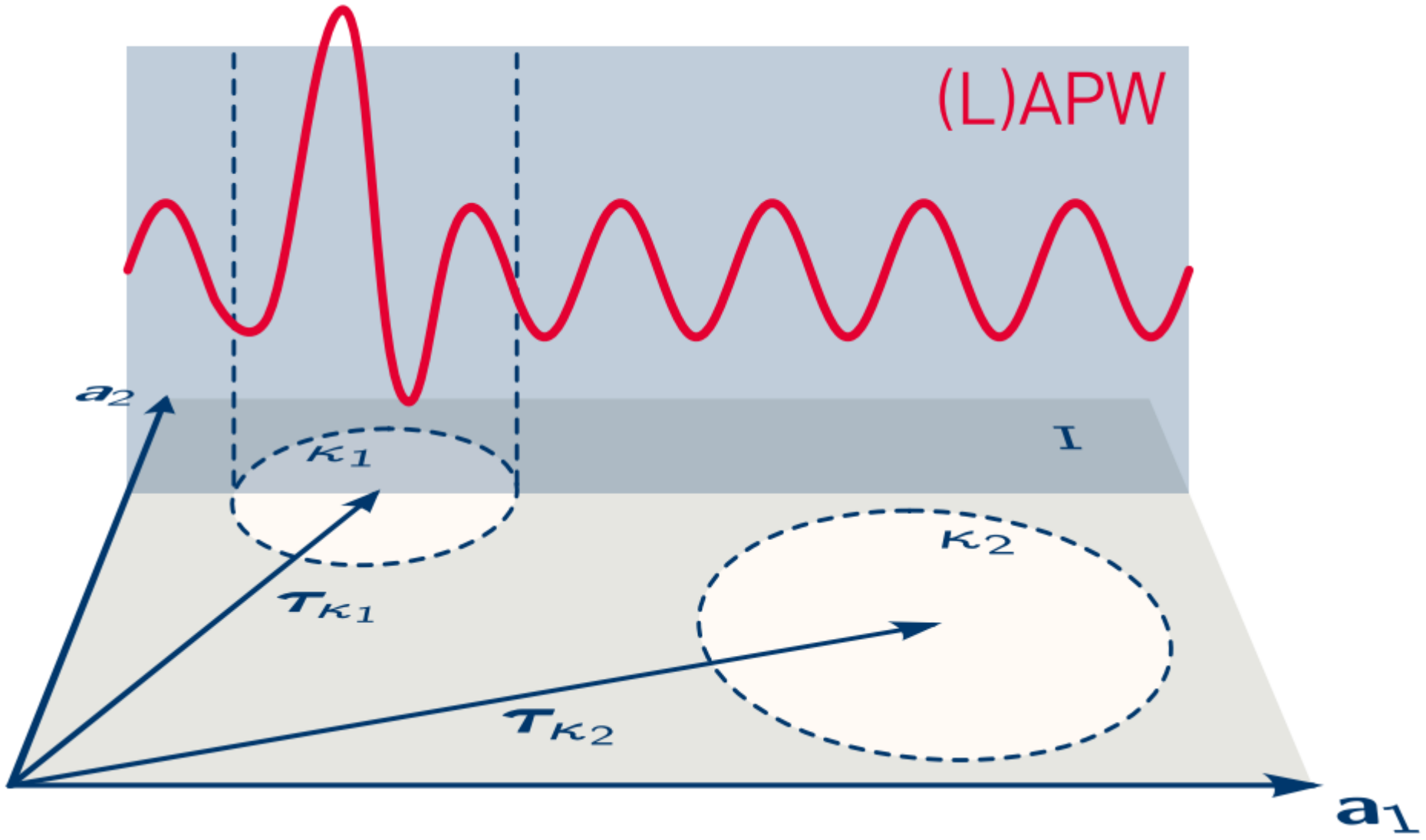
- Size of the basis set controlled by parameter

$R_{\mathrm{MT}} G_{\max}$ (rgkmax)

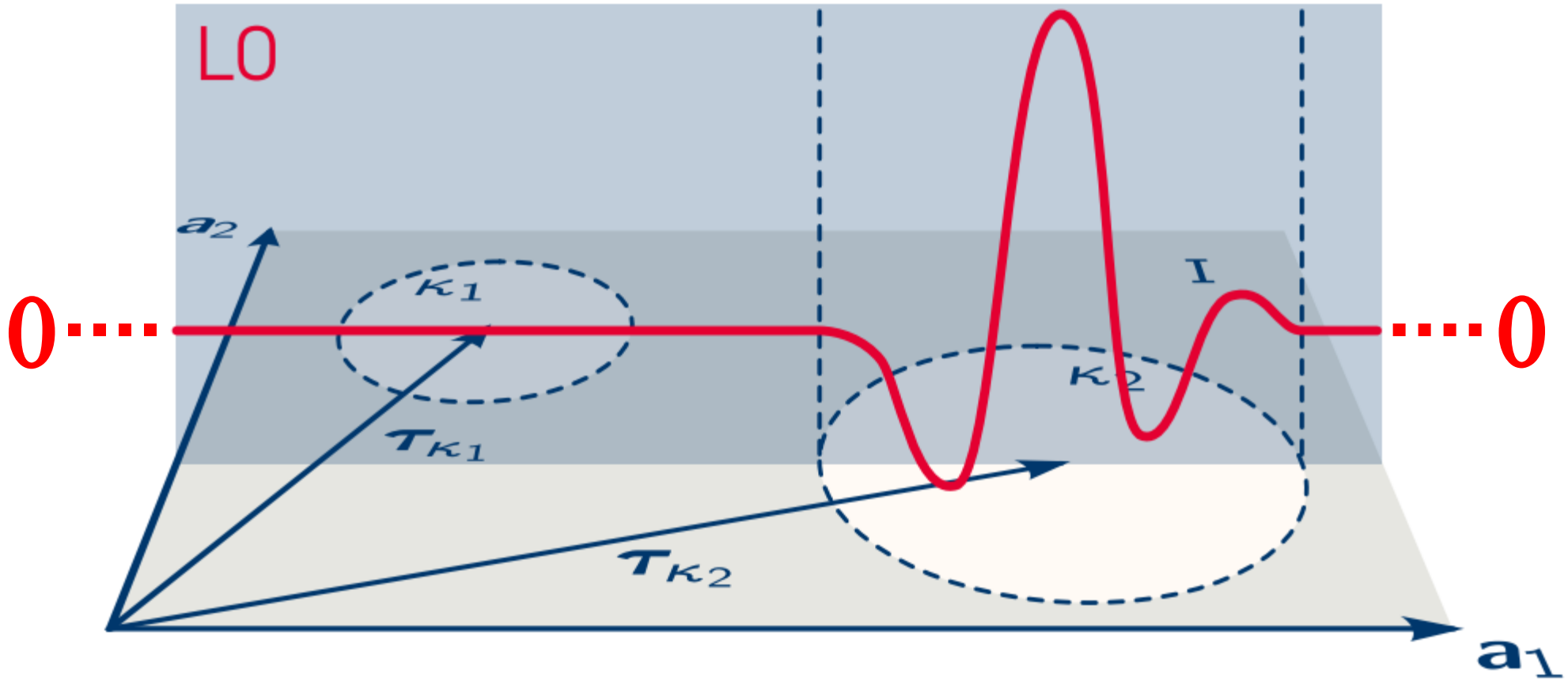
Muffin-tin (MT) and imterstitial (I) regions



(Linear) augmented plane waves: (L)APW



Local orbitals: LO



exciting ``species´´ file

```
chemicalSymbol="C" name="carbon"
```

```
<spdb>
   <sp chemicalSymbol="C" name="carbon" z="-6.00000" mass="21894.16673">
      <muffinTin rmin="0.100000E-04" radius="1.4500" rinf="21.0932" radialmeshPoints="250"/>
      <atomicState n="1" l="0" kappa="1" occ="2.00000" core="true"/>
      <atomicState n="2" l="0" kappa="1" occ="2.00000" core="false"/>
      <atomicState n="2" l="1" kappa="1" occ="1.00000" core="false"/>
      <atomicState n="2" l="1" kappa="2" occ="1.00000" core="false"/>
      <basis>
         <default type="lapw" trialEnergy="0.1500" searchE="false"/>
         <custom l="0" type="apw+lo" trialEnergy="0.1500" searchE="true"/>
         <custom l="1" type="apw+lo" trialEnergy="0.1500" searchE="true"/>
      </basis>
   </sp>
</spdb>
```

```
l="1" type="apw+lo" trialEnergy="0.1500"
```

DFT in exciting

- Secular equations (matrix equations)

$$\sum_{n'} \left(H_{n,n'} - \varepsilon_n S_{n,n'} \right) c_{n'} = 0$$

- Brillouin-zone integration:

$$\sum_{n} \int_{\mathrm{BZ}} d^3k F(\mathbf{k}) \rightarrow \sum_{\mathbf{k}} [w(\mathbf{k}) \cdot F(\mathbf{k})]$$

Regular grid of points in reciprocal space (`ngridk`)

Functionalities

- **Groundstate properties (DFT)**
  - Lattice constants, elastic moduli, EOS, forces, lattice relaxation, phonons
  - KS electronic band structure, KS DOS
  - Spin-polarized calculations
- **Excitations (MBPT+TDDFT)**
  - GW, BSE
  - Quasi-particle (QP) band structure
  - Theoretical spectroscopy

Main exciting Reference

IOP Publishing

Journal of Physics: Condensed Matter

J. Phys.: Condens. Matter **26** (2014) 363202 (24pp)

doi:10.1088/0953-8984/26/36/363202

exciting: a full-potential all-electron package implementing density-functional theory and many-body perturbation theory

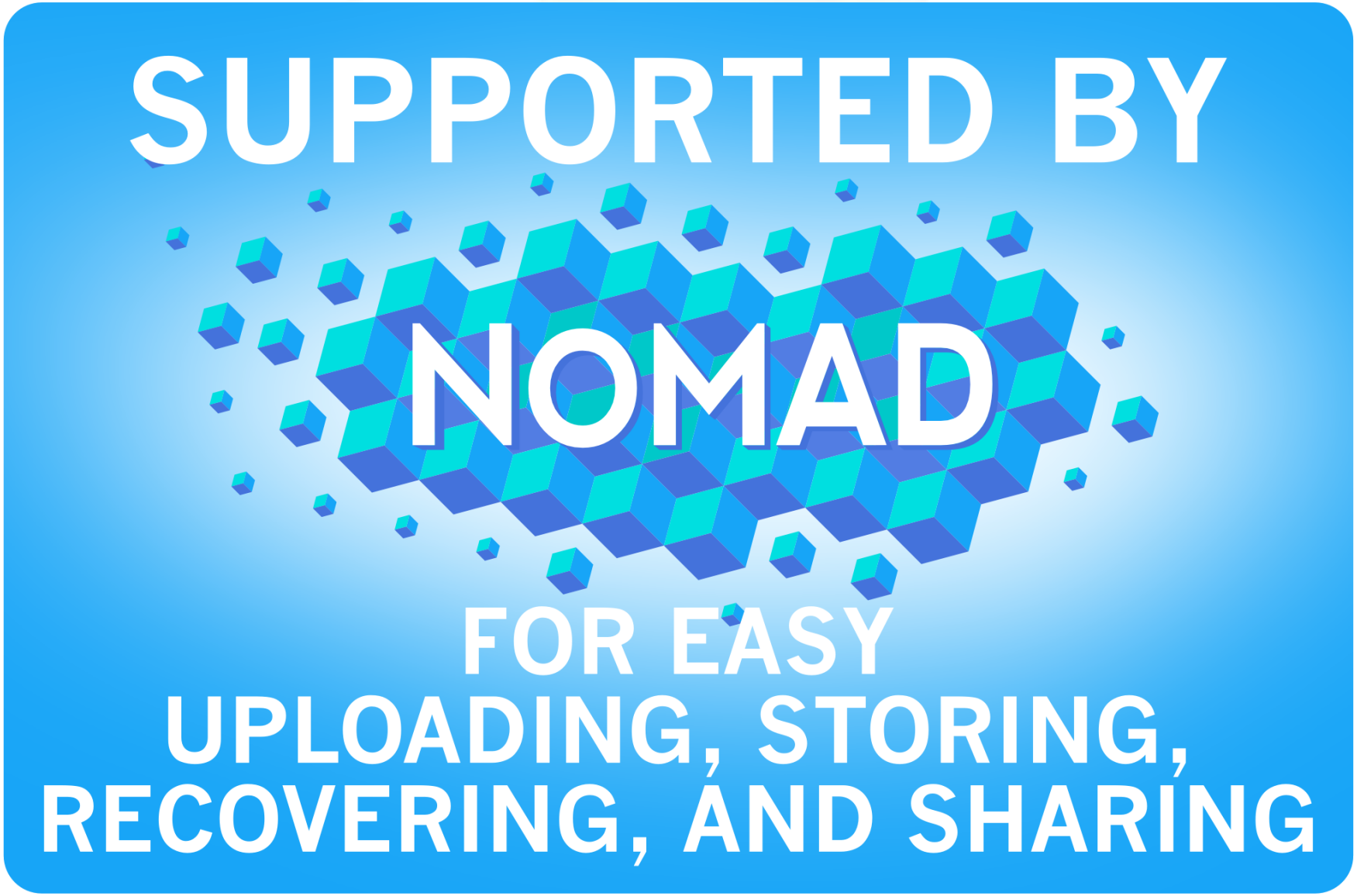
Andris Gulans[1], Stefan Kontur[1], Christian Meisenbichler[1], Dmitrii Nabok[1], Pasquale Pavone[1], Santiago Rigamonti[1], Stephan Sagmeister[2], Ute Werner[1] and Claudia Draxl[1,3]

J. Phys: Condens. Matter 26 (2014) 363202

exciting: Tools & more

- ElaStic (talk)
- CELL (talk)
- LayerOptics
- NOMAD project

The NOMAD Project



exciting Input Format

```
<input>

   <title>Diamond</title>

   <structure speciespath="$EXCITINGROOT/species">

      <crystal scale="6.7274">
         <basevect>0.0   0.5   0.5</basevect>
         <basevect>0.5   0.0   0.5</basevect>
         <basevect>0.5   0.5   0.0</basevect>
      </crystal>

      <species speciesfile="C.xml">
         <atom coord="0.00 0.00 0.00"/>
         <atom coord="0.25 0.25 0.25"/>
      </species>

   </structure>

   <groundstate
      ngridk="4 4 4"
      outputlevel="normal"
      xctype="GGA_PBE_SOL">
   </groundstate>

</input>
```

Input Format

- eXtensible Markup Language (XML)
- Input validation syntax
  - Elements -> actions
  - Attributes -> parameter

input.xml

```
<input>
   <title> Title </title>

   <structure …> … </structure>

   …

</input>
```

input.xml

```
<input>
   <title> Title </title>

   <structure speciespath=´´/path/species´´>
      …
   </structure>

   …

</input>
```

input.xml

```
<input>
   <title> Title </title>

   <structure …> … </structure>

   <groundstate …> … </groundstate>

   …


</input>
```

input.xml

```
<input>
   <title> Title </title>

   <structure …> … </structure>

   <groundstate ngridk=´´8 8 8´´ …>
    …
   </groundstate>
   …

</input>
```

input.xml

```
<input>
   <title> Title </title>

   <structure …> … </structure>

   <groundstate …> … </groundstate>

   <relax …>
   </relax>
   …
</input>
```

input.xml

```
<input>

   …

   <phonon …> … </phonon>

</input>
```

Website: Input Reference

exciting **Neon**

exciting Website

HOME ABOUT TEAM REFERENCES EVENTS INTERNAL

exciting

a full-potential all-electron package implementing linearized augmented planewave methods

DOWNLOAD FORUM

About exciting

exciting is a full-potential all-electron density-functional-theory package implementing linearized augmented planewave methods. It can be applied to all kinds of materials, irrespective of the atomic species involved and allows for exploring the physics of core electrons. As the name tells, **exciting** has a particular focus on excitations.

READ MORE

Current developments

Following our **exciting fluorine** release, we are already working hard on upcoming features. Here are some examples:

- Adaptively-compressed exchange
- Iterative eigensolver
- Speedy BSE

DEVELOPMENT TEAM

Tutorials

Follow our numerous step-by-step tutorials which guide you through basic, as well as advanced features of **exciting**.

GET STARTED

exciting Website

News

How exciting! 2023

Our event series HoW exciting! is back, with its hands-on part followed by an international workshop. Join us at **HoW exciting! 2023** in Berlin, Germany, August 2-10, 2023.

LEARN MORE

New release: exciting fluorine

We are happy to present **exciting fluorine**, the newest main release of the **exciting** code. New features comprise density-functional perturbation theory for phonons, the implementation of the library SIRIUS for tackling large systems, and more.

LEARN MORE

Our webpage in a new look

Do you like to learn about the most **exciting** features, explore our tutorials, or get to know our team? Or are you interested in our events? If so, just enjoy our new webpage!

MORE NEWS

exciting Website

HoW exciting! 2023

Welcome | Program | Registration | Arrival

Welcome to HoW exciting! 2023

Excitations in solids are among the most exciting phenomena in condensed-matter physics. In this context, density-functional theory (DFT) is the first level in a hierarchical set of models which are used to describe and understand these phenomena in real materials. Based on this, time-dependent DFT as well as Green-function based methods allow us to treat light-matter interaction, in terms of phtoemission, optical and core-level spectroscopy, resonant inelastic x-ray scattering (RIXS), electron energy loss spectroscopy, and more. These are most prominent topics of our lectures and hands-on training. Moreover, we will address electron-phonon coupling, charge and heat transport, and non-equilibrium processes.

The aim of this event is to survey the state-of-the-art of theoretical and computational approaches to describe different kinds of excitations (optical, magnetic, vibrational, etc.) in condensed-matter systems, to discuss future perspectives of these methodologies and their applications in different research fields, and to confront advances in theoretical and computational methods with the latest developments in experimental techniques as well as applications.

Hands-on Tutorials

☛ Instructions for the "HoW exciting! 2023" Hands-on Sessions

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Hands-on Tutorials

HoW exciting! 2023 Hands-on Sessions

1. Instructions for the "HoW exciting! 2023" Hands-on Sessions

Please click here for fundamental information on how to set `exciting` before starting with the calculations performed in the hands-on tutorials!

2. Special Instructions for Running the Jupyter Tutorials

- Click here for instructions on running the Jupyter tutorials!

Hands-on Tutorials

Instructions for "HoW exciting! 2023"

by Pasquale Pavone for exciting *neon*

Purpose: Here, it will be given fundamental information on how to set **exciting** before starting with the calculation performed in the hands-on tutorials.

Fold

Table of Contents

Recommendations

- Sit always at the same workstation
- Run all tutorial exercises on the local disk: `/home/tutorials`
- Follow all instructions

Hands-on Tutorials

Tutorials for exciting Neon

Here, **atomic units (Hartree, Bohr, etc.)** are always used!

Tutorials describing ***basic*** features are indicated by 【b】

Tutorials describing ***advanced*** features are indicated by 【a】

INSTRUCTIONS FOR PARTICIPANTS OF 'HoW exciting! 2023'

- Instructions for "HoW exciting! 2023"

GETTING STARTED

【b】 How to start an exciting calculation
【b】 Simple convergence tests
【b】 Electronic band-structure and density of states
【a】 Understanding the exciting species files

The Last Slide: We are so Excited!