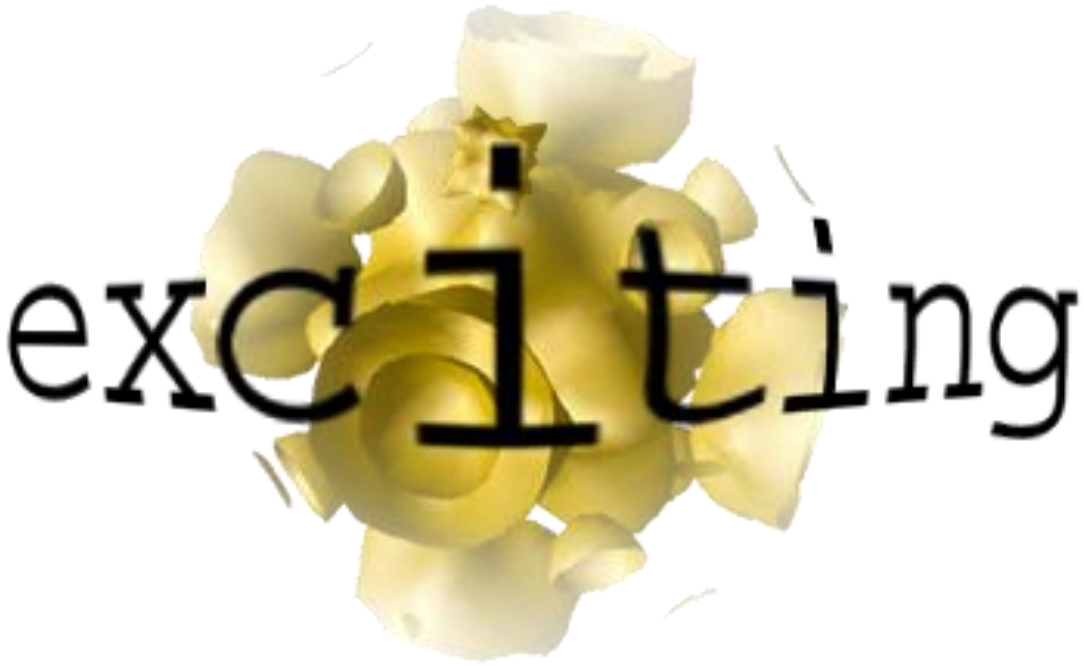
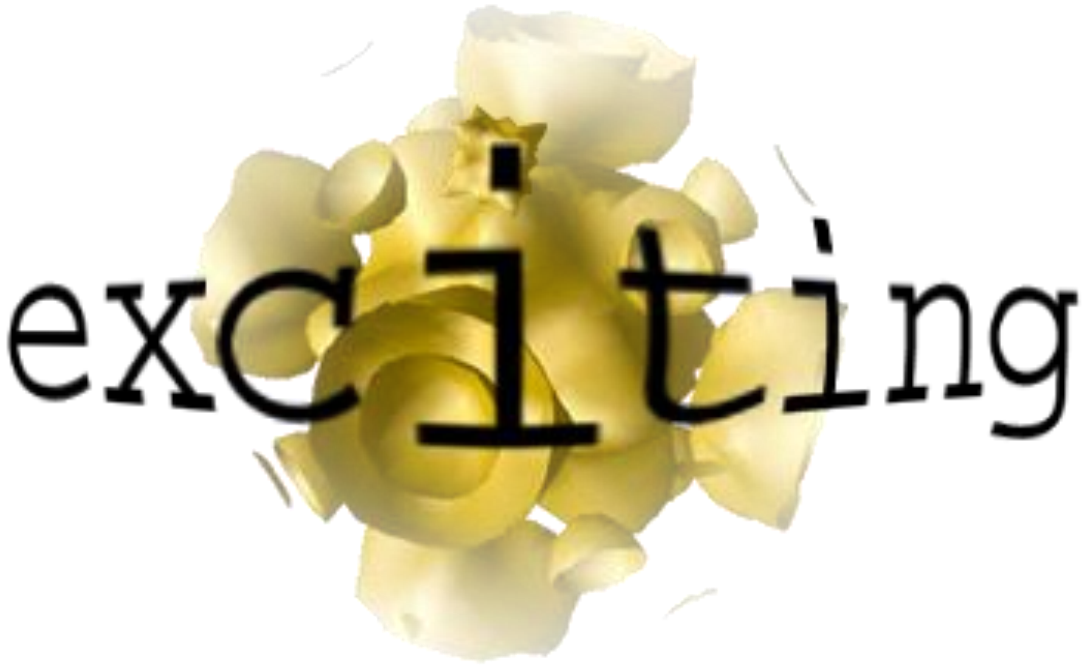
http://exciting-code.org



„**exciting** in a nutshell“

Pasquale Pavone
Humboldt-Universität zu Berlin

http://exciting-code.org



„exciting in a (coco)nutshell“

Pasquale Pavone
Humboldt-Universität zu Berlin

Outline

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

The 5W Rule

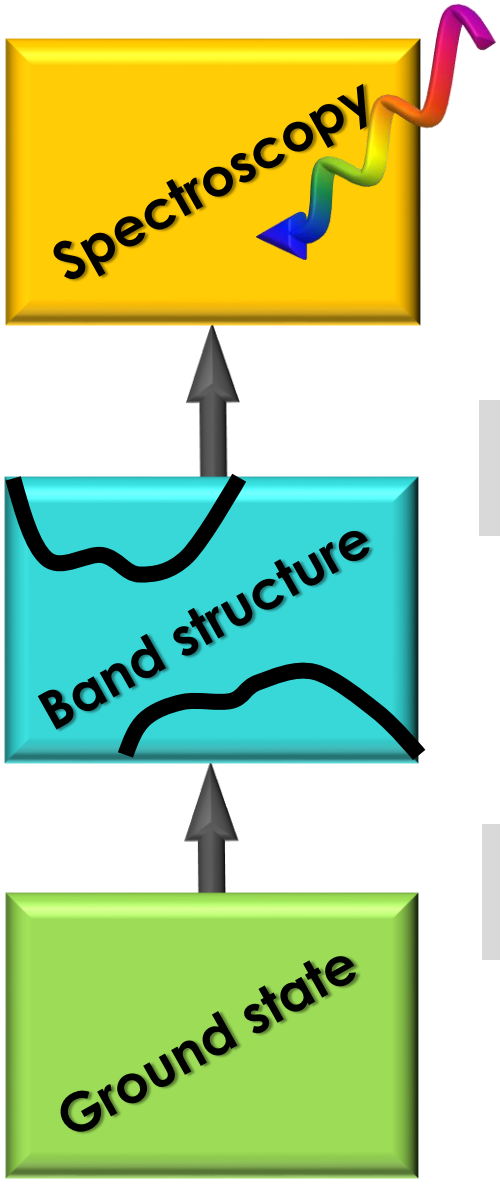
- What?
- Why?
- Who?
- Where?
- When?

What is exciting ?

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

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

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

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 ?

Where is exciting?

When?

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)

Stockholm / Oslo

Linköping

Leoben

Where is exciting?

DFT in exciting

- Solution of Kohn-Sham (KS) equations:

$$\left[-\frac{1}{2}\nabla^2 + v_{\mathrm{KS}}(\mathbf{r})\right]\psi_{\mathbf{ik}}(\mathbf{r}) = \epsilon_{\mathbf{ik}}\psi_{\mathbf{ik}}(\mathbf{r})$$

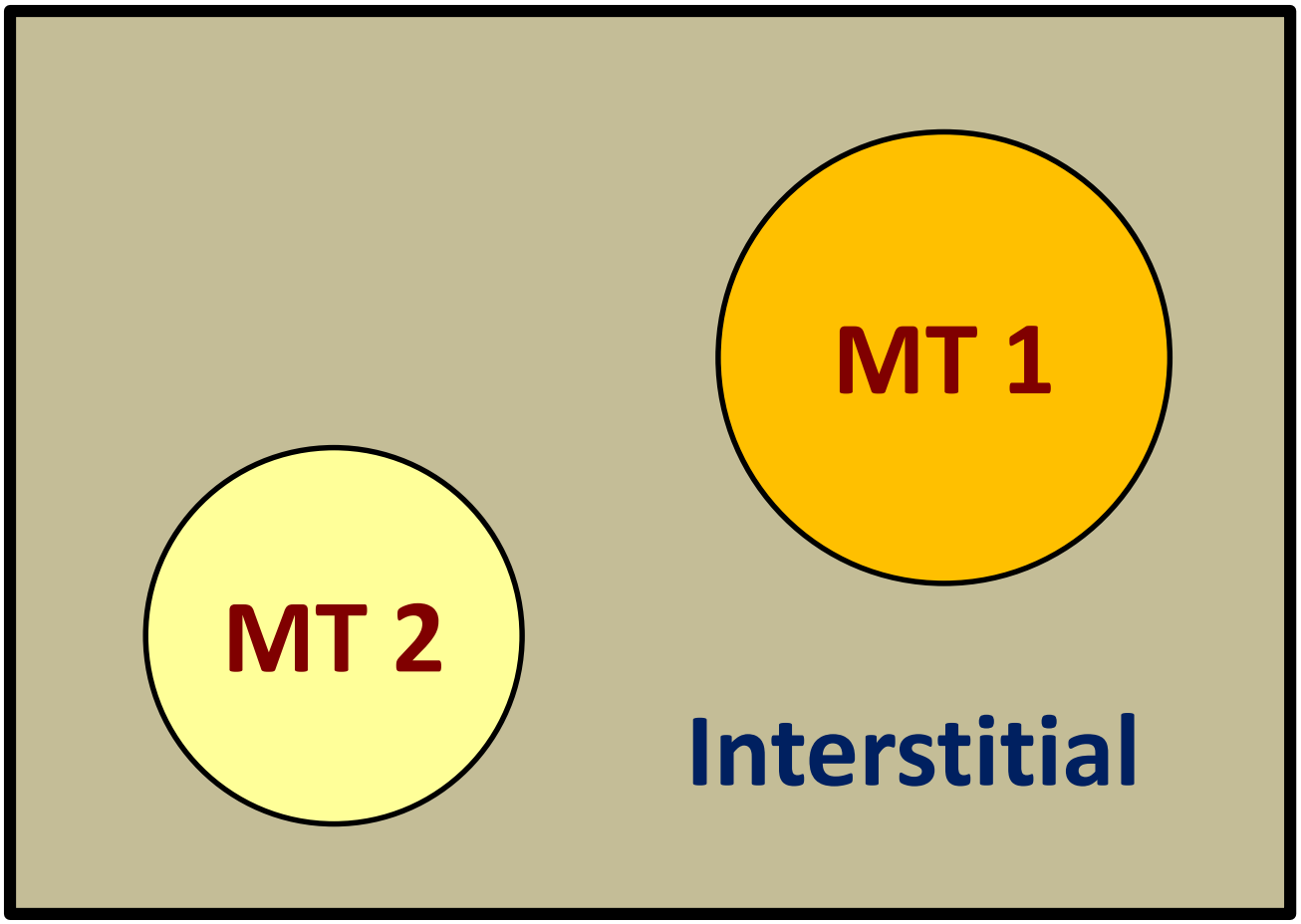
- Expansion in basis functions (APW+lo)

$$\psi_{\mathbf{ik}}(\mathbf{r}) = \sum_{\mathbf{G}} C^{\mathbf{k}}_{\mathbf{iG}}\phi_{\mathbf{G+k}}(\mathbf{r})$$

- Size of the basis set controlled by parameter

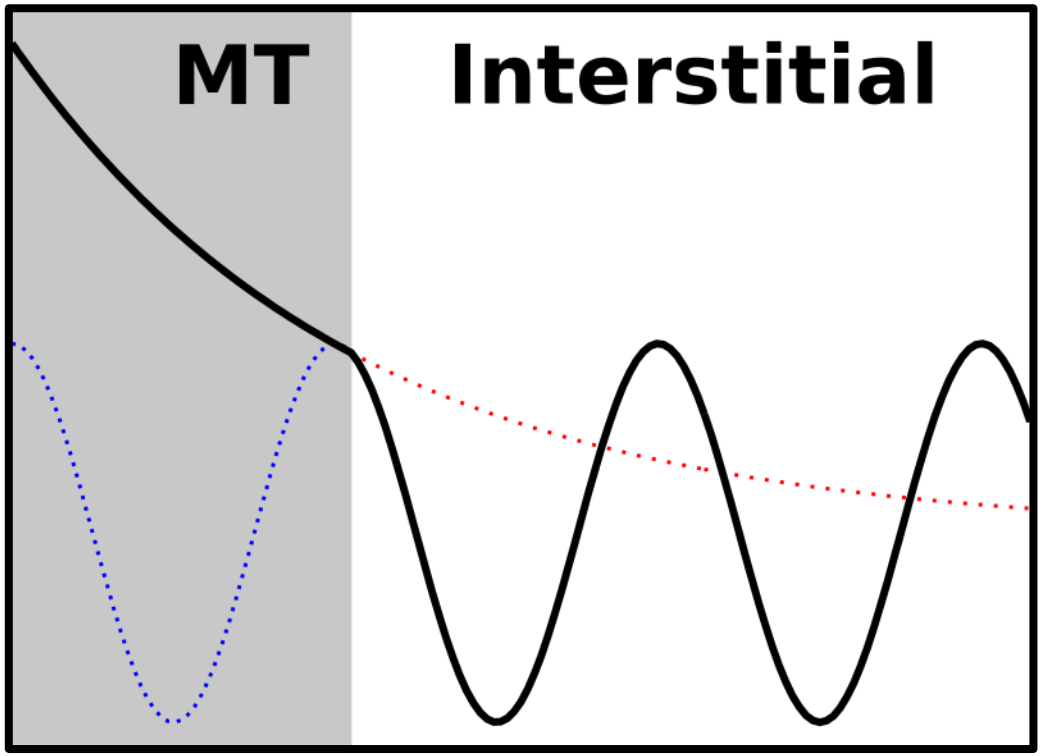
$$R_{\mathrm{MT}}G_{\mathrm{max}}$$ (rgkmax)

Muffin-Tin vs. Interstitial



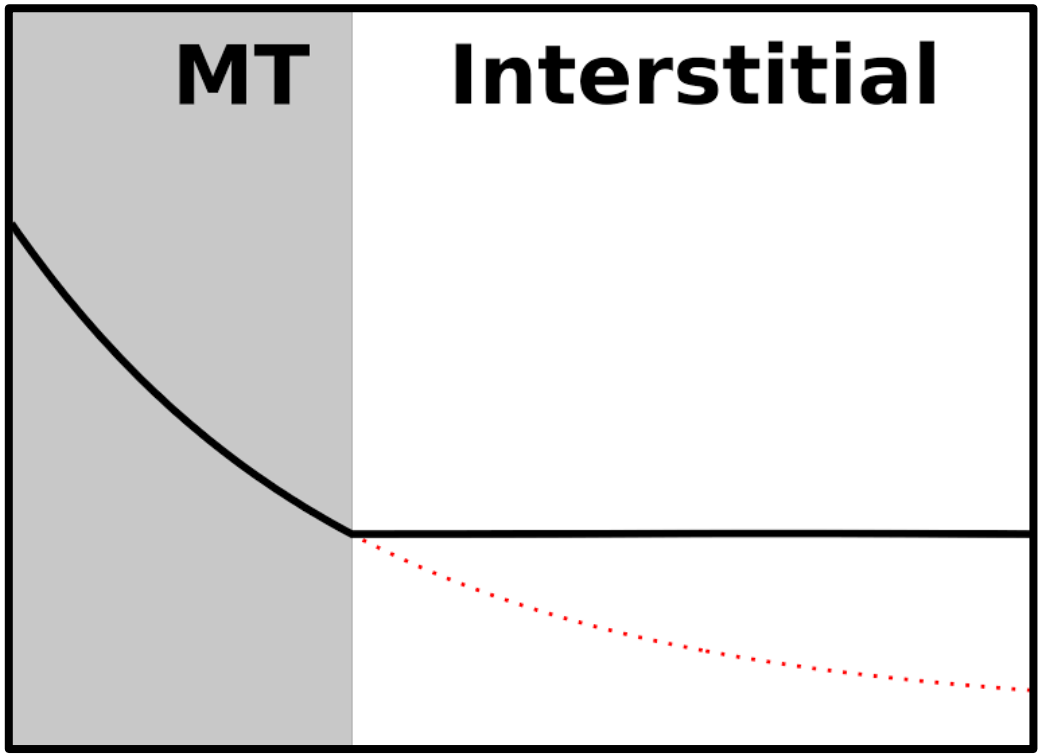
APW Basis: Dual Nature

$$\phi_{\mathbf{G}+\mathbf{k}}(\mathbf{r}) = \begin{cases} \text{“atomic-like“ wavefunction in MT} \\ \text{plane wave in Interstitial} \end{cases}$$



Local Orbital Basis

$$\phi_\mu(\mathbf{r}) = \begin{cases} \text{“atomic-like“ wavefunction in MT} \\ \text{zero in Interstitial} \end{cases}$$



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)

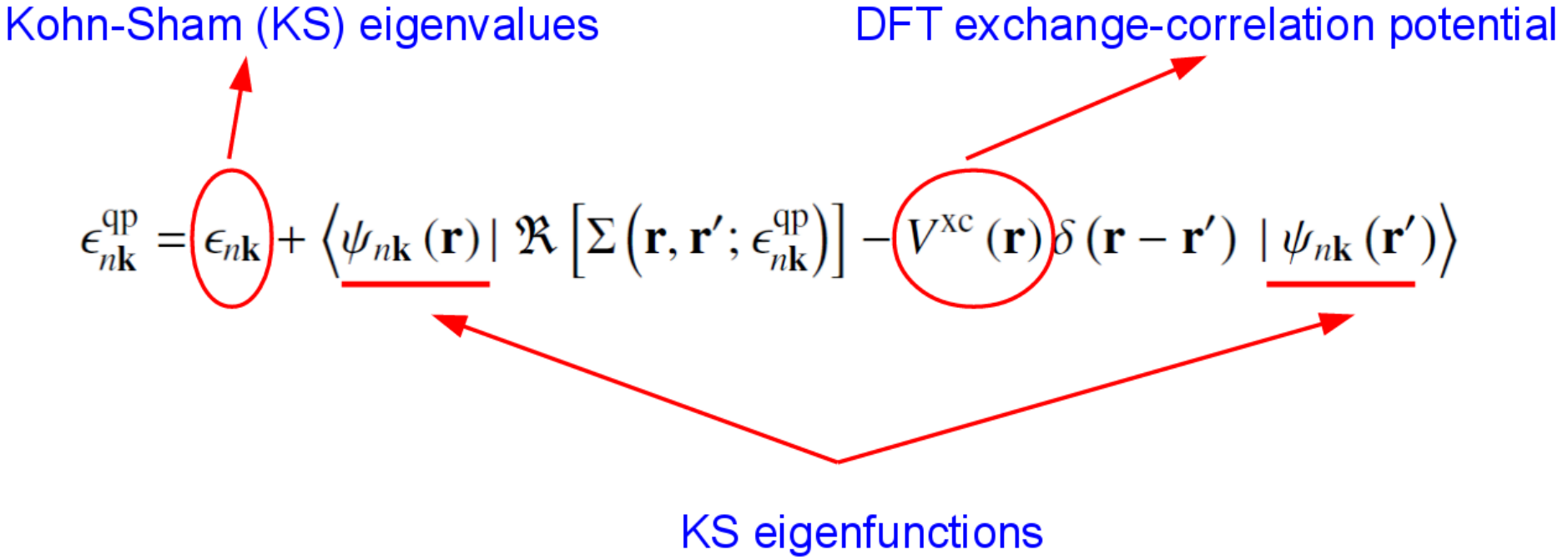
$$H^{\mathbf{k}}\, C^{\mathbf{k}} = \epsilon^{\mathbf{k}}\, S^{\mathbf{k}}\, C^{\mathbf{k}}$$

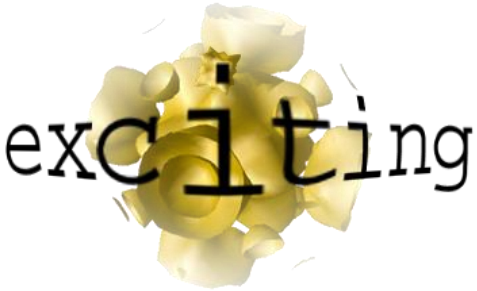
- Brilloiun zone integration:

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

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

MBPT in exciting





Functionalities

- **Groundstate properties (DFT)**
  - Lattice constants, elastic moduli, EOS, forces, lattice relaxation
  - 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)

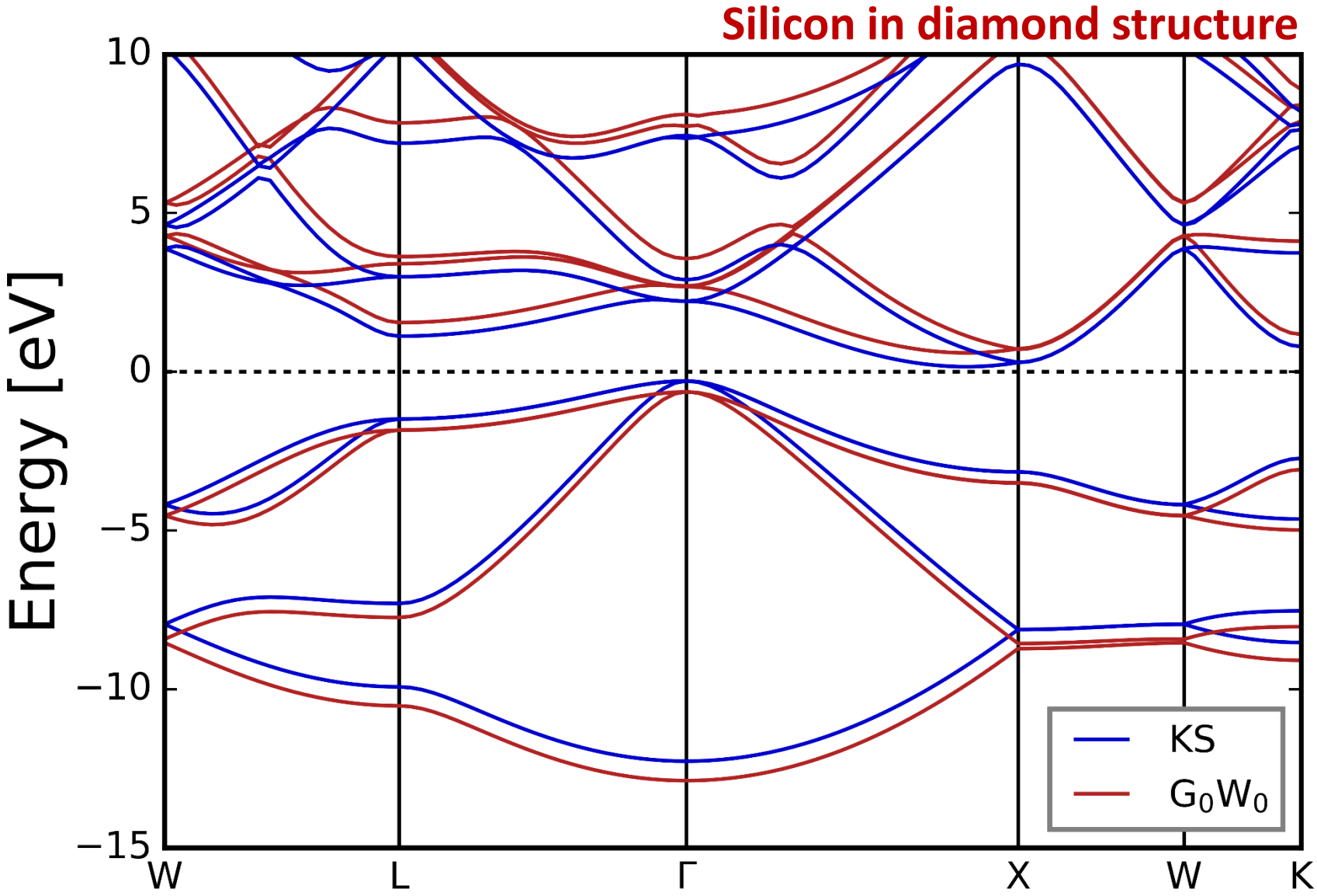
doi:10.1088/0953-8984/26/36/363202

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

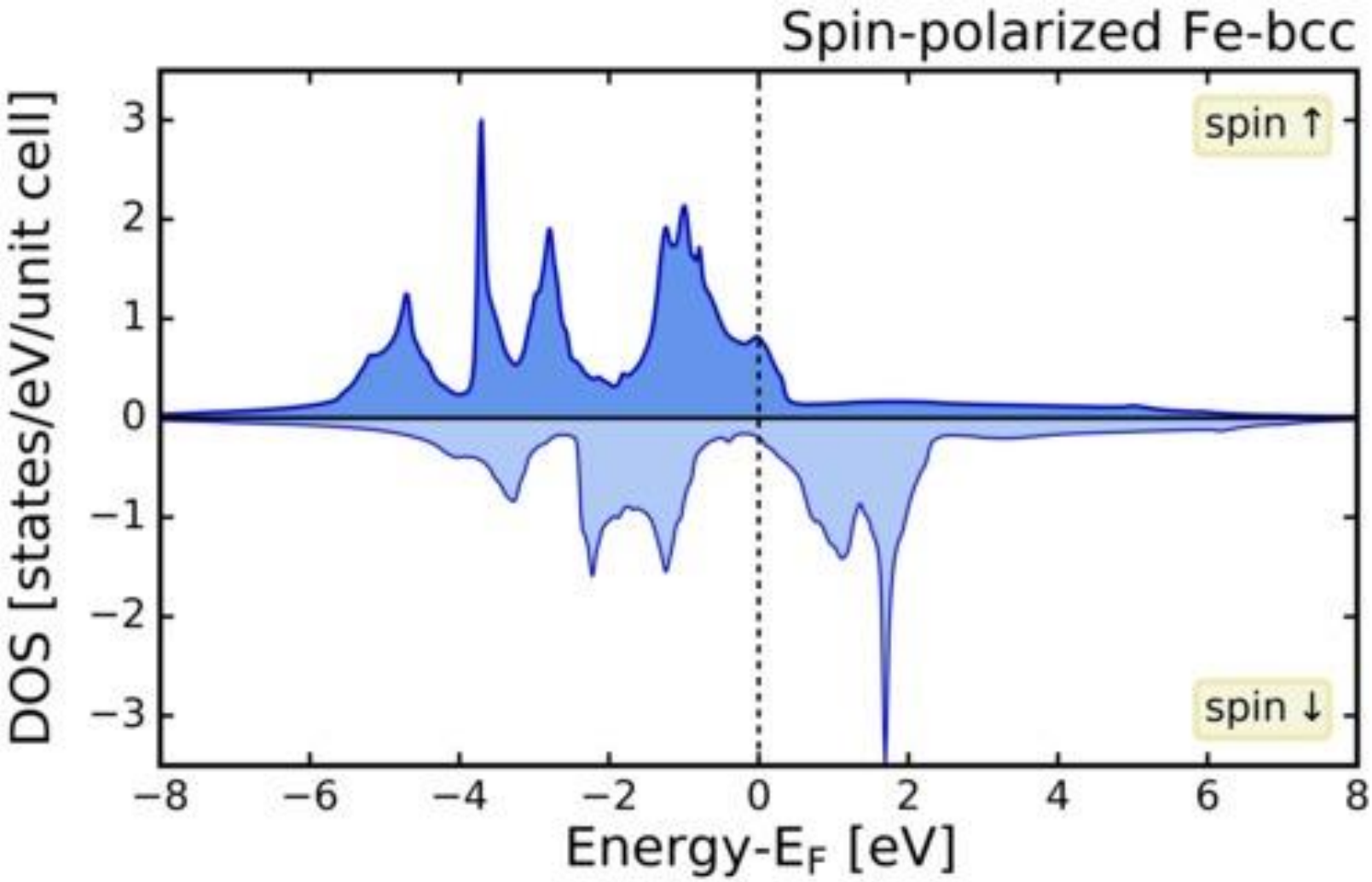
Andris Gulans[1], Stefan Kontur[1], Christian Meisenbichler[1], Dmitrii Nabok[1], Pasquale Pavone[1], Santiago Rigamonti[1], Stephan Sagmeister[2], Ute Werner[1] and Claudia Draxl[1,3]

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

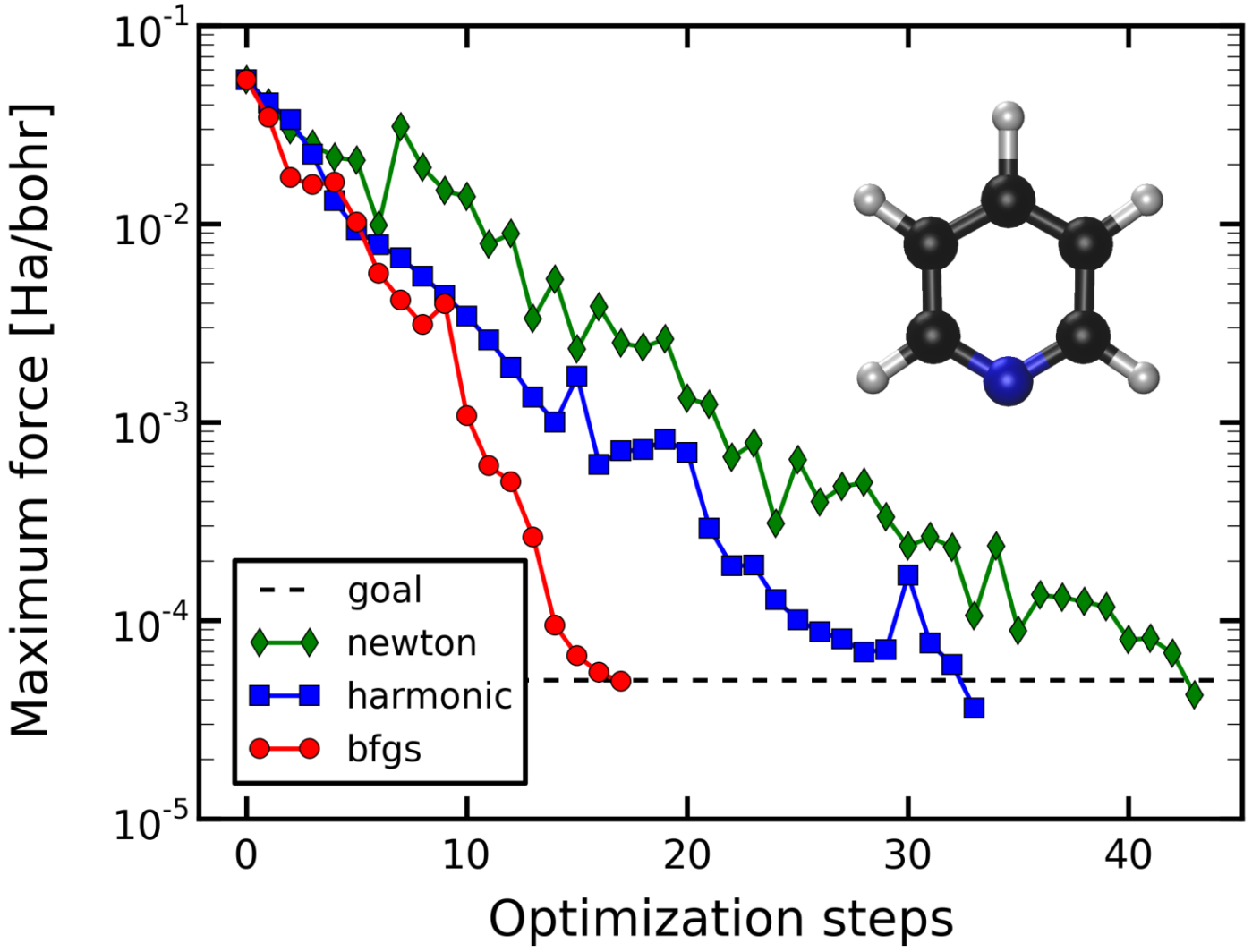
Electronic Band Structure



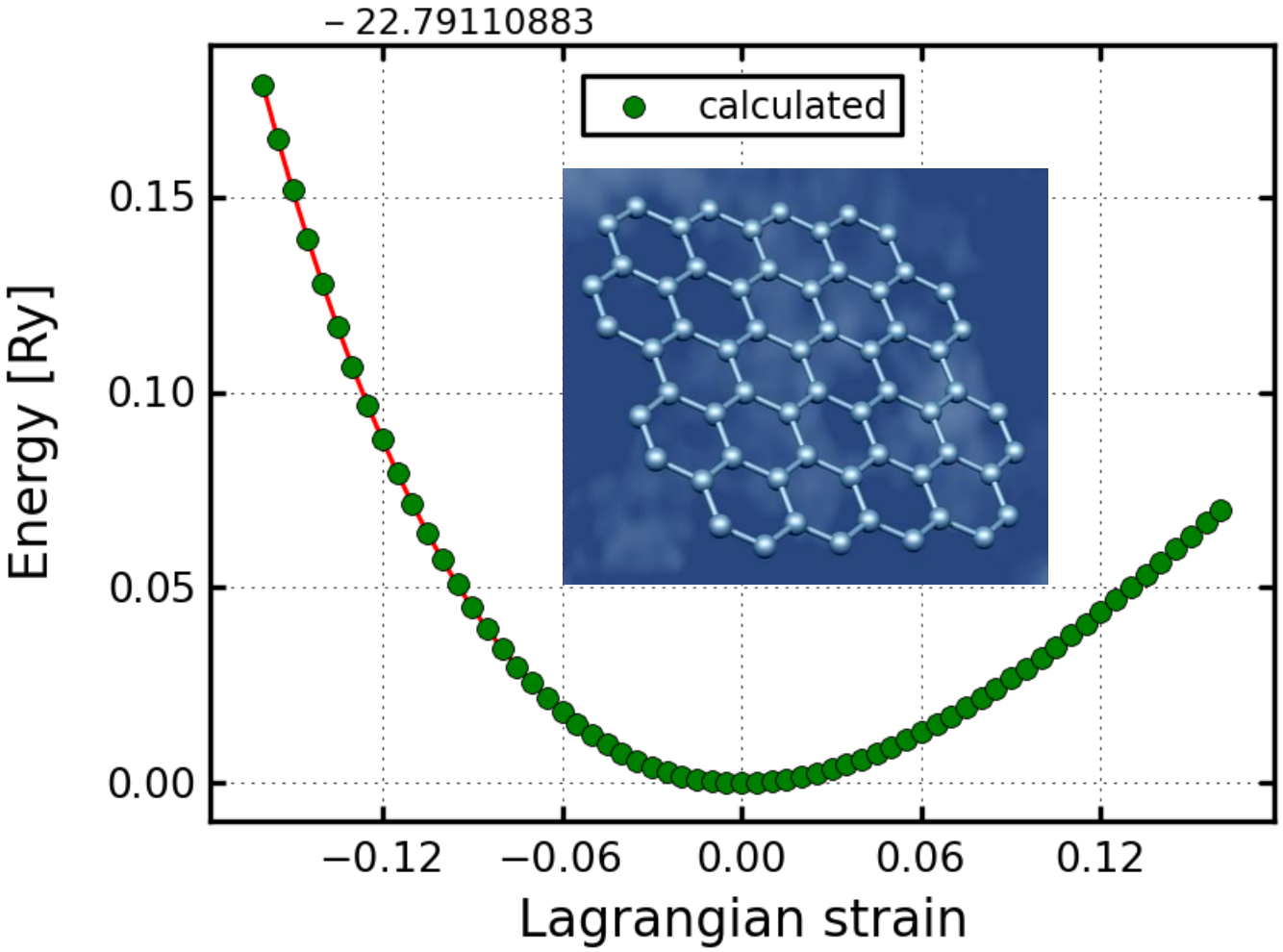
Spin-polarized bcc Fe



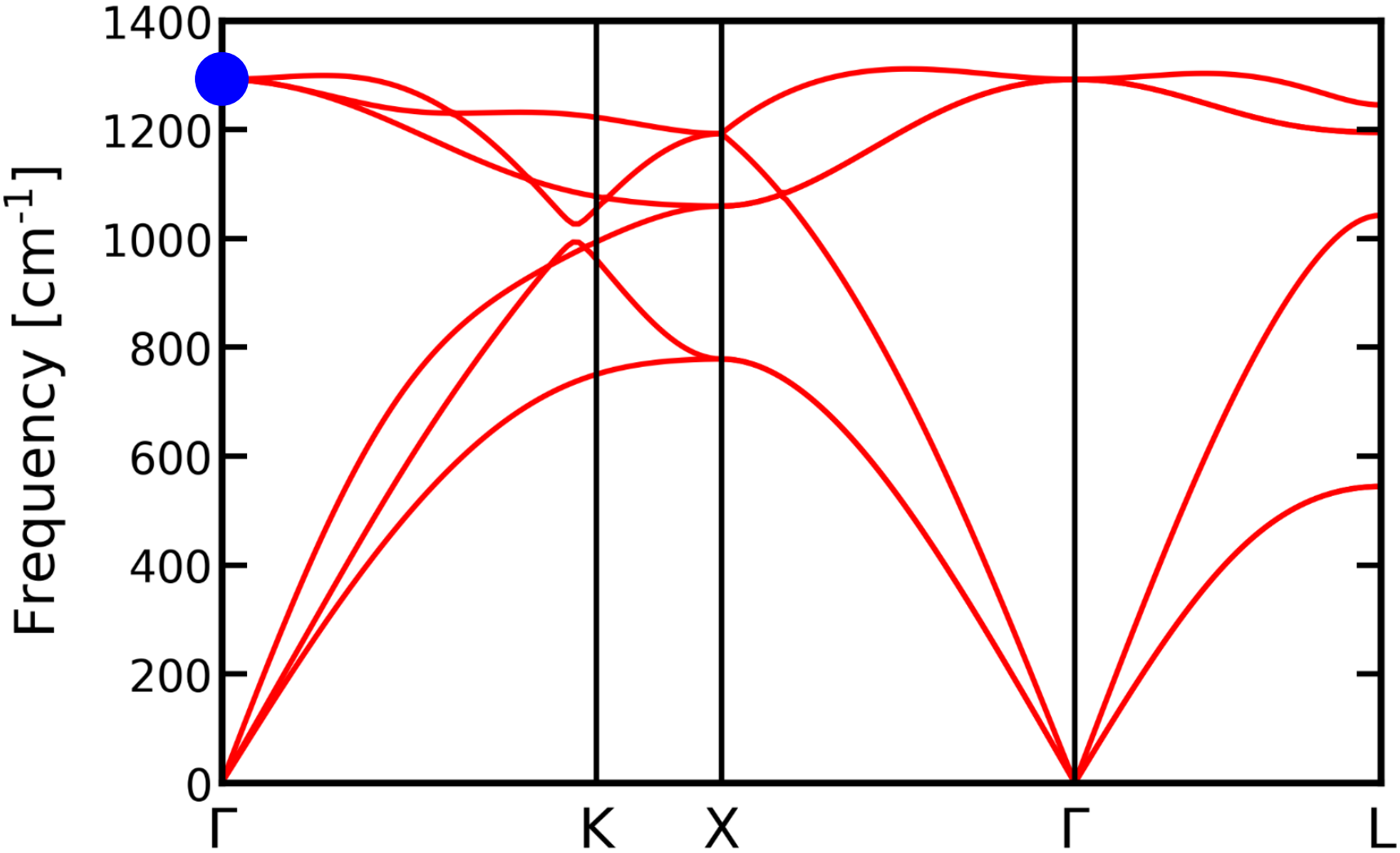
Relaxation of Pyridine



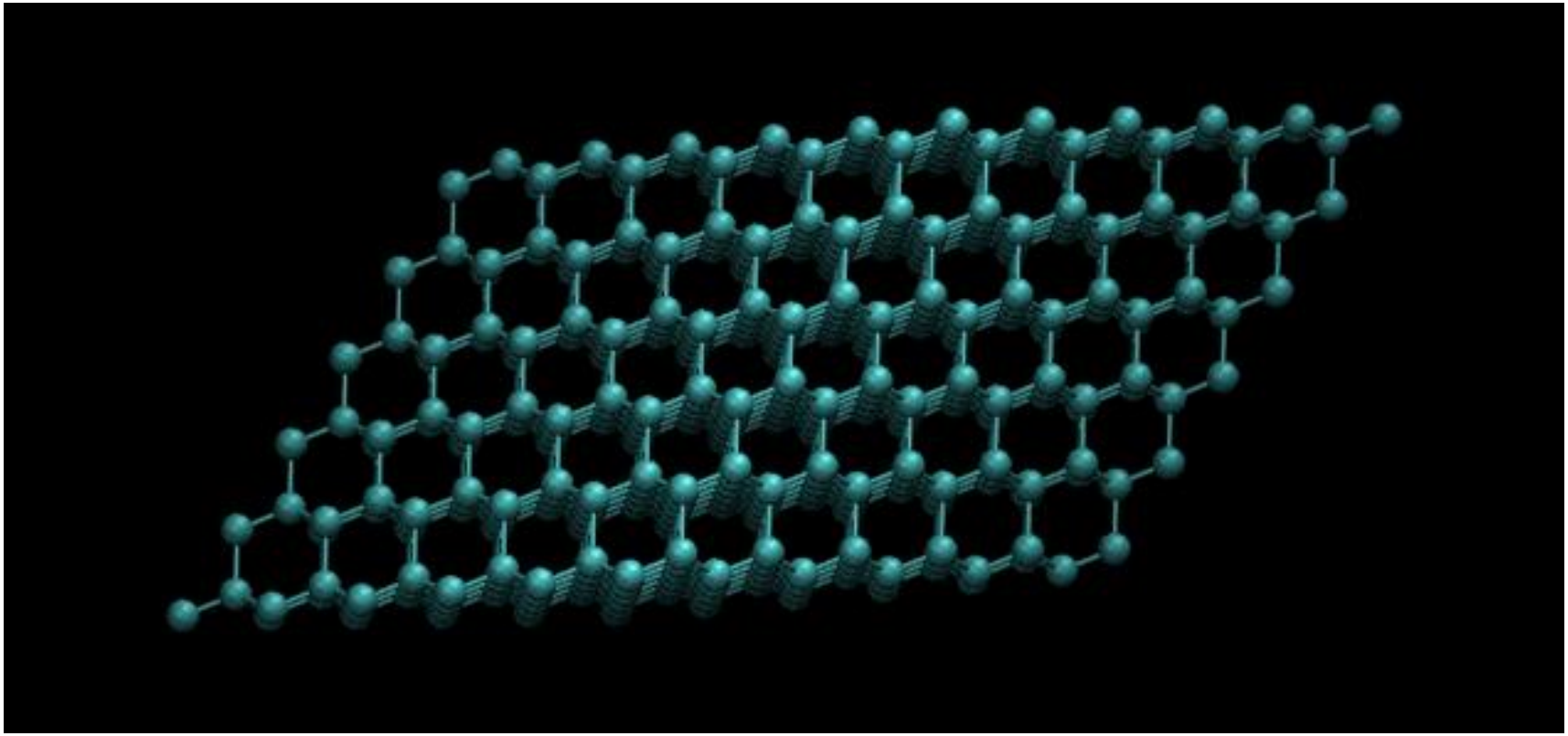
Graphene (100) Strain



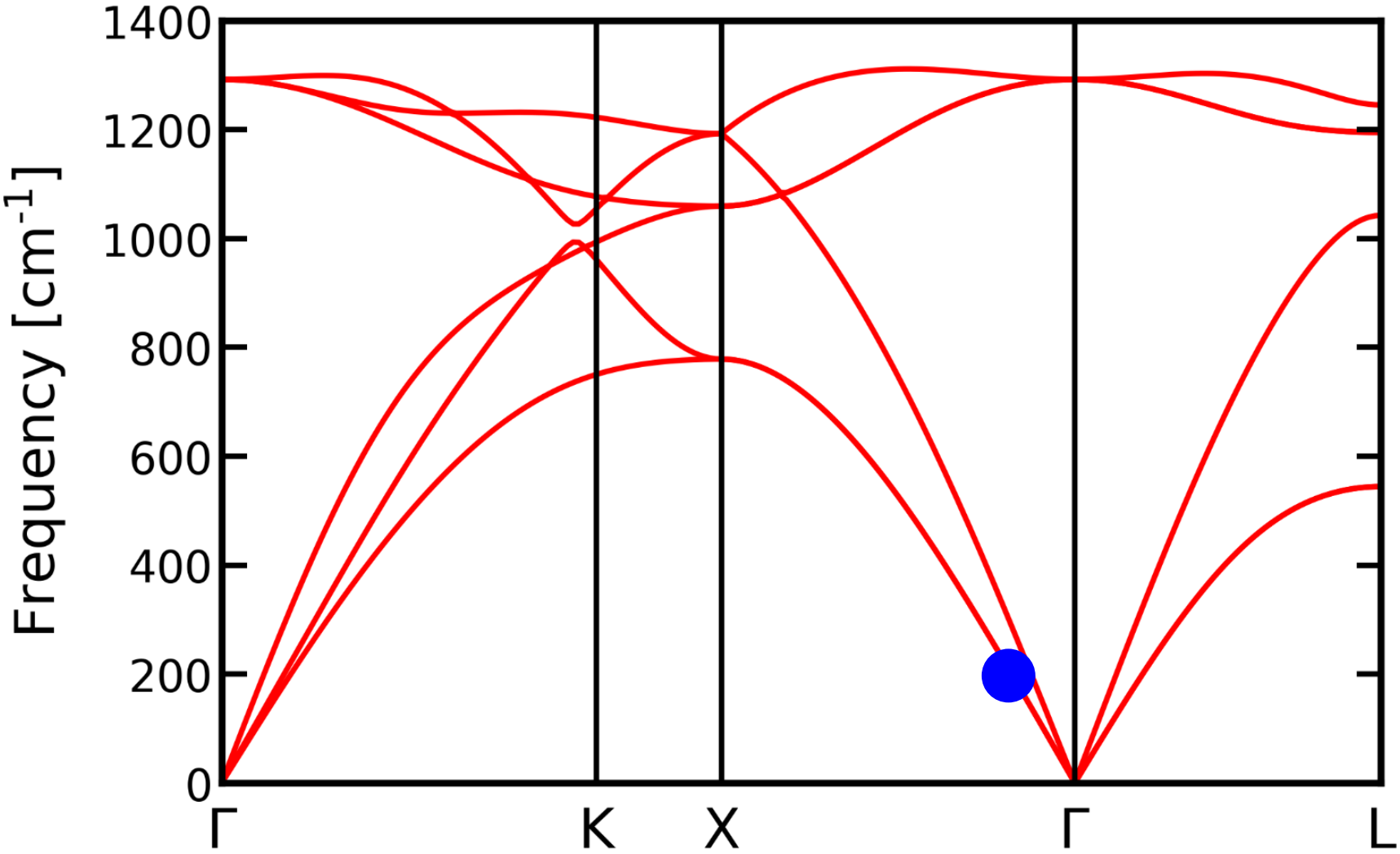
Phonon Dispersion of diamond



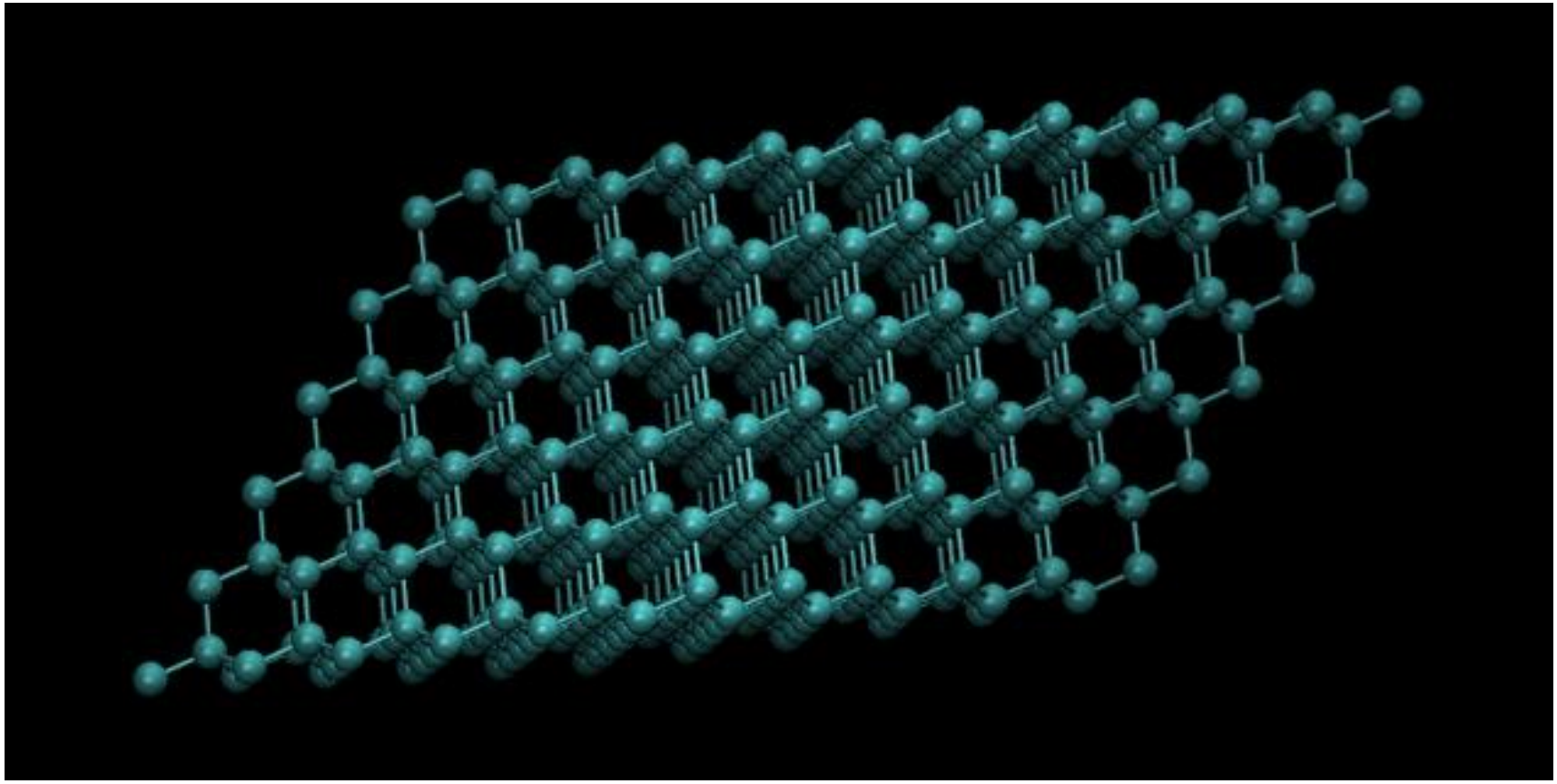
Animated Phonon Modes



Phonon Dispersion of diamond

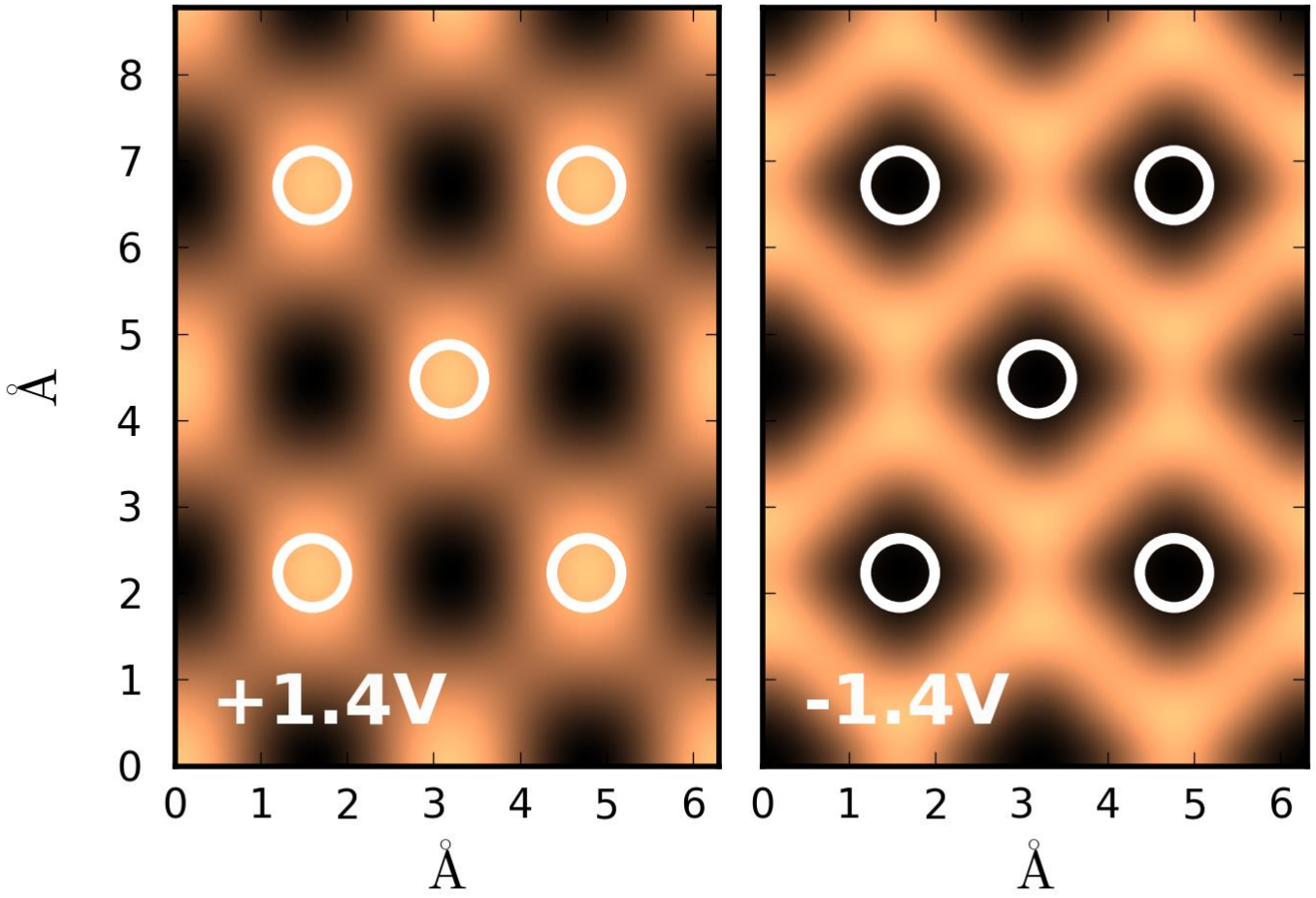


Animated Phonon Modes

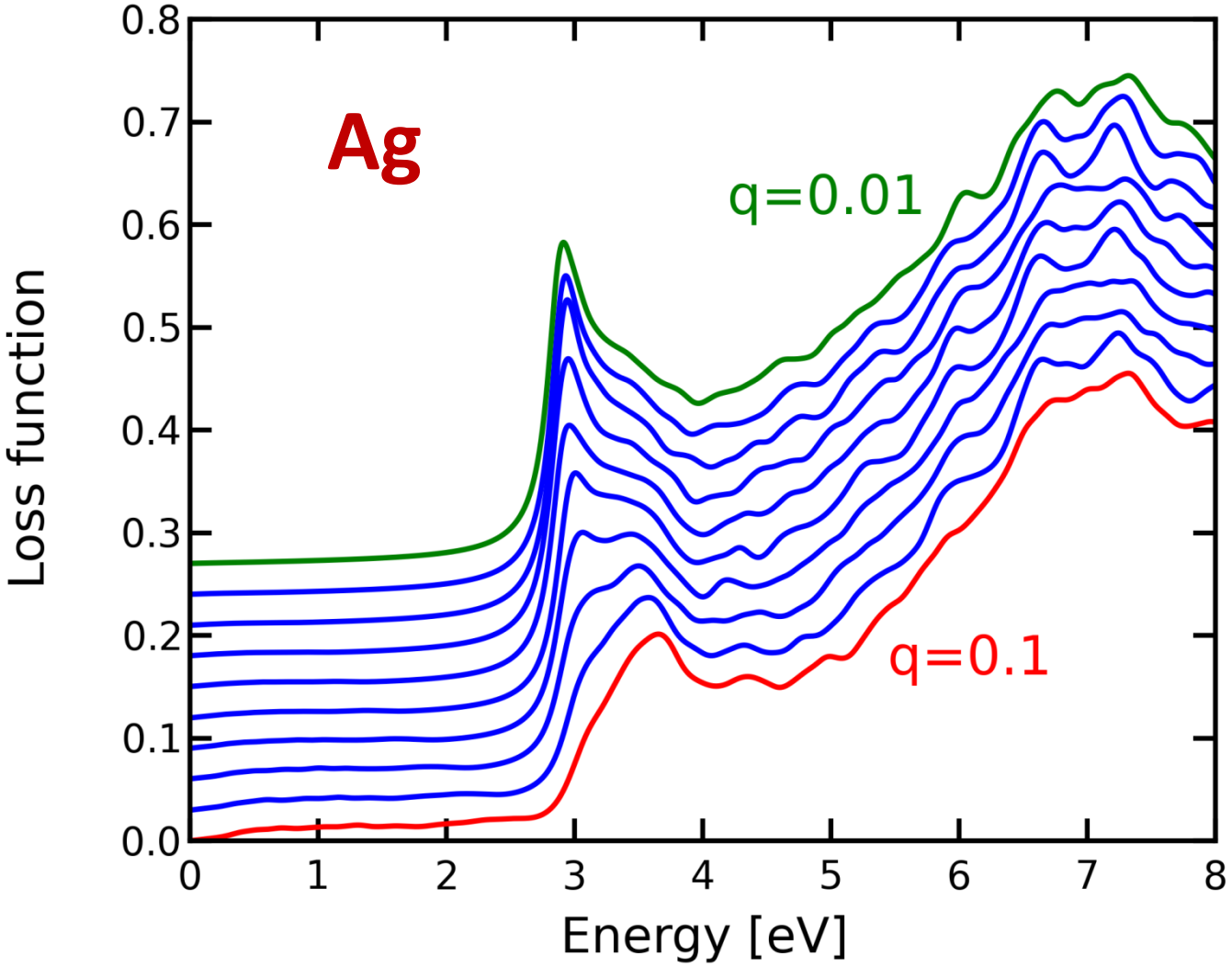


STM Images

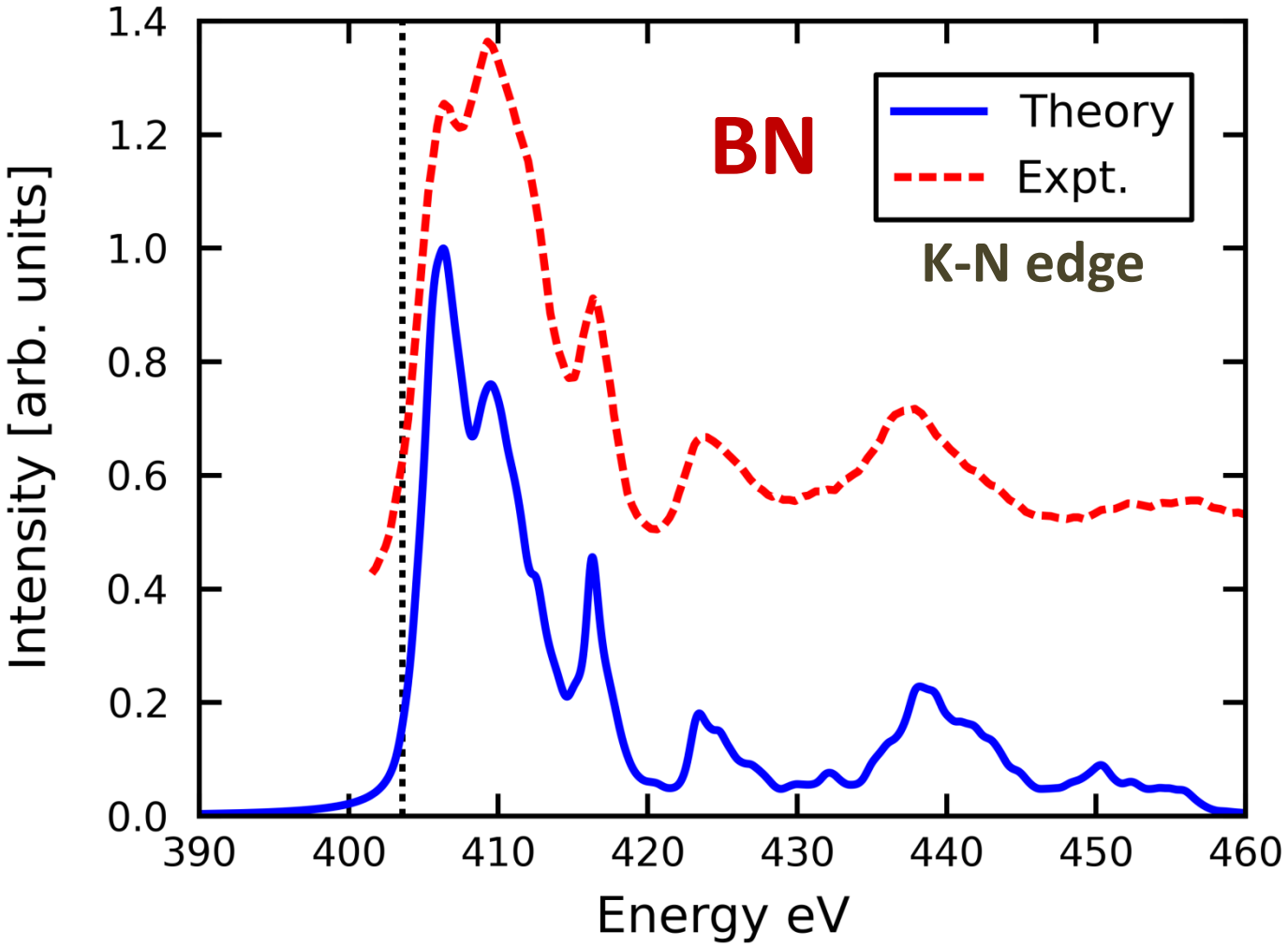
W(110)



Electron-Loss Spectra (TDDFT)



Core-Level Spectra (BSE)



Validation of Ab-Initio Calculation

Science AAAS

Home News Journals Topics Careers

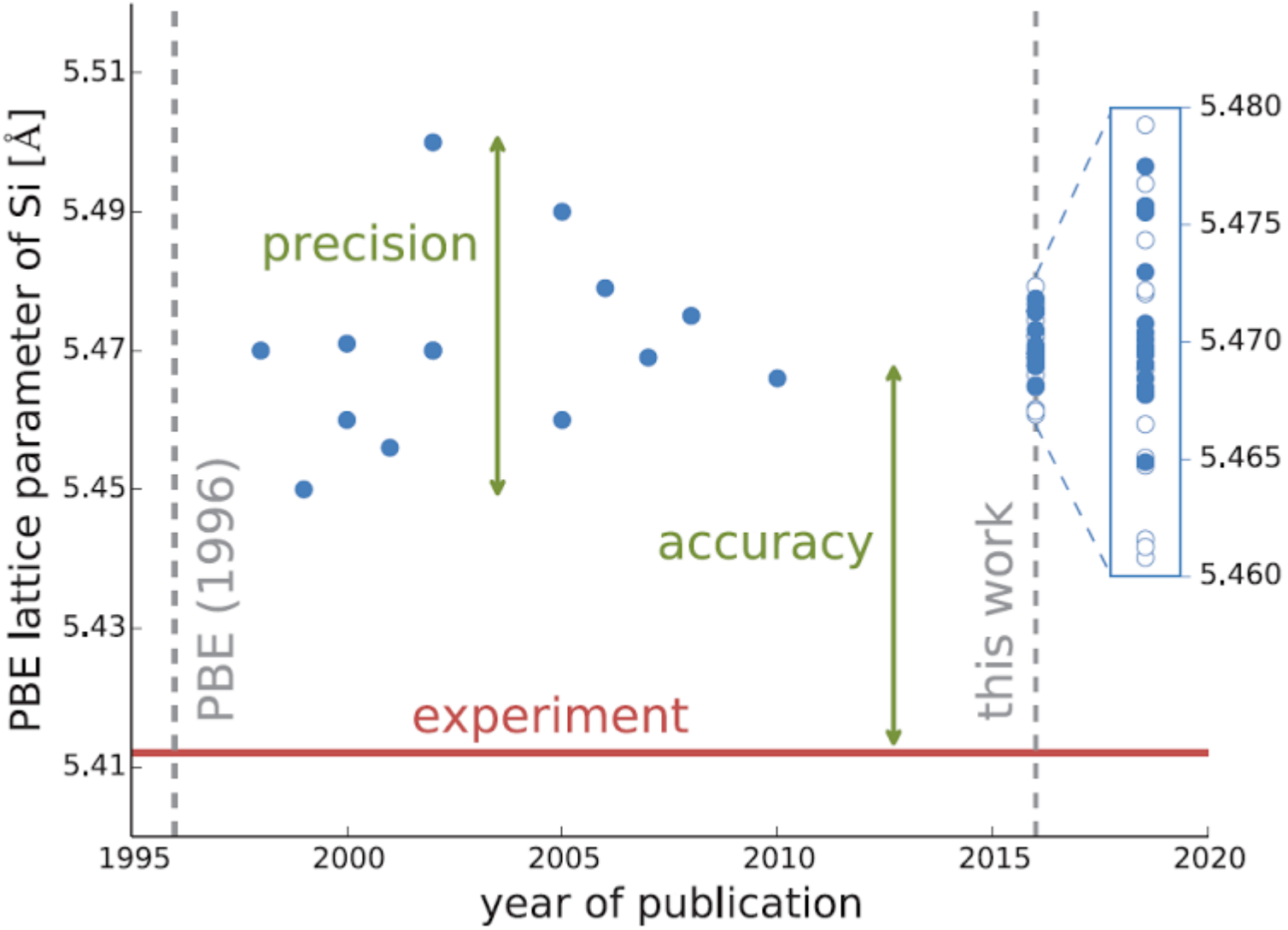
Science Science Advances Science Immunology Science Robotics Science Signaling Science Translational Medicine

RESEARCH ARTICLE SUMMARY

DFT METHODS

Reproducibility in density functional theory calculations of solids

Validation of Ab-Initio Calculation



Excitons in van-der-Waals Materials

PHYSICAL REVIEW B **97**, 241114(R) (2018)

Rapid Communications

Dimensionality of excitons in stacked van der Waals materials: The example of hexagonal boron nitride

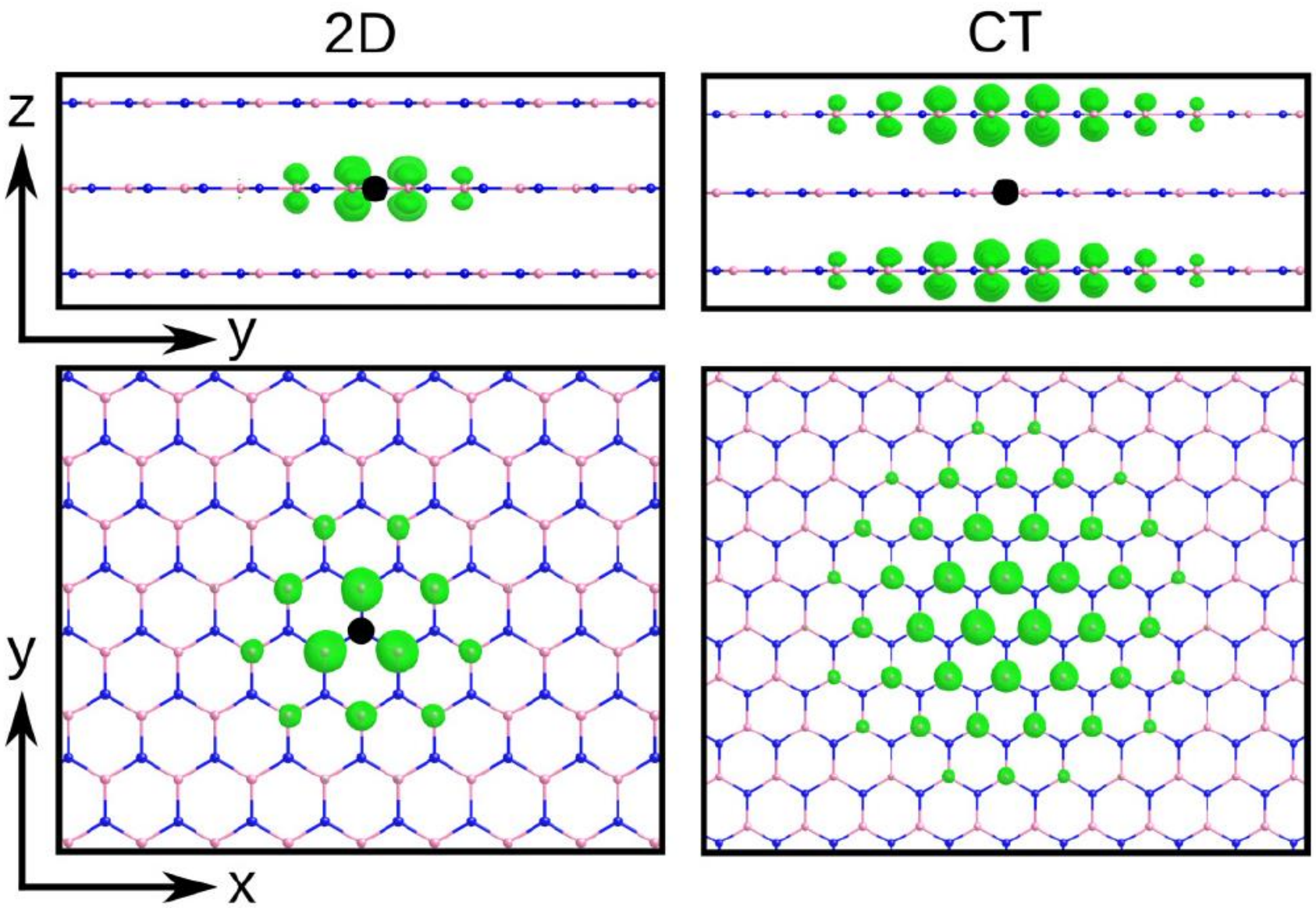
Wahib Aggoune,[1,2] Caterina Cocchi,[1,3,*] Dmitrii Nabok,[1,3] Karim Rezouali,[2] Mohamed Akli Belkhir,[2] and Claudia Draxl[1,3,†]

[1] *Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany*

[2] *Laboratoire de Physique Théorique, Faculté des Sciences Exactes, Université de Bejaia, 06000 Bejaia, Algeria*

[3] *European Theoretical Spectroscopic Facility (ETSF)*

Excitons in van-der-Waals Materials



Predicting ground-state configurations

CHEMISTRY OF MATERIALS

Review

pubs.acs.org/cm

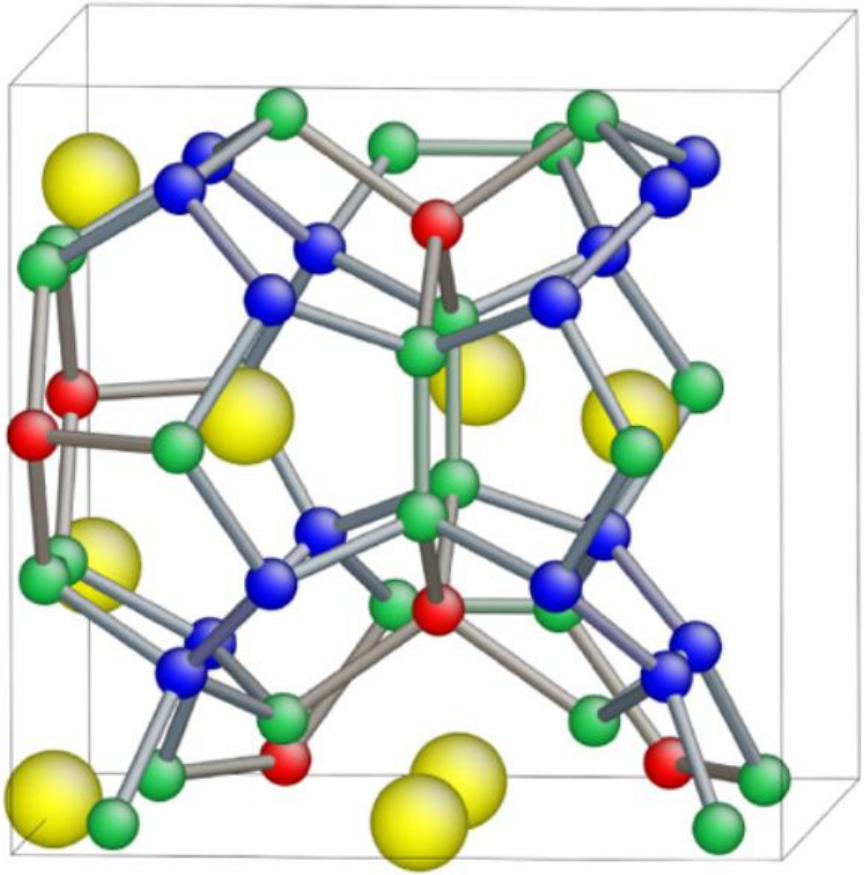
Predicting Ground-State Configurations and Electronic Properties of the Thermoelectric Clathrates $Ba_8Al_xSi_{46-x}$ and $Sr_8Al_xSi_{46-x}$

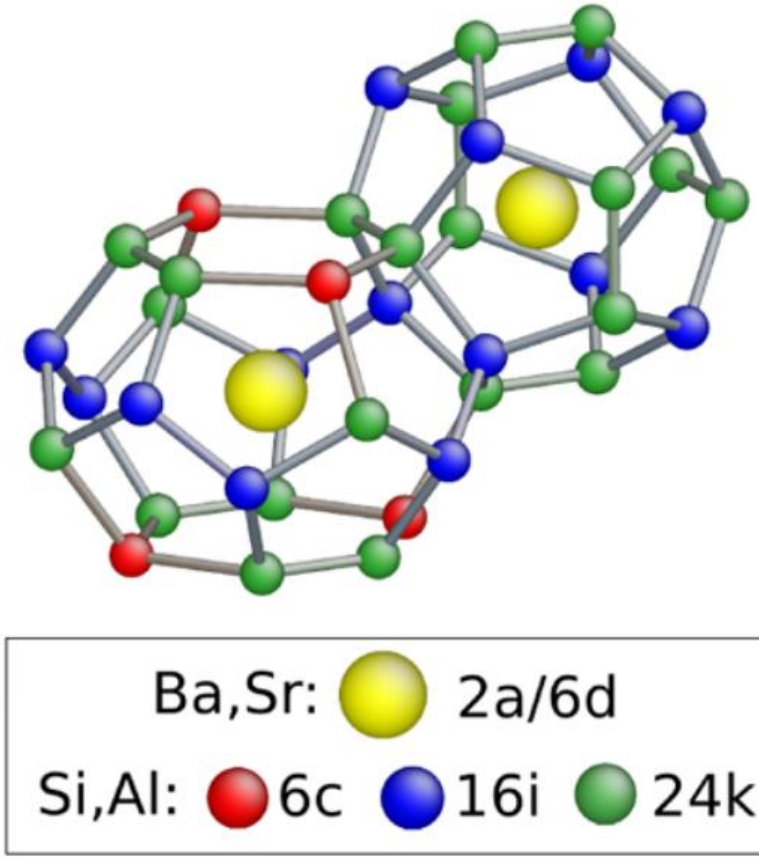
Maria Troppenz,[†] Santiago Rigamonti,[†] and Claudia Draxl*[,†,‡]

[†]Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

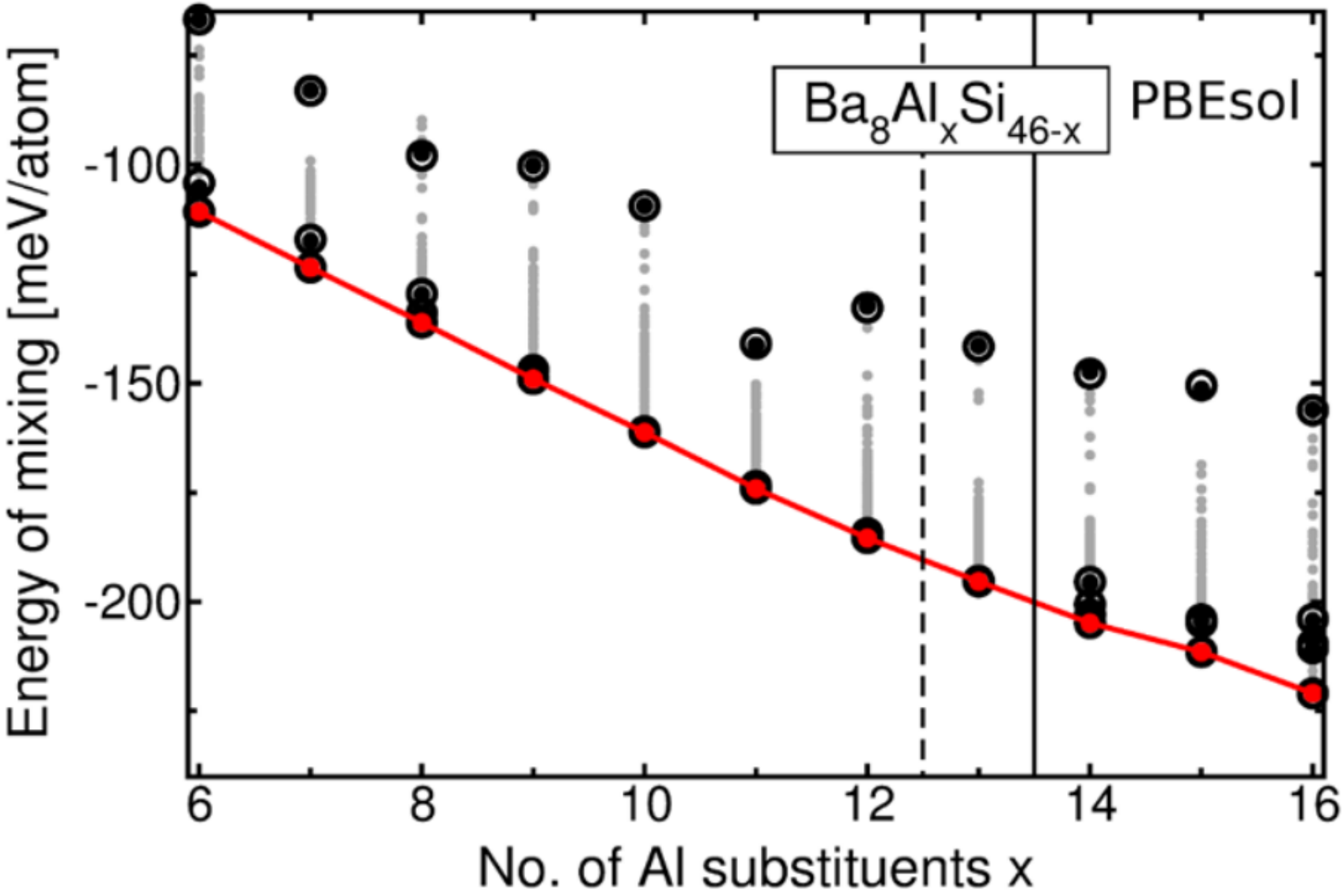
[‡]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany

Predicting ground-state configurations





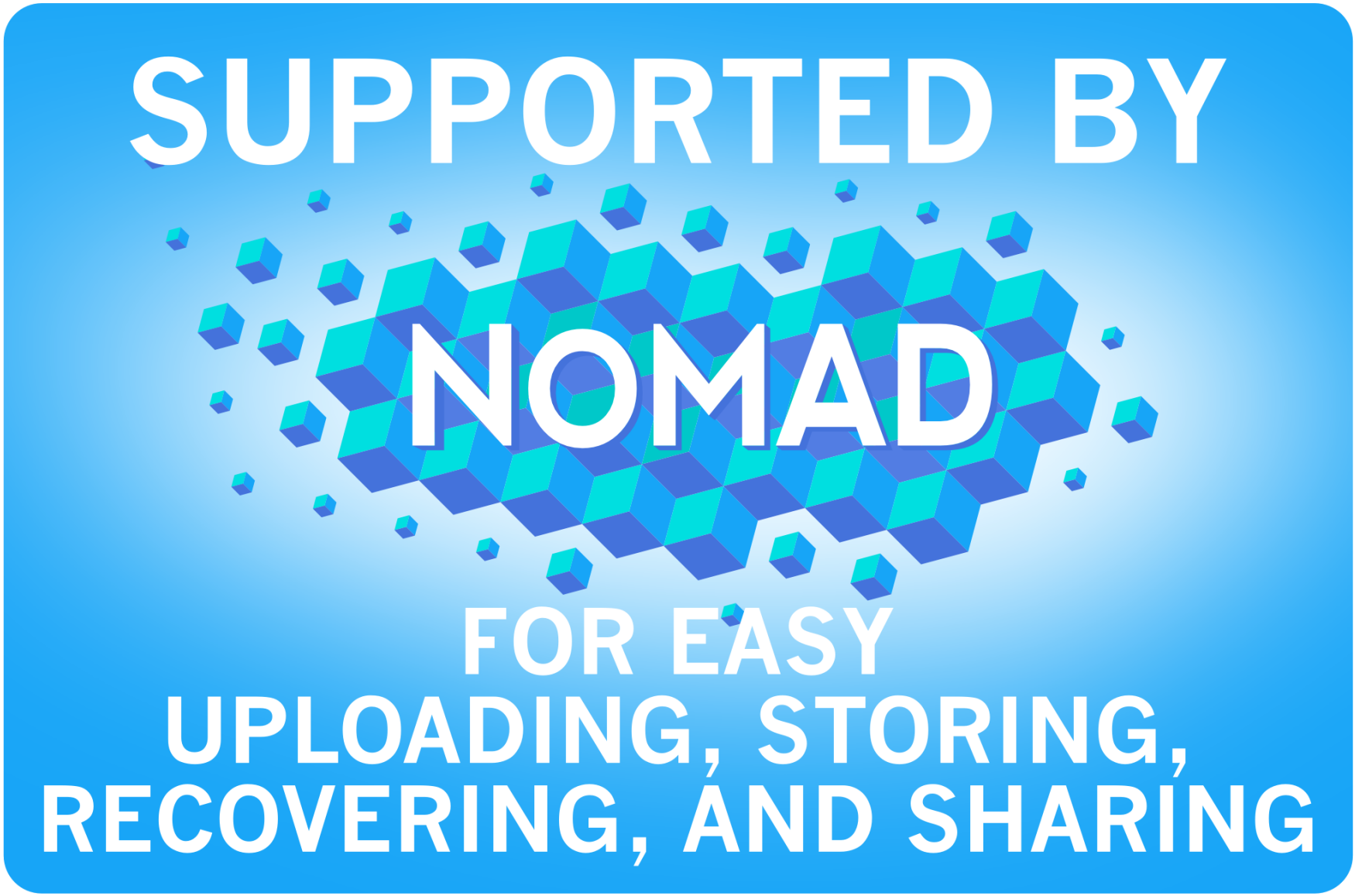
Predicting ground-state configurations

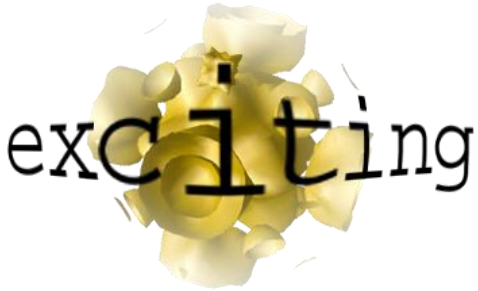


exciting: Tools & more

- ElaStic
- LayerOptics
- CELL
- NOMAD project

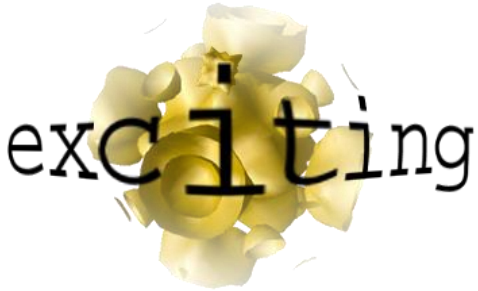
The NOMAD Project





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

   …


</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

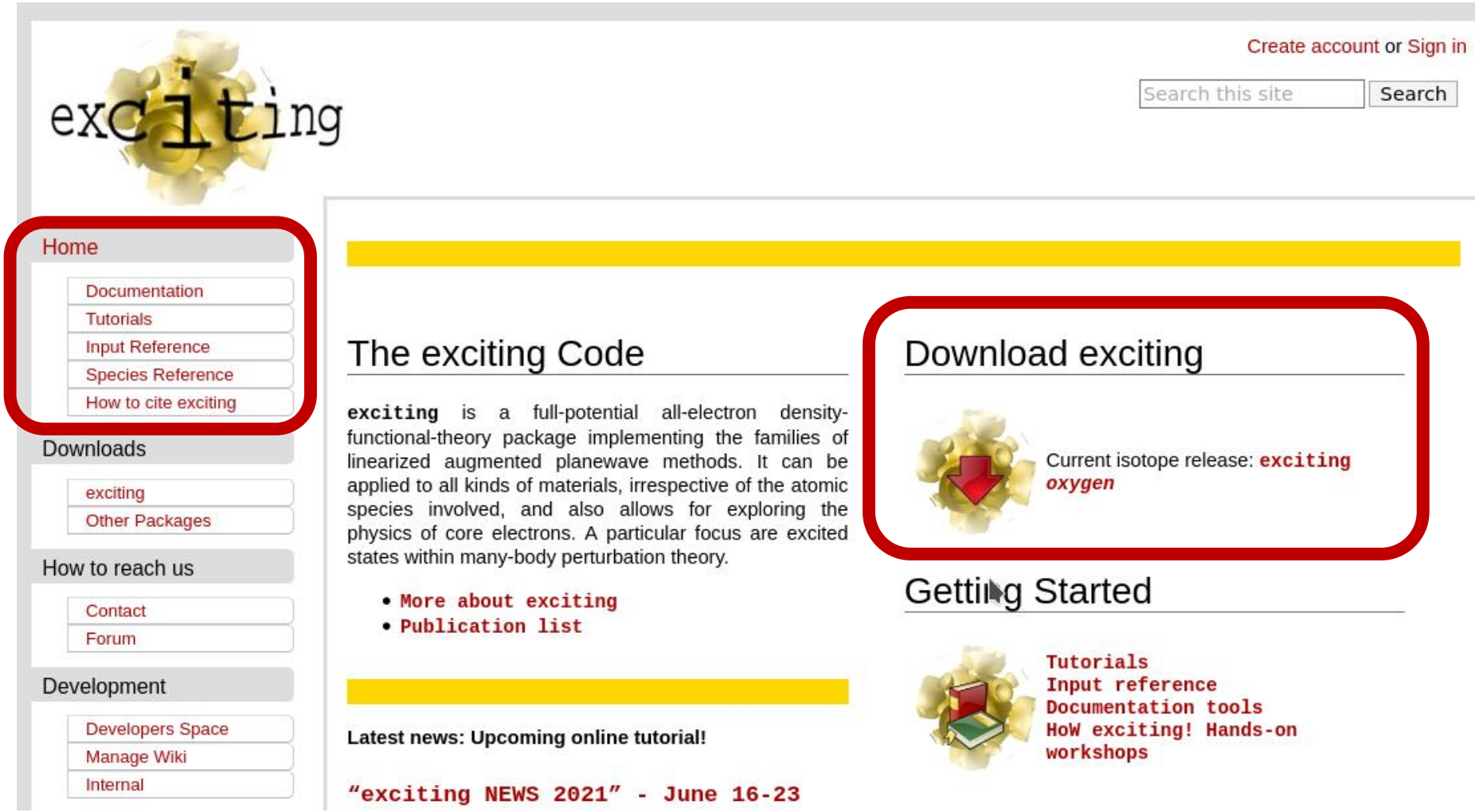
Download

http://exciting-code.org

exciting *oxygen*

June 15, 2021

exciting Website



Tutorials

Home

- Documentation
- Tutorials
- Input Reference
- Species Reference
- How to cite exciting

Downloads

exciting Tutorials

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

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

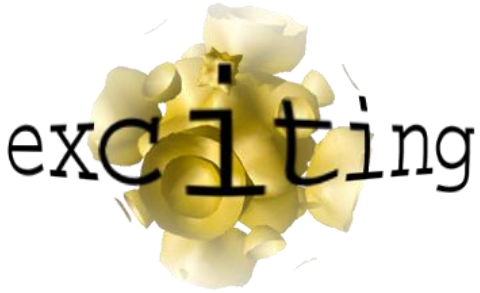
Tutorials describing ***advanced*** features are indicated by 【a】

READ BEFORE STARTING

【b】 How to set environment variables for tutorial scripts

GETTING STARTED

【b】 Download and compile exciting
【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



Tutorials

Tutorial Scripts and Environment Variables

by Pasquale Pavone for exciting *oxygen*

Purpose: Here, it will be explained how to set those **environment variables** which are needed for running examples presented in the tutorials. Furthermore, some general information is given about the scripts that are used in **exciting** tutorials.

Fold

Table of Contents

Tutorials

1. Setting environment variables

The next instructions have to be executed only once before starting your first tutorial!

Very important: Before starting, the following environment variable **must** be set by the user

- **EXCITINGROOT** = full path of the directory **exciting** after download, *e.g.*: **/home/tutorials/exciting** .

The above variable is used to define other environment variables

- **EXCITINGTOOLS** = Directory where the tutorial scripts are located, defined as **$EXCITINGROOT/tools** .
- **TIMEFORMAT** = Output format for writing on the screen the running elapsed time, used in some script.

```
#=============================================================================
# The following shell variables are needed for executing scripts in exciting tutorials
#
export EXCITINGROOT=/home/tutorials/exciting
export EXCITINGTOOLS=$EXCITINGROOT/tools
#-----------------------------------------------------------------------------
export TIMEFORMAT="   Elapsed time = %0lR"
#-----------------------------------------------------------------------------
export WRITEMINMAX="1"
#-----------------------------------------------------------------------------
export PYTHONPATH=$PYTHONPATH:$EXCITINGTOOLS/stm
export PATH=$PATH:$EXCITINGTOOLS:$EXCITINGROOT/bin:$EXCITINGTOOLS/stm
#=============================================================================
```

Tutorials

- Linux kernel version 4.19.0-13-amd64
- Intel-2019 compiler
- Bash shell
- Python 2.7.16
- Matplotlib 2.2.13
- Gnuplot 5.2 patchlevel 6
- xmgrace Grace-5.1.25
- vmd for LinuxAMD64, version 1.9
- xcrysden-1.5.24
- vesta 3.4.6

exciting Tutorials

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

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【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

Tutorials

Download and Compile exciting

by Alexander Buccheri & Pasquale Pavone for exciting *oxygen*

Purpose: In this tutorial you will learn how to download and quickly compile **exciting**.

```
$ tar xvf exciting.oxygen.tar.gz
```

exciting Tutorials

Download and Compile exciting

by **Alexander Buccheri** & **Pasquale Pavone** for **exciting** ***oxygen***

Purpose: In this tutorial you will learn how to download and quickly compile **exciting**.

---

compile with Intel ifort:

```
$ cd $EXCITINGROOT
$ cp build/platforms/make.inc.ifort build/make.inc
$ make smp
```

compile with GCC gfortran:

```
$ cd $EXCITINGROOT
$ cp build/platforms/make.inc.gfortran build/make.inc
$ make smp
```

Tutorials

```
$ time exciting_smp
```

```
$ make serial    # full serial version                    --> exciting_serial
$ make smp       # shared-memory multiprocessing version --> exciting_smp
$ make mpi       # mpi-parallelised version              --> exciting_purempi
$ make mpiandsmp # hybrid smp-mpi parallelised version   --> exciting_mpismp
```

Tutorials

☛ GROUND STATE

☛ METHODS:

【b】 Exchange-correlation functionals
【b】 How to visualize Kohn-Sham states
【b】 Spin-polarized calculations for bcc Fe
【b】 Spin-orbit coupling
【a】 Hybrid-functional calculations
【a】 Exact-exchange calculations
【a】 Van-der-Waals corrections
【a】 Dipole correction for surface calculations
【a】 DFT-1/2

☛ ELECTRONIC PROPERTIES:

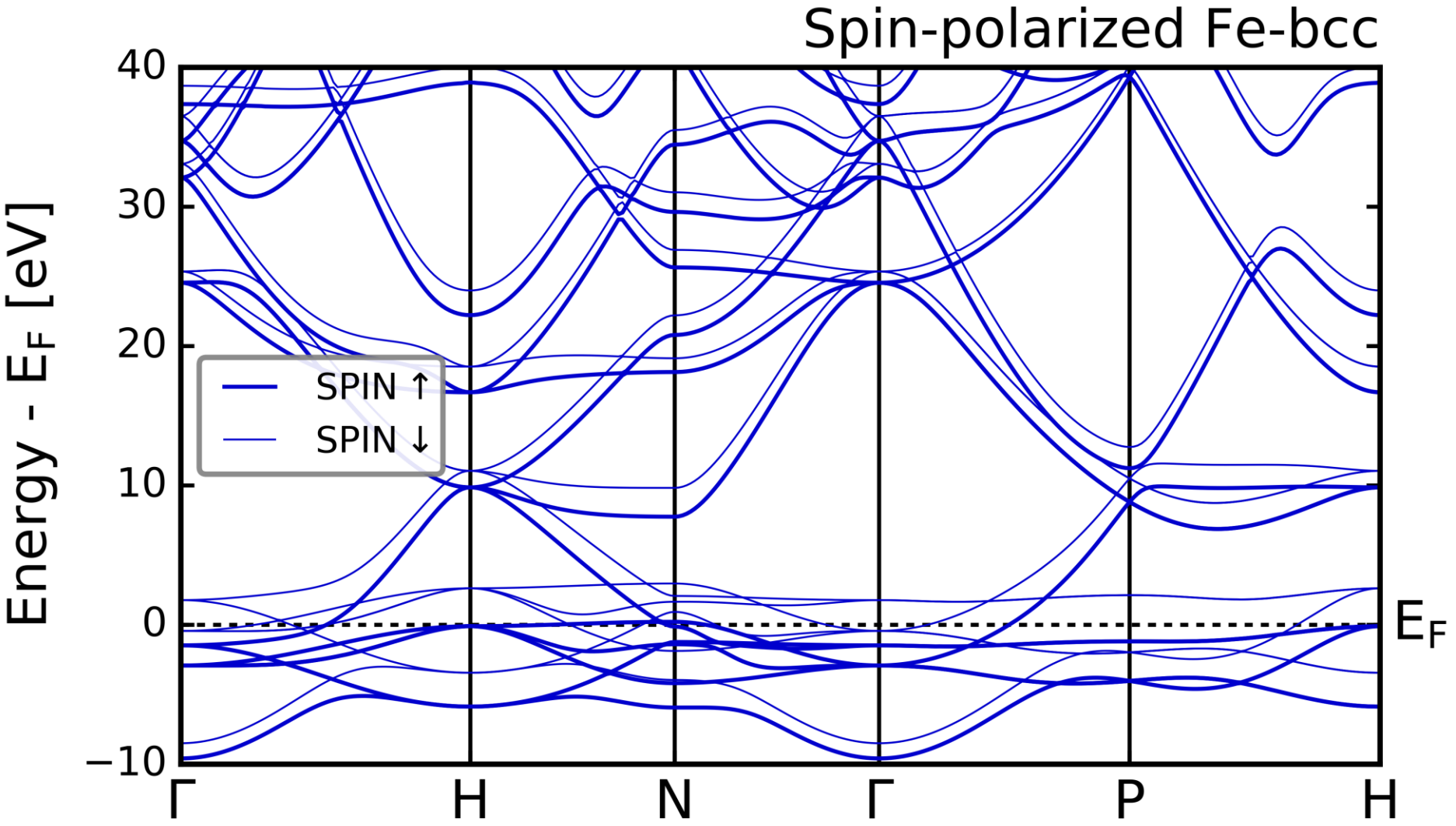
【a】 Wannier functions for interpolation in reciprocal space
【a】 Fermi surface visualization
【a】 Spin-texture calculation

Tutorials

☛ PLOTTING TOOLS

【b】 The python script "PLOT-band-structure.py"
【b】 The python script "PLOT-dos.py"
【b】 The python script "PLOT-files.py"
【a】 The python script "PLOT-spintext.py"
【a】 The python script "PLOT-multitask.py"

exciting **Tutorials**



Recommendation

We assume you are familiar with

Linux

The Last Slide: We are so Excited!

... and let‘s give a try!