



The Basics of FHI-aims

James A. Green, Konstantin Lion, and Andrei Sobolev

Molecular Simulations from First Principles (MS1P) e.V., Berlin, Germany



Hands-on Workshop on Electronic-Structure Theory and Artificial Intelligence for Materials Science

🕒 Nov. 5-8, 2025

📍 Shanghai, China



The FHI-aims Code



- Community based DFT and beyond code with an open development platform.
- Contributions from **over 200 people** all over the world from Berlin, Duke, UNC, Beijing, Helsinki, Warwick, Cardiff, Dalhousie, etc, with **20+ years of development**

Coordinators: V. Blum, S. Kokott, M. Rossi, M. Scheffler

Joseph Abbott, Alaa Akkoush, Heiko Appel, Victor Atalla, Kurt Baarmann, Carsten Baldauf, Alexej Bagrets, Jörg Behler, Daniel Berger, Josh Berryman, Sheng Bi, Benedikt Biedermann, Bjoern Bieniek, Volker Blum, Saeed Bohloul, Tiago Botari, Connor Box, Danilo Brambila, Gabriel Bramley, Daniel Bultrini, María Camarasa-Gómez, Christian Carbogno, Fabio Caruso, Marco Casadei, Michele Ceriotti, Amit Chaudhari, Wael Chibani, Sucismita Chutia, Francisco Antonio Delesma, Fabio Della Sala, Maria Dragoumi, Andreas Dolfen, Marc Dvorak, Simon Erker, Ferdinand Evers, Eduardo Fabiano, Matt Farrow, Nicola Ferri, Karen Fidanyan, Jakob Filser, Lukas Gallandi, Ralf Gehrke, Simiam Ghan, Luca Ghiringhelli, Mark Glass, Vivekanand Gobre, Dorothea Golze, Matthias Gramzow, James Green, Johannes Jan Günzl, Patrick Guetlein, Stefan Gutzeit, Volker Haigis, Sam Hall, Felix Hanke, Paula Havu, Ville Havu, Joscha Hekele, Olle Hellman, Uthpala Herath, Jan Hermann, Daniel Hernagómez-Pérez, Oliver Hofmann, Johannes Hoja, Xiaojuan Hu, William Huhn, Lukas Hörmann, Arvid Ihrig, Timo Jacob, Adam Jackson, Osama Jalil, Svenja Janke, Ran Jia, Rainer Johanni, Erin Johnson, Werner Jürgens, Juhan Matthias Kahk, Yosuke Kanai, Elisabeth Keller, Levi Keller, Roman Kempt, Matthias Kick, Woo Youn Kim, Jan Kloppenburg, Alexander Knoll, Florian Knoop, Franz Knuth, Simone Koecher, Gabrielle Koknat, Sebastian Kokott, Hagen-Henrik Kowalski, Raul Laasner, Lucas Lang, Bjoern Lange, Marvin Lechner, Susi Lehtola, Maja-Olivia Lenz, Moritz Leucke, Sergey Levchenko, Alan Lewis, Jiachen Li, Xinzhen Li, Kailai Lin, Xinyi Lin, Konstantin Lion, Werner Lipsunen, Yair Litman, Chi Liu, Qing-Long Liu, Andrew Logsdail, Michael Lorke, Andreas Marek, Thomas Markovich, Reinhard Maurer, Florian Merz, Joerg Meyer, Wenhui Mi, Evgeny Moerman, Dylan Morgan, Jack Morgenstein, Christoph Muschielok, Mohammad Nakhaee, Lydia Nemec, Norbert Nemec, Kane O'Donnell, Harald Oberhofer, Berk Onat, Alberto Otero de la Rosa, Ramon L. Panades-Barrueta, Hao Peng, Mariia Pogodaeva, Eszter Pos, Alastair Price, Thomas Purcell, Jingkai Quan, Nathaniel Raimbault, Markus Rampp, Karsten Rasim, Xinguo Ren, Karsten Reuter, Norina Richter, Stefan Ringe, Patrick Rinke, Herzain Rivera, Matti Ropo, Mariana Rossi, Tuomas Rossi, Adrienn Ruzsinszky, Nikita Rybin, Georg Michelitsch, Andrea Sanfilippo, Matthias Scheffler, Markus Schneider, Christoph Schober, Franziska Schubert, Honghui Shang, Tonghao Shen, Markus Sinstein, Justin Clifford Smith, Andrey Sobolev, Ari-Pekka Soikkeli, Ruyi Song, Aloysius Soon, Pavel Stishenko, Muhammad Tahir, Jun Tang, Alexandre Tkatchenko, Thomas Theis, Oscar van Vuren, Alvaro Vazquez Mayagoitia, Daniel Waldschmidt, Suzy Wallace, Tianlin Wang, Yanyong Wang, Jürgen Wieferink, Scott Woodley, Jianhang Xu, Yong Xu, Yi Yao, Mina Yoon, Ted Yu, Victor Yu, Zhenkun Yuan, Marios Zacharias, Guo-Xu Zhang, Igor Ying Zhang, Min-Ye Zhang, Wentao Zhang, Wenxing Zhang, Rundong Zhao, Ruiyi Zhou, Yuanyuan Zhou, Tong Zhu

Thank you to everyone!

“Original” FHI-aims implementation paper (2009):

Computer Physics Communications 180 (2009) 2175–2196

Ab initio molecular simulations with numeric atom-centered orbitals

Volker Blum*, Ralf Gehrke, Felix Hanke, Paula Havu, Ville Havu, Xinguo Ren, Karsten Reuter, Matthias Scheffler*

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Read the FHI-aims
roadmap on arXiv

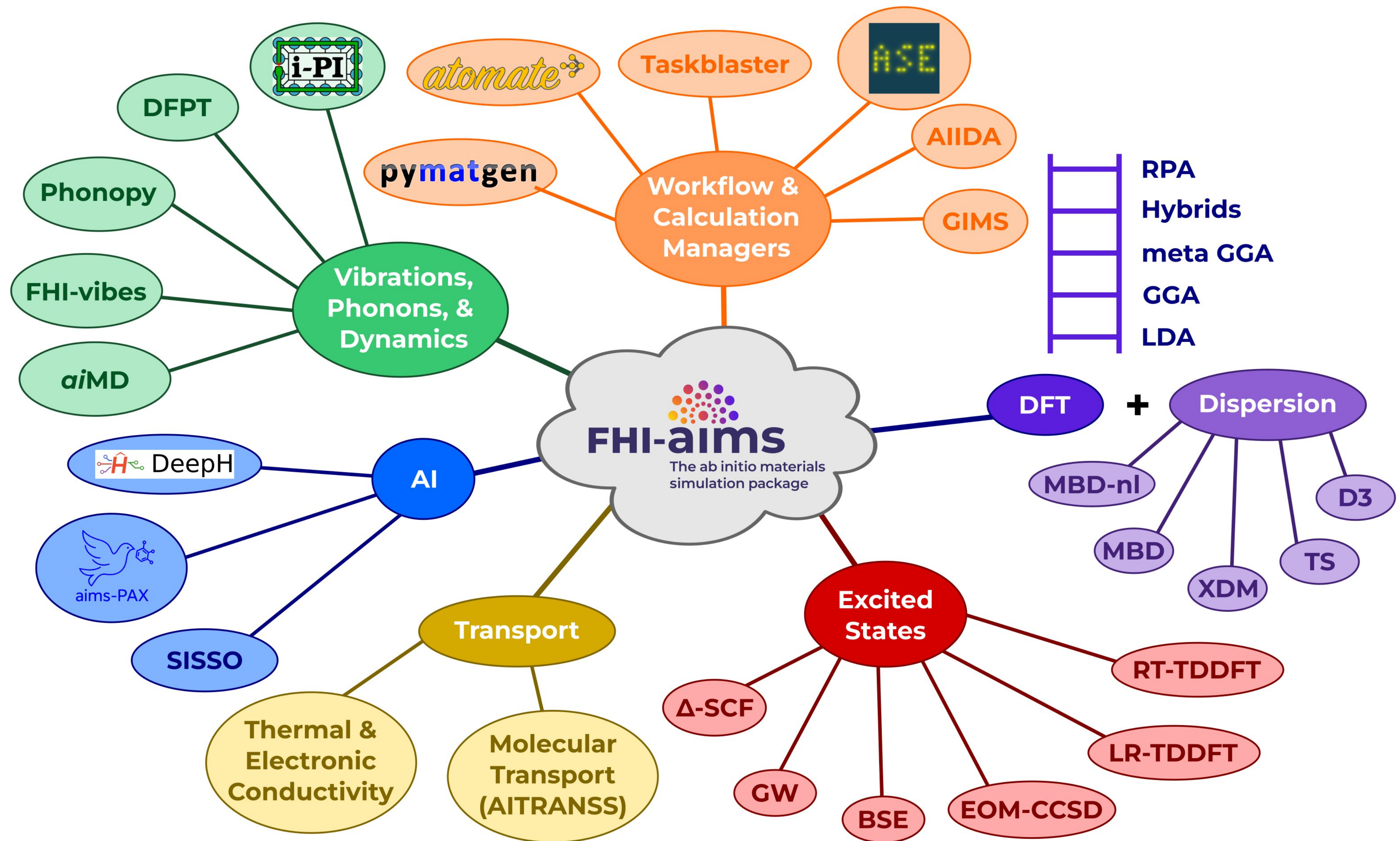


FHI-aims roadmap 2025 paper : 30+ sections, 200+ authors

Roadmap on Advancements of the FHI-aims Software Package

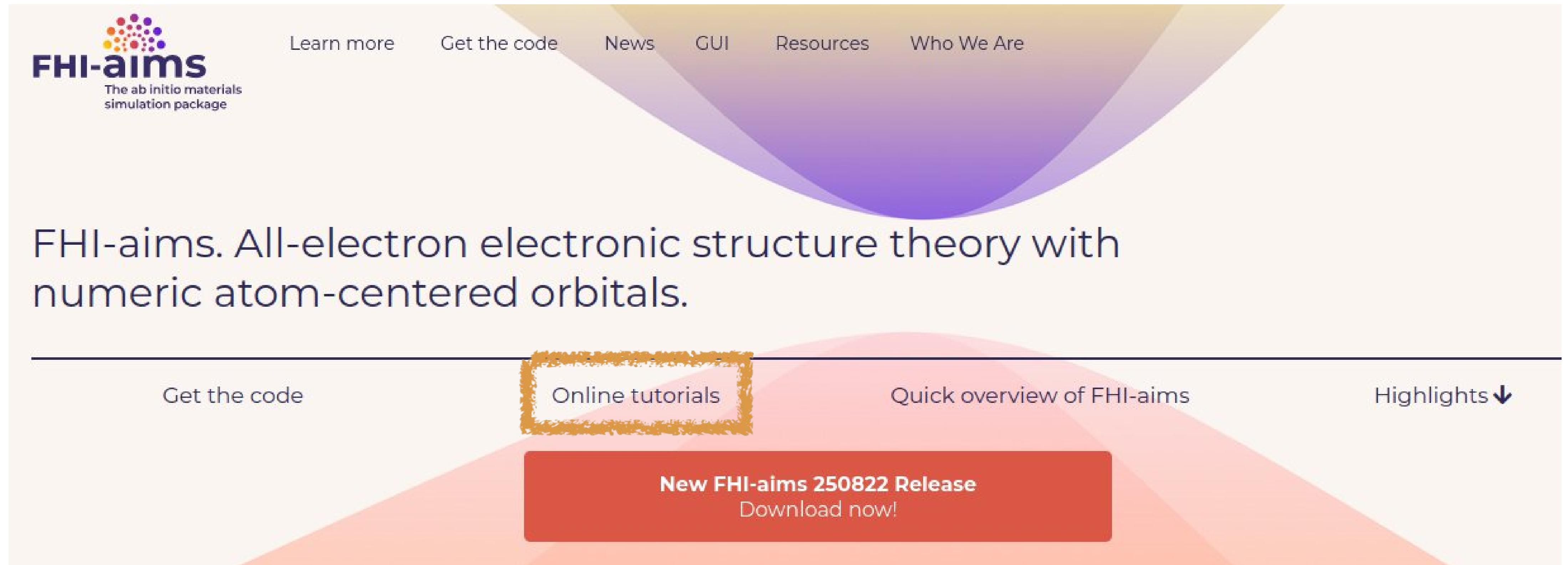
Joseph W. Abbott, Carlos Mera Acosta, Alaa Akkoush, Alberto Ambrosetti, Viktor Atalla, Alexej Bagrets, Jörg Behler, Daniel Berger, Björn Bieniek, Jonas Björk, Volker Blum, Saeed Bohloul, Connor L. Box, Nicholas Boyer, Danilo Simoes Brambila, Gabriel A. Bramley, Kyle R. Bryenton, María Camarasa-Gómez, Christian Carbogno, Fabio Caruso, Sucismita Chutia, Michele Ceriotti, Gábor Csányi, William Dawson, Francisco A. Delesma, Fabio Della Sala, Bernard Delley, Robert A. DiStasio Jr., Maria Dragoumi, Sander Driessen, Marc Dvorak, Simon Erker, Ferdinand Evers, Eduardo Fabiano, Matthew R. Farrow, Florian Fiebig, Jakob Filser, Lucas Foppa, Lukas Gallandi, Alberto Garcia, Ralf Gehrke, Simiam Ghan, Luca M. Ghiringhelli, Mark Glass, Stefan Goedecker, Dorothea Golze, Matthias Gramzow, James A. Green, Andrea Grisafi, Andreas Grüneis, Jan Günzl, Stefan Gutzeit, Samuel J. Hall, Felix Hanke, Ville Havu, Xingtao He, Joscha Hekele, Olle Hellman, Uthpala Herath, Jan Hermann, Daniel Hernangómez-Pérez, Oliver T. Hofmann, Johannes Hoja, Simon Hollweger, Lukas Hörmann, Ben Hourahine, Wei Bin How, William P. Huhn, Marcel Hülberg, Timo Jacob, Sara Panahian Jand, Hong Jiang, Erin R. Johnson, Werner Jürgens, J. Matthias Kahk, Yosuke Kanai, Kisung Kang, Petr Karpov, Elisabeth Keller, Roman Kempt, Danish Khan, Matthias Kick, Benedikt P. Klein, Jan Kloppenburg, Alexander Knoll, Florian Knoop, Franz Knuth, Simone S. Köcher, Jannis Kockläuner, Sebastian Kokott, Thomas Körzdörfer, Hagen-Henrik Kowalski, Peter Kratzer, Pavel Kůs, Raul Laasner, Bruno Lang, Björn Lange, Marcel F. Langer, Ask Hjorth Larsen, Hermann Lederer et al. (102 additional authors not shown)

What Can You Do With FHI-aims?



Where Can You Find FHI-aims?

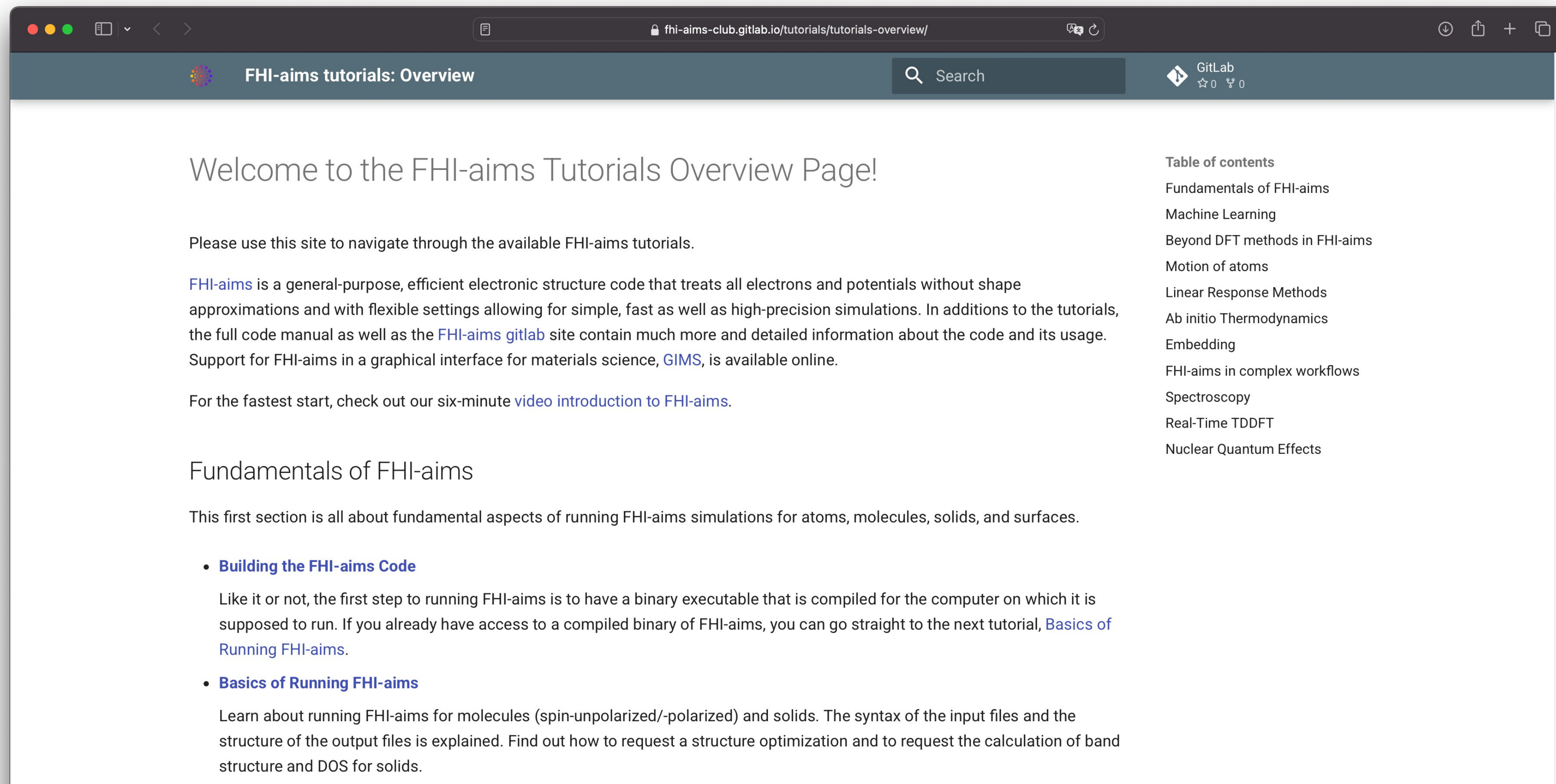
<https://fhi-aims.org/>



The screenshot shows the homepage of the FHI-aims website. At the top left is the FHI-aims logo, which consists of a cluster of colored dots above the text 'FHI-aims' and the tagline 'The ab initio materials simulation package'. To the right of the logo is a navigation bar with links: 'Learn more', 'Get the code', 'News', 'GUI', 'Resources', and 'Who We Are'. Below the navigation bar is a large heading: 'FHI-aims. All-electron electronic structure theory with numeric atom-centered orbitals.' Below this heading is a horizontal line. Underneath the line are four links: 'Get the code', 'Online tutorials' (which is highlighted with a yellow hand-drawn rectangle), 'Quick overview of FHI-aims', and 'Highlights ↓'. Below these links is a red rectangular button with the text 'New FHI-aims 250822 Release' and 'Download now!' below it.

Extensive and Growing List of Tutorials

<https://fhi-aims-club.gitlab.io/tutorials/tutorials-overview/>



The screenshot shows a web browser window displaying the "FHI-aims tutorials: Overview" page. The browser's address bar shows the URL `fhi-aims-club.gitlab.io/tutorials/tutorials-overview/`. The page has a dark header with the title "FHI-aims tutorials: Overview", a search bar, and a GitLab logo. The main content area has a light background and contains the following text:

Welcome to the FHI-aims Tutorials Overview Page!

Please use this site to navigate through the available FHI-aims tutorials.

[FHI-aims](#) is a general-purpose, efficient electronic structure code that treats all electrons and potentials without shape approximations and with flexible settings allowing for simple, fast as well as high-precision simulations. In additions to the tutorials, the full code manual as well as the [FHI-aims gitlab](#) site contain much more and detailed information about the code and its usage. Support for FHI-aims in a graphical interface for materials science, [GIMS](#), is available online.

For the fastest start, check out our six-minute [video introduction to FHI-aims](#).

Fundamentals of FHI-aims

This first section is all about fundamental aspects of running FHI-aims simulations for atoms, molecules, solids, and surfaces.

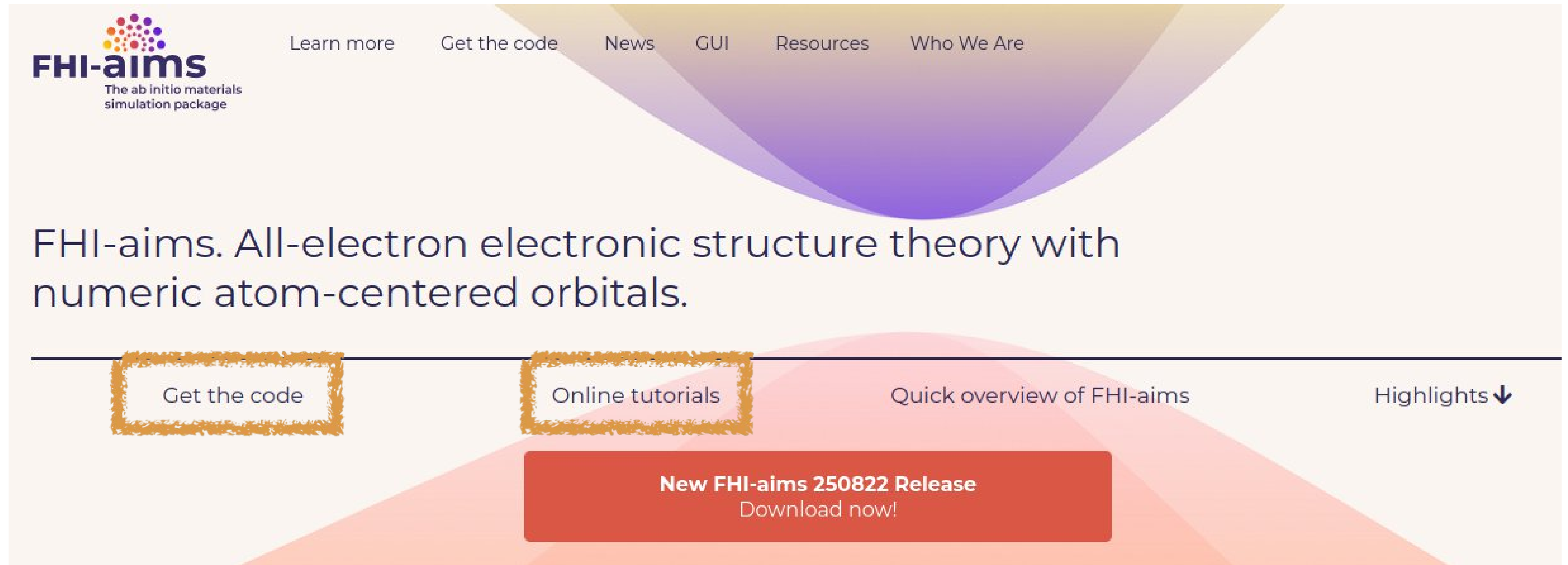
- **Building the FHI-aims Code**
Like it or not, the first step to running FHI-aims is to have a binary executable that is compiled for the computer on which it is supposed to run. If you already have access to a compiled binary of FHI-aims, you can go straight to the next tutorial, [Basics of Running FHI-aims](#).
- **Basics of Running FHI-aims**
Learn about running FHI-aims for molecules (spin-unpolarized/-polarized) and solids. The syntax of the input files and the structure of the output files is explained. Find out how to request a structure optimization and to request the calculation of band structure and DOS for solids.

On the right side of the page, there is a "Table of contents" section with the following links:

- Table of contents
- Fundamentals of FHI-aims
- Machine Learning
- Beyond DFT methods in FHI-aims
- Motion of atoms
- Linear Response Methods
- Ab initio Thermodynamics
- Embedding
- FHI-aims in complex workflows
- Spectroscopy
- Real-Time TDDFT
- Nuclear Quantum Effects

FHI-aims Website

<https://fhi-aims.org/>



The screenshot shows the FHI-aims website homepage. At the top left is the FHI-aims logo with the tagline 'The ab initio materials simulation package'. To the right of the logo is a navigation bar with links: 'Learn more', 'Get the code', 'News', 'GUI', 'Resources', and 'Who We Are'. Below the navigation bar is a large heading: 'FHI-aims. All-electron electronic structure theory with numeric atom-centered orbitals.' Below this heading is a horizontal line with four buttons: 'Get the code', 'Online tutorials', 'Quick overview of FHI-aims', and 'Highlights ↓'. The 'Get the code' and 'Online tutorials' buttons are highlighted with orange borders. Below the 'Online tutorials' button is a red button that says 'New FHI-aims 250822 Release Download now!'.

FHI-aims
The ab initio materials simulation package

Learn more Get the code News GUI Resources Who We Are

FHI-aims. All-electron electronic structure theory with numeric atom-centered orbitals.

Get the code Online tutorials Quick overview of FHI-aims Highlights ↓

New FHI-aims 250822 Release
Download now!

Getting the Code

Get the code

```
!****p* FHI-aims/aims_real
!  NAME
!    aims_real -- Program to call the top-level FHI-aims subroutine
!  SYNOPSIS
!
!    program aims_real
!
!  PURPOSE
!
!    This is FHI-aims code, which creates the standard FHI-aims executable program.
!
!    Please keep this top level program minimally complex. If you plan for more
!    complex uses of the aims() subroutine, please create a separate code to do so.
!
!    In principle, FHI-aims can also be built as a library. In that case, aims
!    is called as a subroutine aims() (see main.f90). The present program embeds
!    this subroutine for the standalone executable.
```

For Academia and Community

For Industry

For Cloud Computing

FHI-aims is developed by a large community of scientists worldwide, without whom this code would not exist. Licenses for academia and industry can be obtained from the nonprofit association Molecular Simulations from First Principles (MS1P) e.V. In addition, we also offer support for cloud computing with FHI-aims. For more details, click on the appropriate field above. If you have any questions, please contact aims-coordinators@ms1p.org .

Any FHI-aims license revenue that MS1P receives goes back into development, maintenance and community support of the FHI-aims project.

Getting the Code

Academia and Community

FHI-aims is a code based in academia, created by a large community. And yes, we want to you use FHI-aims, and we are immensely grateful to anyone who chooses to contribute to the code. Please follow the steps below.

For members of a group that already holds an FHI-aims license

Please register for access at the [Registration site \(aimsclub\)](#). In order to register, you will need the user ID (and approval) of the main license holder, most likely your group leader or PI.

We invite you to become part of an active community. The [FHI-aims GitLab server](#) and the [FHI-aims Slack workspace](#) are effectively the main support sites for the code. We need to manually invite users to those resources. Once you are registered in the aimsclub, please ask us for Slack workspace and GitLab access by e-mailing: aims-coordinators@mslp.org.

For external groups that do not have an FHI-aims license yet

We look forward to having you as a part of our active FHI-aims community. To obtain FHI-aims, you need to obtain a license from Molecular Simulations from First Principle e.V. (MS1P e.V.). We offer these types of licenses:

Academic license

Use of FHI-aims in an academic setting by a single research group (at a university, non-profit research labs, etc.), with:

- up to five users - price: 2,000 Euro (+ VAT), [PDF License Agreement](#) ↓
- up to 20 users - price: 4,000 Euro (+ VAT), [PDF License Agreement](#) ↓

The payment is voluntary. It helps to run the website, distribute the code, and other small things. It does not pay the code developers. Please fill in the [academic license form](#) in any case. If needed, add a handwritten change to the payment amount and send a short explanation to aims-coordinators@mslp.org. In case of questions please contact aims-coordinators@mslp.org.

Design Principles of FHI-aims

The Vision

Quantum mechanics-based simulations of real, complex molecules and materials and their properties without a priori precision and accuracy limitations.

- **Key design choice:** Which basis functions to use?

Gaussians



TURBOMOLE



Plane Waves/ Pseudopotentials



CASTEP

Numeric Atom- Centered Orbitals

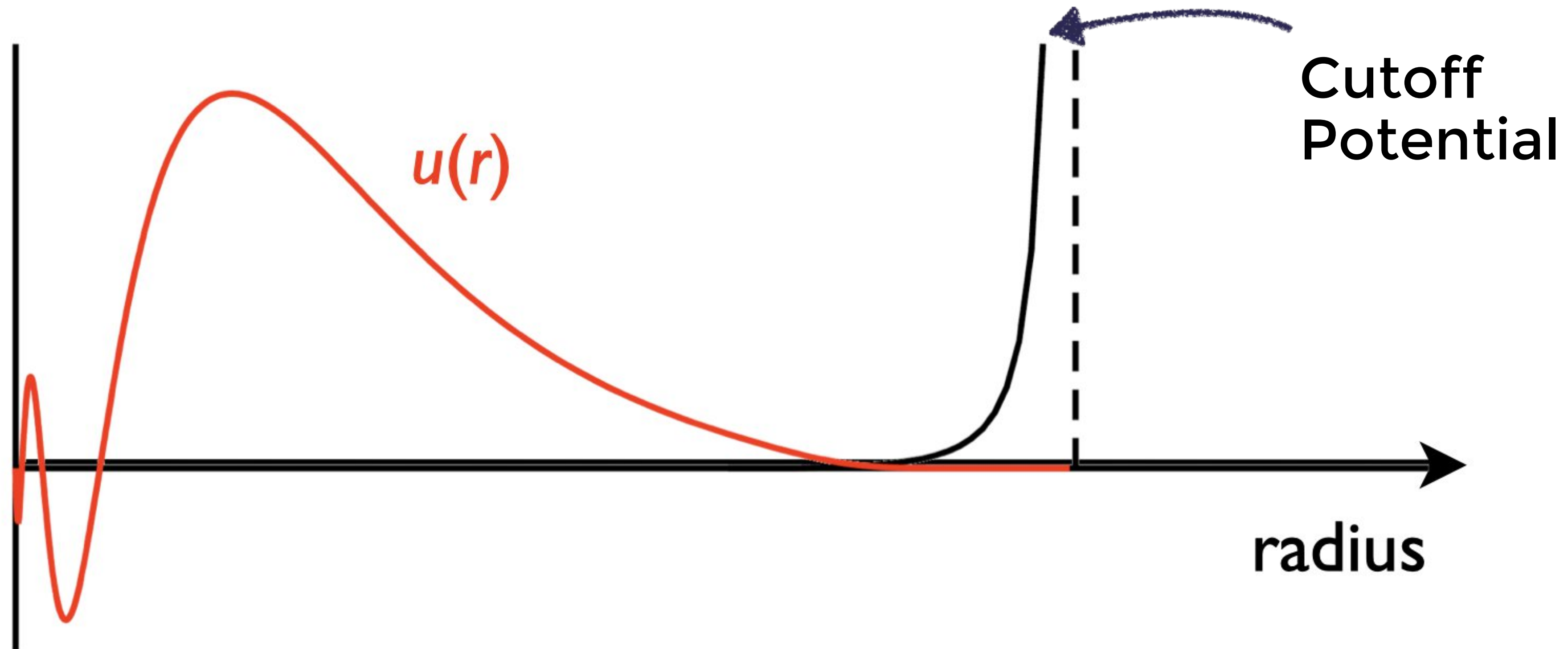


siesta

Basis Set Expansion

$$\psi_k(\mathbf{r}) = \sum_i c_{ki} \varphi_i(\mathbf{r})$$

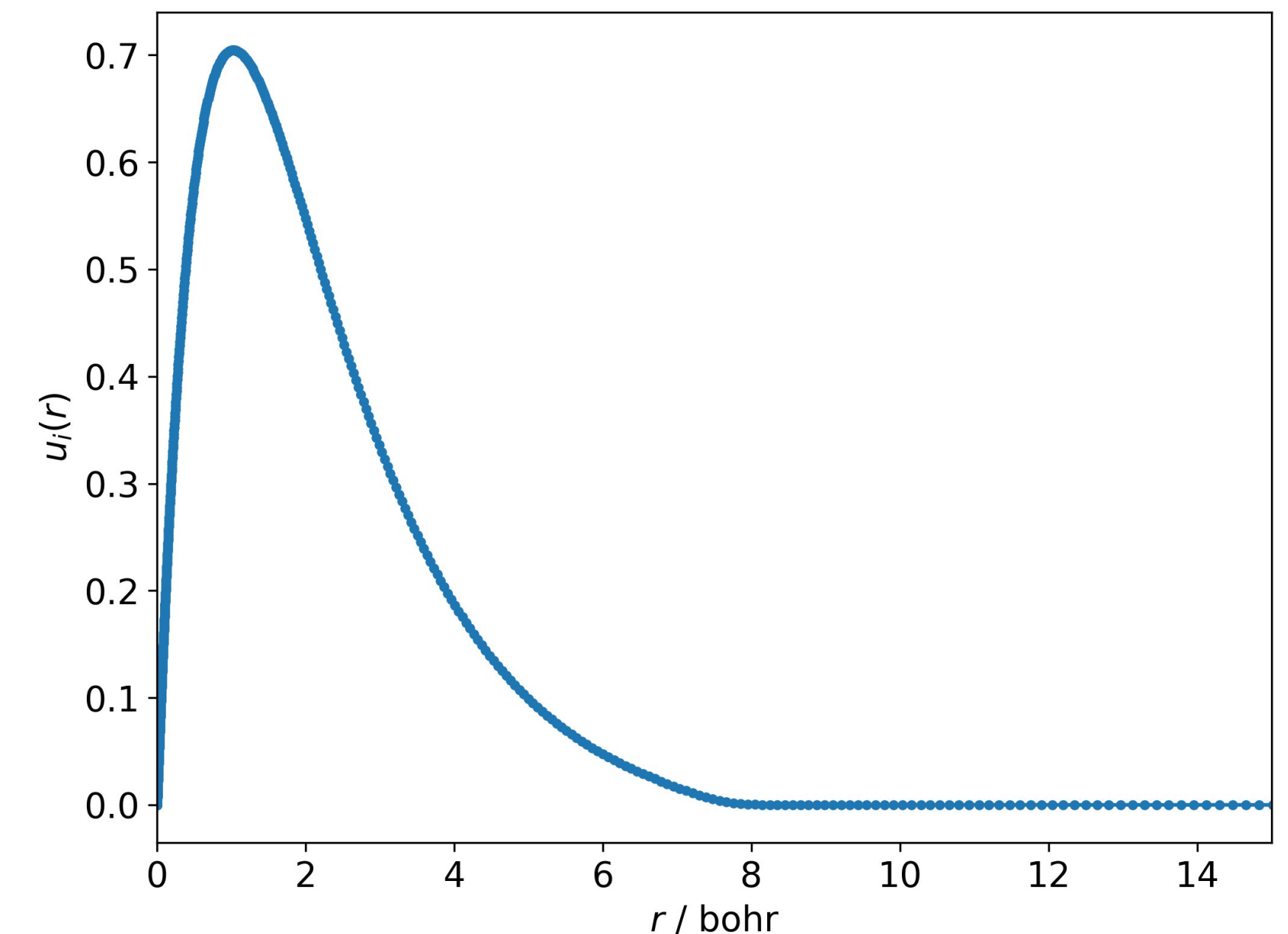
$$\varphi_{i[lm]}(\mathbf{r}) = \frac{u_i(r)}{r} \cdot Y_{lm}(\Omega)$$



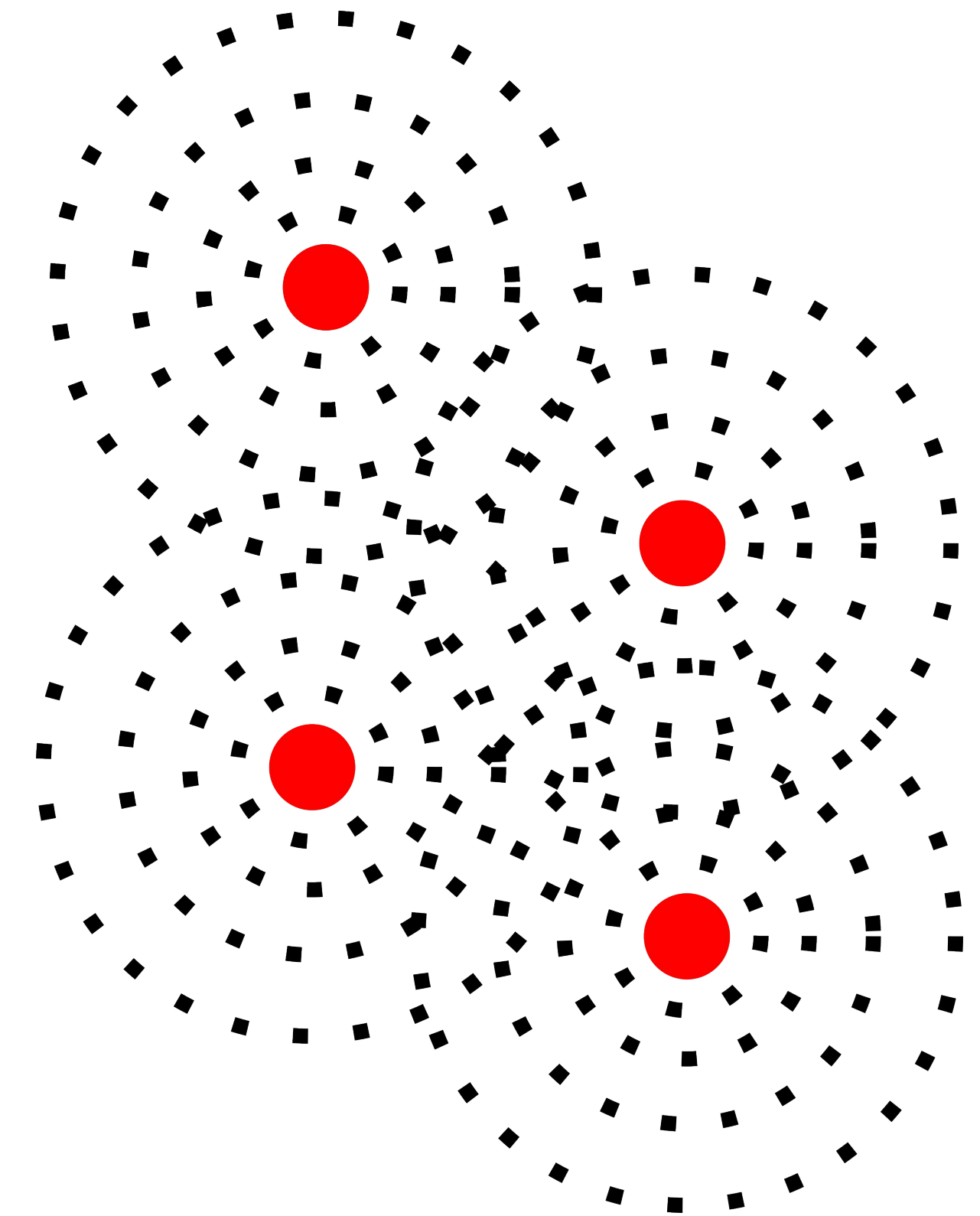
- Solve radial Schrodinger eq on dense 1D logarithmic grid

$$\left[-\frac{1}{2} \frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + v_i(r) + v_{\text{cut}}(r) \right] u_i(r) = \epsilon_i u_i(r)$$

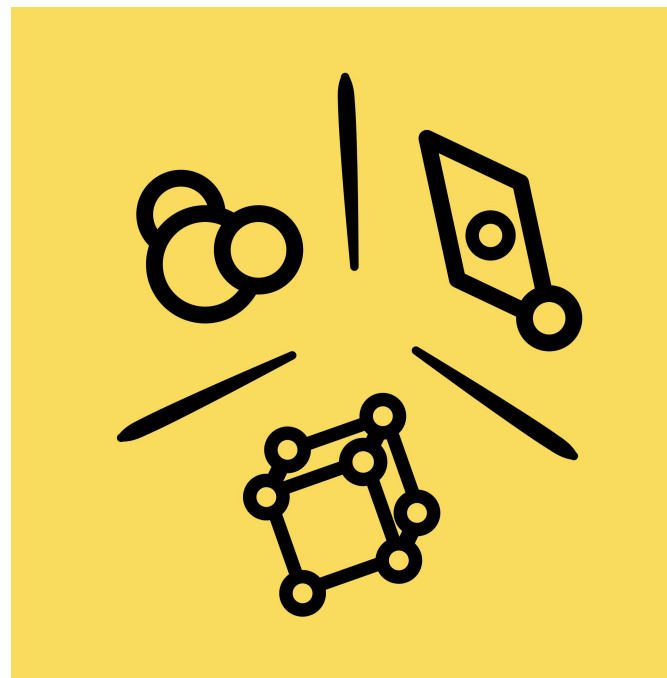
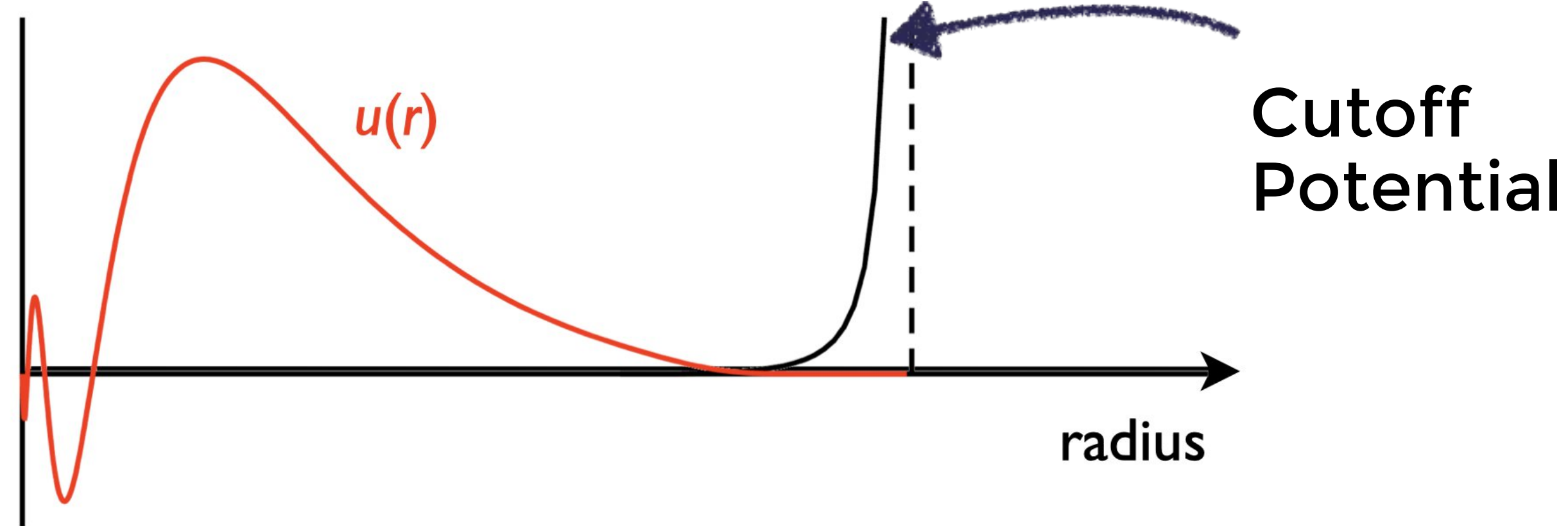
- Free atom like (minimal basis) $v_i(r) = v_{\text{free atom}}^{\text{DFT}}(r)$
- Hydrogen-like $v_i(r) = z/r$
- Free ions, Gaussians etc



- In FHI-aims there are pre-calculated “species defaults” for elements 1-102 which contain basis functions, but not only...
- Include parameters for: cut-off potential, angular and radial grids, hartree potential, as well as species name, atomic mass, and atomic number
- Pre-calculated defaults, ranging from fast-qualitative to meV-converged calculations (Total energy, DFT)
- Also freely user customizable
- More later in practical aspects...



Why This Choice of NAOs?



Versatile

Non-periodic and
periodic systems on
same footing



Precise + Accurate

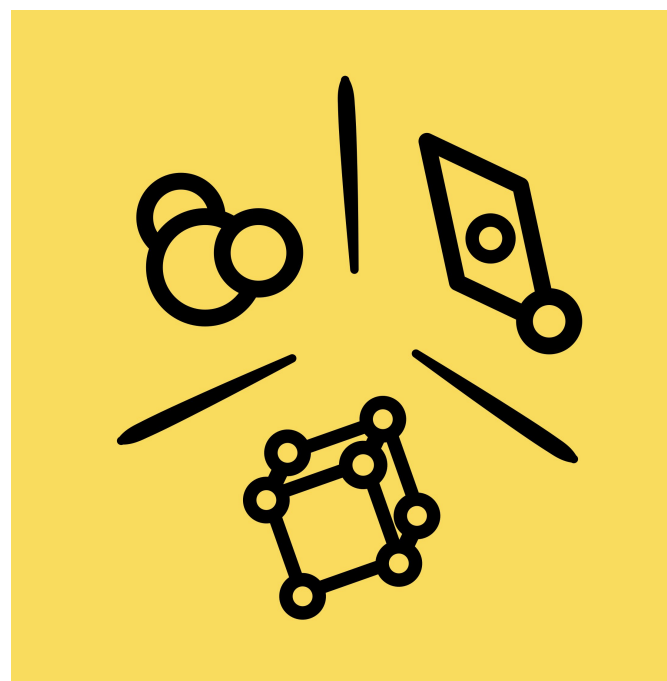
Flexible shape and all-
electron description
for DFT and correlated
methods (RPA, GW, ...)



Scalable

Localizable NAOs - $O(N)$
scaling.
From laptops to HPC, and
from tens to thousands of
atoms

Examples of FHI-aims' Precision, Accuracy, Scalability and Versatility



High Precision for DFT - “Delta Test”

Reproducibility in Density-Functional Calculations of Solids,
K. Lejaeghere, ... 68 coauthors! ..., S. Cottenier, Science 351, aad3000 (2016).

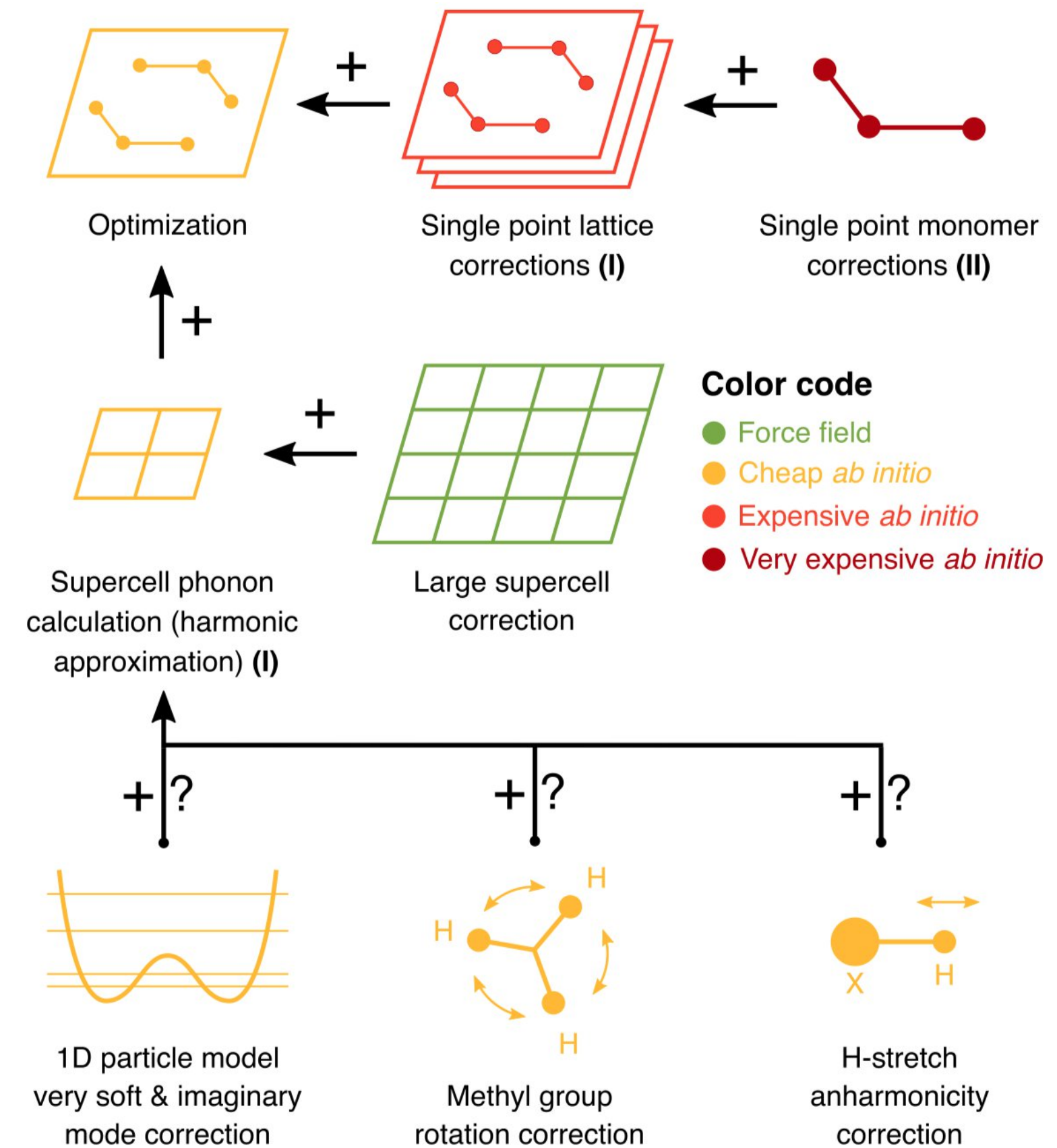
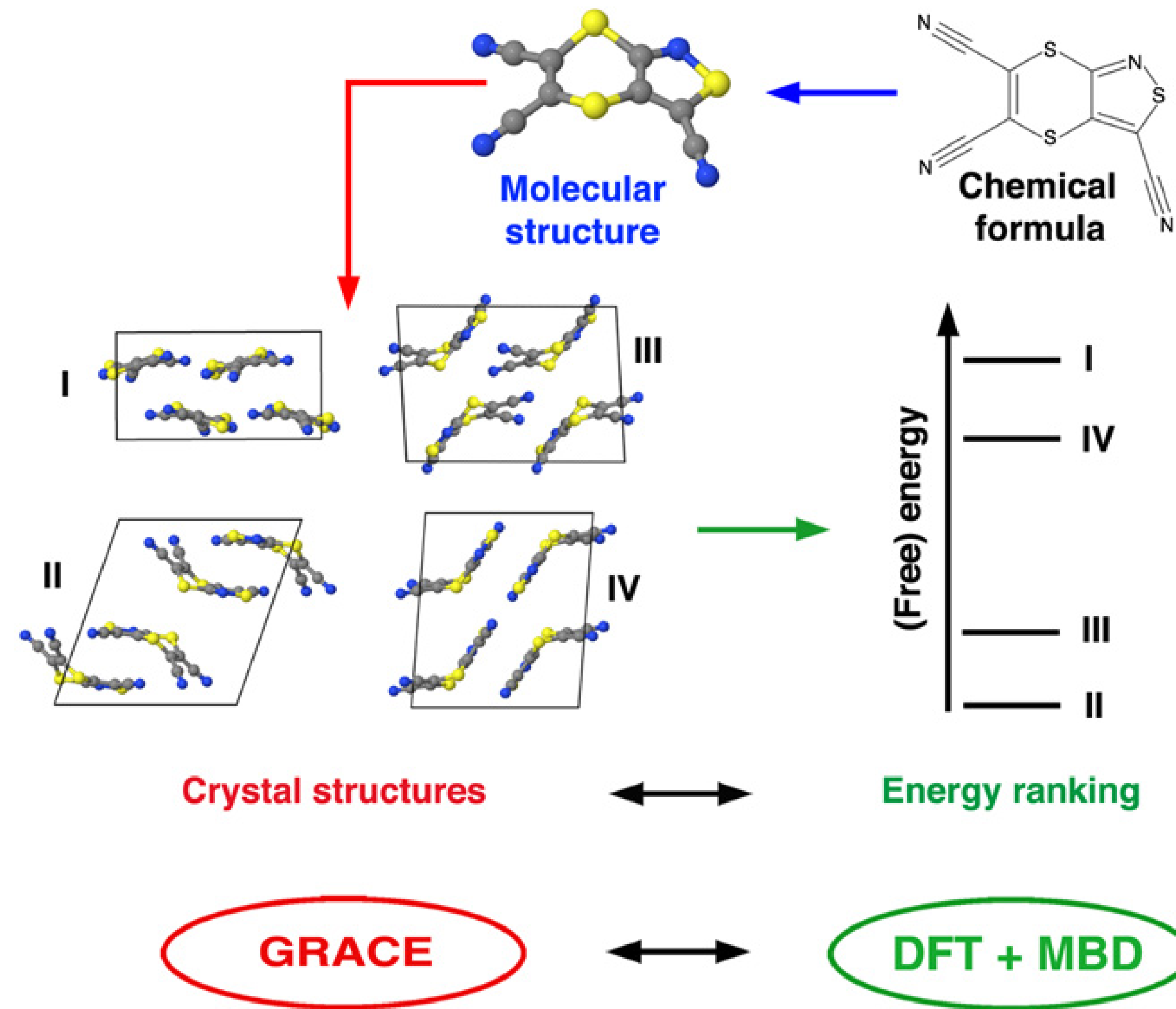
E(V) for 71 elemental solids - 15 codes, all-electron & 40 pseudopotential sets

Code	Basis	Electron treatment	Delta (meV)
Wien2k 13.1	LAPW/APW+lo	All-electron	0
FHI-aims 081213*	NAO, tier2	All-electron (scalar rel. atomic ZORA)	0.2
Exciting (dev.)	LAPW+xlo	All-electron	0.2
Quantum Espresso 5.1	plane waves	SSSP accuracy (mixed NC/US/PAW library)	0.3
VASP 5.2.12	plane waves	PAW 2015	0.3
FHI-aims 081213*	NAO, tier2	All-electron (scalar rel., scaled ZORA)	0.3
ELK 3.1.5	APW+lo	All-electron	0.3

* Results: Marcin Dulak, DTU (Copenhagen)

Slide: Courtesy of V. Blum

High Accuracy in Crystal Structure Prediction

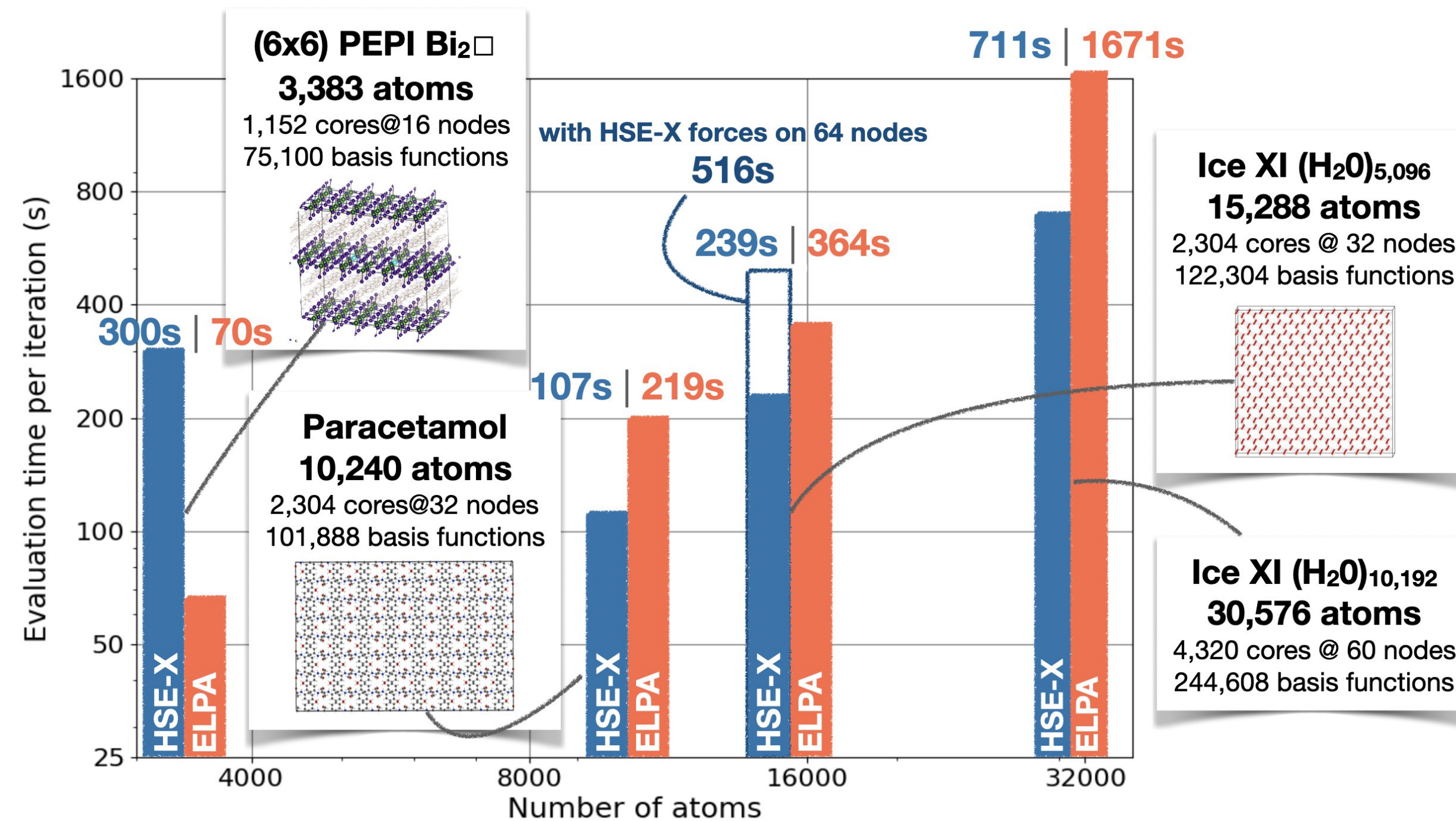


J. Hoja et al., Sci. Adv. 5, eaau3338 (2019)

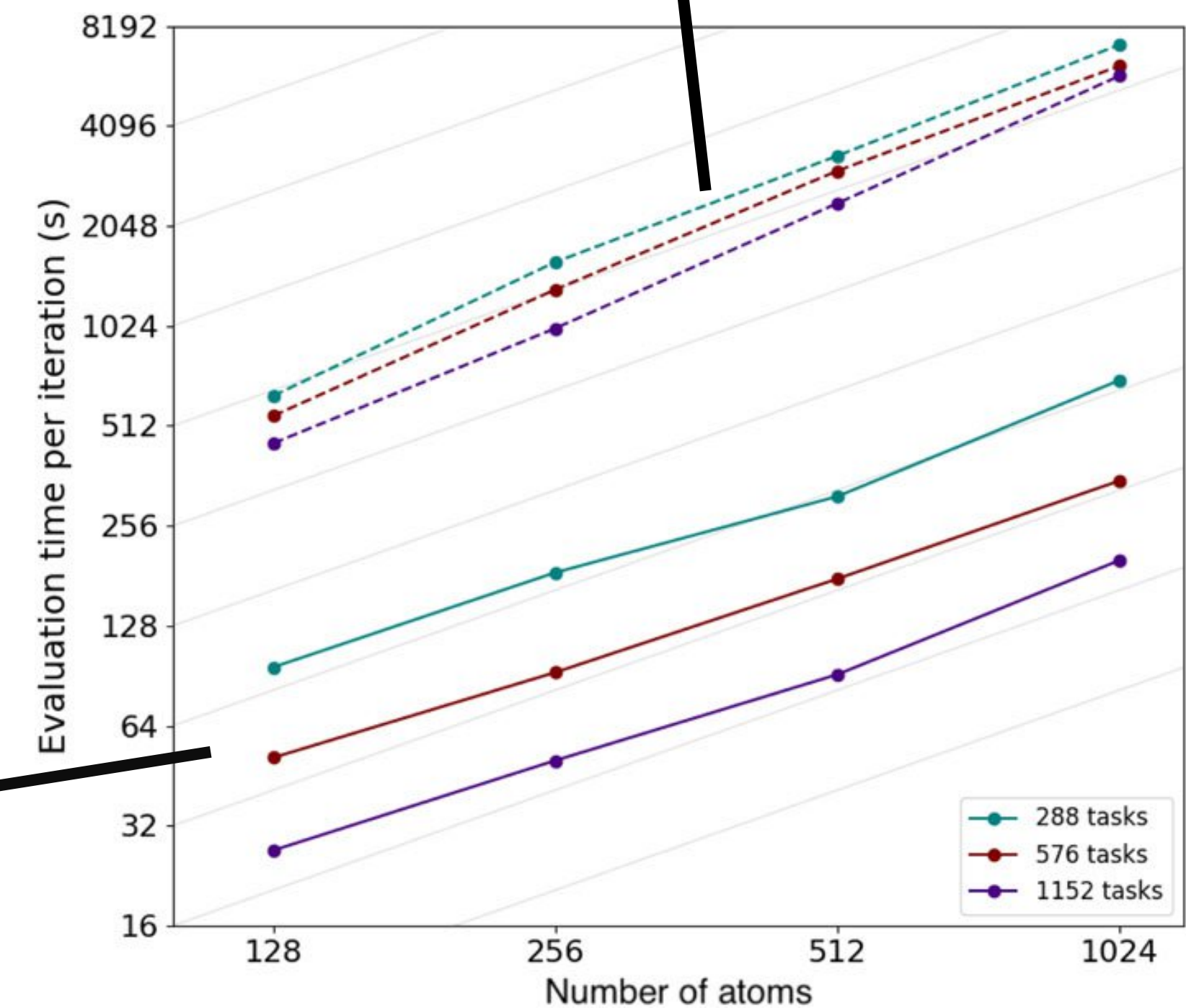
D. Firaha et al., Nature 623, 324–328 (2023)

- Best performing method in the 7th Crystal Structure Prediction blind test: Hunnisett et al., J. Acta. Cryst., B80, 517-574, (2024)

Scalability for Hybrid DFT



Original implementation:
S. Levchenko et. al., Comp.
Phys. Comm., 192, (2015), 60-69



RESEARCH ARTICLE | JULY 11 2024

Efficient all-electron hybrid density functionals for atomistic simulations beyond 10 000 atoms

Sebastian Kokott ; Florian Merz ; Yi Yao ; Christian Carbogno ; Mariana Rossi ; Ville Havu; Markus Rampf ; Matthias Scheffler ; Volker Blum



+ Author & Article Information

J. Chem. Phys. 161, 024112 (2024)

<https://doi.org/10.1063/5.0208103> Article history

New
implementation

Efficiency for Creating Machine Learning Datasets

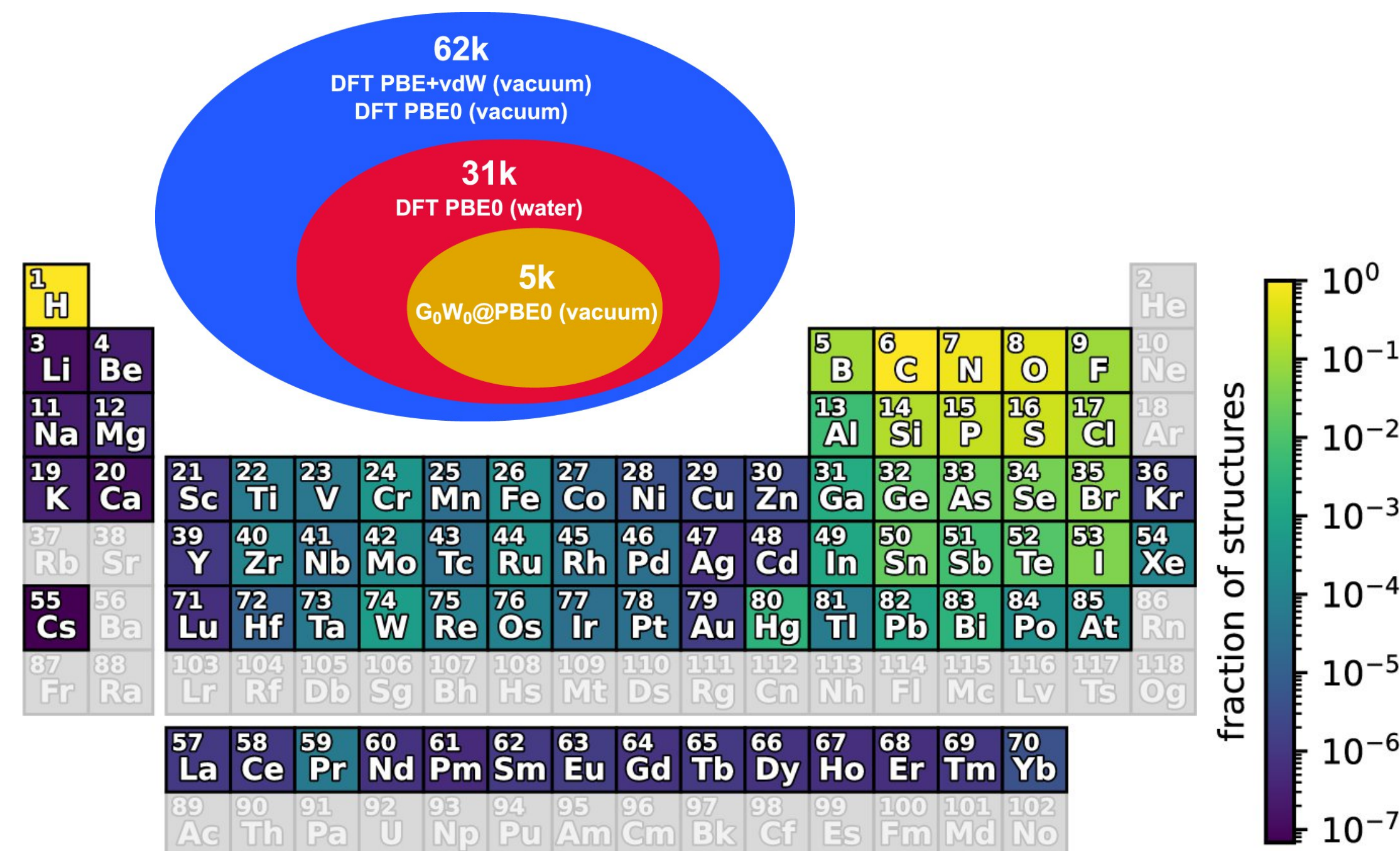
1. OE62 Dataset:

A Stuke et. al., Atomic structures and orbital energies of 61,489 crystal-forming organic molecules, Scientific Data, 7, 58, (2020)

2. QCML Dataset:

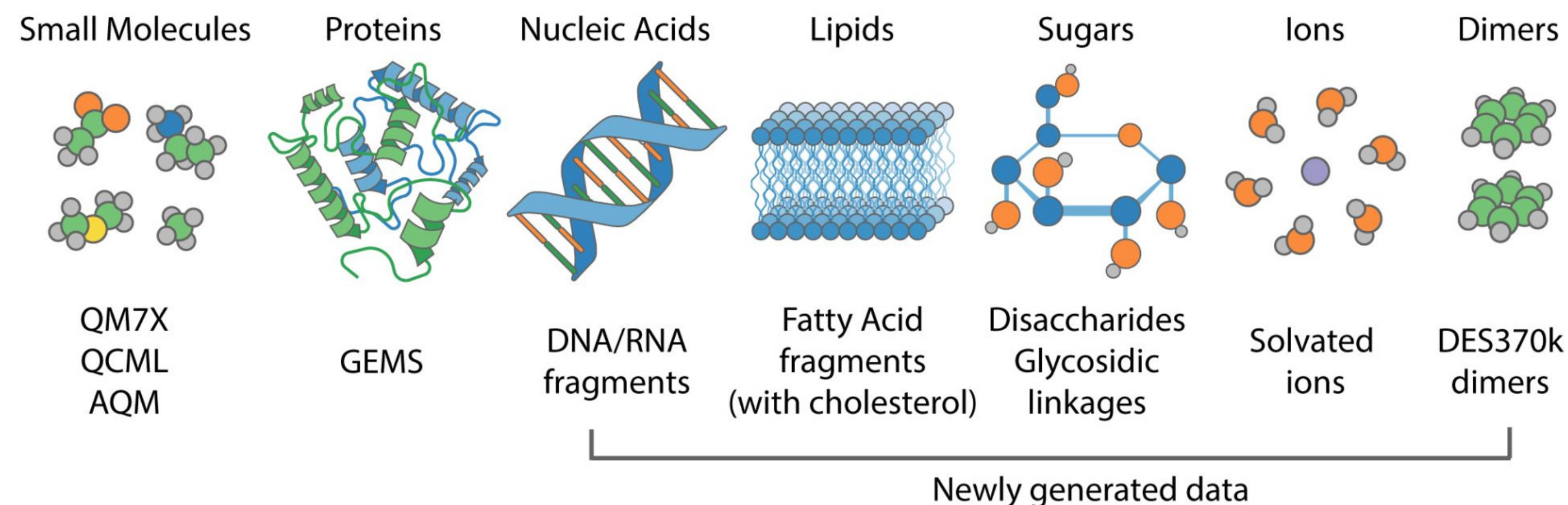


S. Ganscha et. al., The QCML dataset, Quantum chemistry reference data from 33.5M DFT and 14.7B semi-empirical calculations, Scientific Data, 12, 406, (2025)

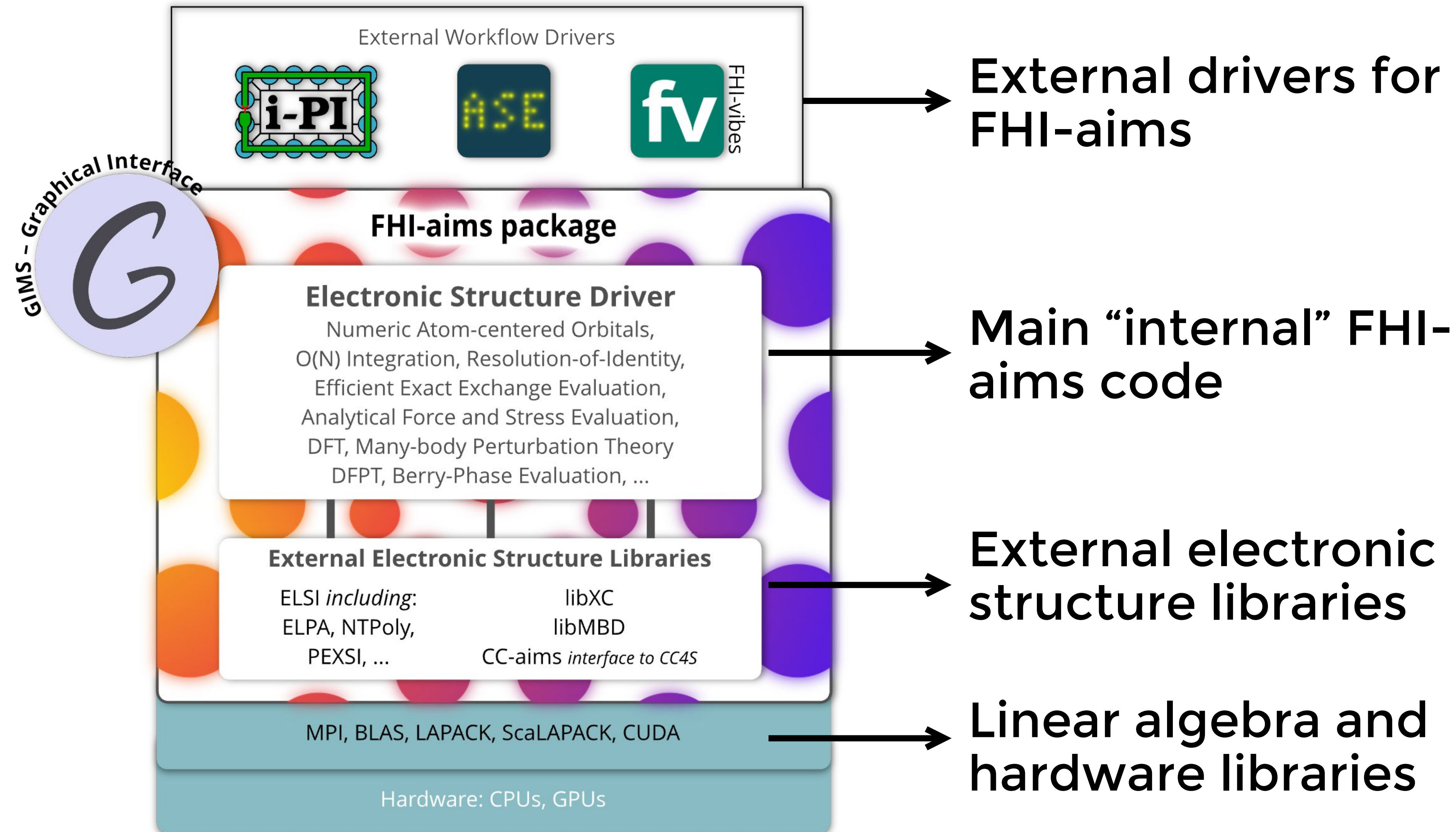


3. QCell Dataset:

A. Kabylda et. al., QCell: Comprehensive Quantum-Mechanical Dataset Spanning Diverse Biomolecular Fragments, (2025) arxiv.org/abs/2510.09939



A Dive into FHI-aims: Modular and Versatile



Practical Aspects of FHI-aims Calculations

Input Files for FHI-aims

FHI-aims works on the command line with text based input/output files. 2 Input files required:

geometry.in

control.in

Non-periodic:

```
atom 0.000000 0.000000 0.000000 O
atom 0.707000 -0.707000 0.000000 H
atom -0.707000 -0.707000 0.000000 H
```

```
xc pbe

[Species defaults attached below]
```

Periodic:

```
lattice_vector 0.00000 2.71500 2.71500
lattice_vector 2.71500 0.00000 2.71500
lattice_vector 2.71500 2.71500 0.00000
```

```
atom_frac 0.00000 0.00000 0.00000 Si
atom_frac 0.25000 0.25000 0.25000 Si
```

```
xc pbe
k_grid 8 8 8

[Species defaults attached below]
```


Species Defaults in FHI-aims : The Basics

species_defaults folder in FHI-aims

light

Fast, less accurate
Used for quick pre-relaxations

intermediate

Fast-ish, reasonably accurate
Go-to for large structures and hybrid DFT

tight

Slower, converged results
meV/atom energy differences

really_tight

Slowest, overconverged
Generally only for benchmarking

- Relative to really_tight



Basis Set Tiers

- Basis set = minimal basis + additional basis functions
- For all species defaults, basis functions are organized into tiers, which can be commented/uncommented for less/more accurate calculations

```
#####  
#  
# Definition of "minimal" basis  
#  
#####  
# valence basis states  
# valence 1 s 1.  
# ion occupancy  
# ion_occ 1 s 0.5  
#####  
#  
# Suggested additional basis functions. For production calculations,  
# uncomment them one after another (the most important basis functions are  
# listed first).  
#  
# Basis constructed for dimers: 0.5 A, 0.7 A, 1.0 A, 1.5 A, 2.5 A  
#  
#####  
# "First tier" - improvements: -1014.90 meV to -62.69 meV  
# hydro 2 s 2.1  
# hydro 2 p 3.5  
# "Second tier" - improvements: -12.89 meV to -1.83 meV  
# hydro 1 s 0.85  
# hydro 2 p 3.7  
# hydro 2 s 1.2  
# hydro 3 d 7  
# "Third tier" - improvements: -0.25 meV to -0.12 meV  
# hydro 4 f 11.2  
# hydro 3 p 4.8  
# hydro 4 d 9  
# hydro 3 s 3.2  
#####
```

More Advanced Species Defaults for Specific Tasks

intermediate_gw
tight_gw
really_tight_gw

Additional auxiliary basis functions
Specific basis sets for periodic GW calculations

NAO-VCC-nZ

"Correlation consistent" basis set for RPA, MP2, or GW
I. Y. Zhang et al., New Journal of Physics 15, 123033 (2013)

Tier2_aug2

FHI-aims' tier2 basis sets plus Gaussian augmentation functions for neutral excitations (BSE@GW, LR-TDDFT)
C. Liu et al., J. Chem. Phys. 152, 044105 (2020)

Running and Output of FHI-aims

```
mpirun -np N aims.x > aims.out
```

```
Leaving FHI-aims.
Date      : 20251010, Time      : 165346.853

Computational steps:
| Number of self-consistency cycles      :          42
| Number of SCF (re)initializations      :           5
| Number of relaxation steps              :           4

Detailed time accounting      : max(cpu_time)    wall_clock(cpu1)
| Total time                        :      1.229 s      3.158 s
| Preparation time                  :      0.107 s      0.283 s
| Boundary condition initialization    :      0.014 s      0.109 s
| Grid partitioning                  :      0.033 s      0.122 s
| Preloading free-atom quantities on grid :      0.026 s      0.091 s
| Free-atom superposition energy       :      0.018 s      0.017 s
| Total time for integrations          :      0.333 s      0.434 s
| Total time for solution of K.-S. equations :      0.030 s      0.187 s
| Total time for EV reorthonormalization :      0.001 s      0.003 s
| Total time for density & force components :      0.283 s      0.307 s
| Total time for mixing                :      0.026 s      0.024 s
| Total time for Hartree multipole update :      0.035 s      0.037 s
| Total time for Hartree multipole sum   :      0.169 s      0.200 s
| Total time for total energy evaluation :      0.004 s      0.004 s
| Total time NSC force correction        :      0.029 s      0.028 s
| Total time for scaled ZORA corrections :      0.000 s      0.000 s

Partial memory accounting:
| Residual value for overall tracked memory usage across tasks:      0.000000 MB (should be 0.000000 MB)
| Peak values for overall tracked memory usage:
|   Minimum:      2.435 MB (on task 1 after allocating hessian_basis_wave)
|   Maximum:      2.455 MB (on task 0 after allocating hessian_basis_wave)
|   Average:      2.444 MB
| Largest tracked array allocation:
|   Minimum:      0.729 MB (previous_rho_gradient_diff on task 2)
|   Maximum:      0.735 MB (previous_rho_gradient_diff on task 0)
|   Average:      0.732 MB
Note: These values currently only include a subset of arrays which are explicitly tracked.
      ... will be greater.
```

```
Have a nice day.
```


Graphical Interface for Materials Simulations (GIMS)

<https://gims.ms1p.org>

- Create input files, analyse output files

The screenshot displays the GIMS web interface. At the top, there is a header with the GIMS logo, the text "Graphical Interface for Materials Simulations", a link to the desktop application, and options to choose the code (FHI-aims or exociting) and the GIMS version (Stable). Below the header, there are two main sections: "Calculation Apps" and "Elemental Apps". The "Calculation Apps" section contains four buttons: "Simple Calculation", "Band Structure", "GW Calculation", and "MD Calculation". The "Elemental Apps" section contains three buttons: "Structure Builder", "Control Generator", and "Output Analyzer". The "Structure Builder" button is highlighted with a thick orange border.

Sebastian Kokott, Iker Hurtado, Christian Vorwerk, Claudia Draxl, Volker Blum, Matthias Scheffler,
GIMS: Graphical Interface for Materials Simulations. Journal of Open Source Software, 6(57), 2767.
<https://doi.org/10.21105/joss.02767>

GIMS: Build a Structure

The screenshot displays the GIMS StructureBuilder web interface. At the top, the title 'Graphical Interface for Materials Simulations / StructureBuilder' is shown. On the right, there are options to 'Choose your code' (FHI-aims, exciting) and 'Choose GIMS version' (Stable). A 'SETTINGS' gear icon is also present. The main workspace shows a 3D model of a crystal structure with atoms represented by colored spheres (Cd: orange, Sr: green, Ta: blue). The structure is enclosed in a unit cell with axes labeled 'a', 'b', and 'c'. A legend on the left identifies the atom types. Above the model, there are buttons for 'CdSrTa.in', '+', 'View options', and a camera icon. An 'Edit structure' toggle is set to 'OFF'. The sidebar on the right contains several sections: 'Import' and 'Export' buttons, 'Lattice Vectors' (with a table of values), 'Atomic Positions', 'Structure Info', 'Supercell', 'Standardized Cells', and 'Surface (Slab) Construction'. The 'Lattice Vectors' section is highlighted with a yellow box.

	All numbers in units of Å			Constraint
a:	7.550000	0.000000	0.000000	☐
b:	0.000000	7.550000	0.000000	☐
c:	0.000000	0.000000	7.550000	☐

☒ Scale atom positions with lattice vectors
☐ Remove lattice vectors

- Import structure from ASE supported formats (e.g. CIF) and export to geometry.in
- Edit / remove lattice vectors
- Add / move / remove atoms, change atomic species
- Simply create supercell / primitive cell
- Plus much more...

Graphical Interface for Materials Simulations (GIMS)

<https://gims.ms1p.org>

- Create input files, analyse output files

The screenshot displays the GIMS web interface. At the top, there is a header with the GIMS logo, the text 'Graphical Interface for Materials Simulations', and a link to the desktop application. To the right, there are options to 'Choose your code' (with buttons for 'FHI-aims' and 'exciting') and 'Choose GIMS version' (with a dropdown menu set to 'Stable'). A 'SETTINGS' gear icon is also present. Below the header, the interface is divided into two sections: 'Calculation Apps' and 'Elemental Apps'. The 'Calculation Apps' section contains four buttons: 'Simple Calculation', 'Band Structure', 'GW Calculation', and 'MD Calculation'. The 'Elemental Apps' section contains three buttons: 'Structure Builder', 'Control Generator', and 'Output Analyzer'. The 'Structure Builder' and 'Control Generator' buttons are highlighted with a thick orange border.

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GIMS: Create a control.in File

Control Generator

Basic Settings

Geometry species

Cd Sr Ta

XC functional

Species Default Settings

Spin

The species defaults are a collection of pre-defined numerical parameters for the integration grids and basis functions.
light: Settings for fast pre-relaxations, structure searches, etc. Usually, no obvious geometry or convergence errors resulted from these settings. Recommended for many household tasks.
intermediate: Only available for a few elements, but can play an important role for large and expensive calculations, especially for hybrid functionals.
tight: Regarding the integration grids, Hartree potential, and basis cutoff potentials, the settings specified here are rather safe, intended to provide meV-level accurate energy differences also for large structures.

K-grid

Structure lattice vectors:

7.550 Å 7.550 Å 7.550 Å

☒ k-points grid

☐ k-points grid density

Å

Post-processing

Structure Optimization, Forces, and Stress

Self-Consistent Field Convergence (optional)

Extra keywords

- A set of mostly used input file keywords with explanation
- A simple mechanism of visibility constraints (certain keyword inputs may not be visible based on other inputs' values) and sanity checks of inputs' values based on other inputs and structure
- Extra keywords table allows building complicated input files

Graphical Interface for Materials Simulations (GIMS)

<https://gims.ms1p.org>

- Create input files, analyse output files

The screenshot displays the GIMS web interface. At the top, there is a header with the GIMS logo, the text "Graphical Interface for Materials Simulations", a link to the desktop application, and options to choose the code (FHI-aims, exociting) and the GIMS version (Stable). Below the header, there are two main sections: "Calculation Apps" and "Elemental Apps". The "Calculation Apps" section includes four buttons: "Simple Calculation", "Band Structure", "GW Calculation", and "MD Calculation". The "Elemental Apps" section includes three buttons: "Structure Builder", "Control Generator", and "Output Analyzer". The "Elemental Apps" section is highlighted with an orange border.

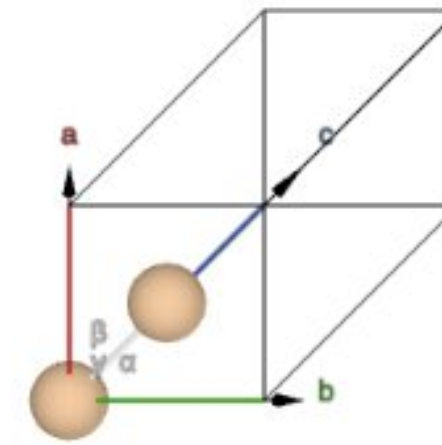
Sebastian Kokott, Iker Hurtado, Christian Vorwerk, Claudia Draxl, Volker Blum, Matthias Scheffler,
GIMS: Graphical Interface for Materials Simulations. Journal of Open Source Software, 6(57), 2767.
<https://doi.org/10.21105/joss.02767>

GIMS: Analyse Output

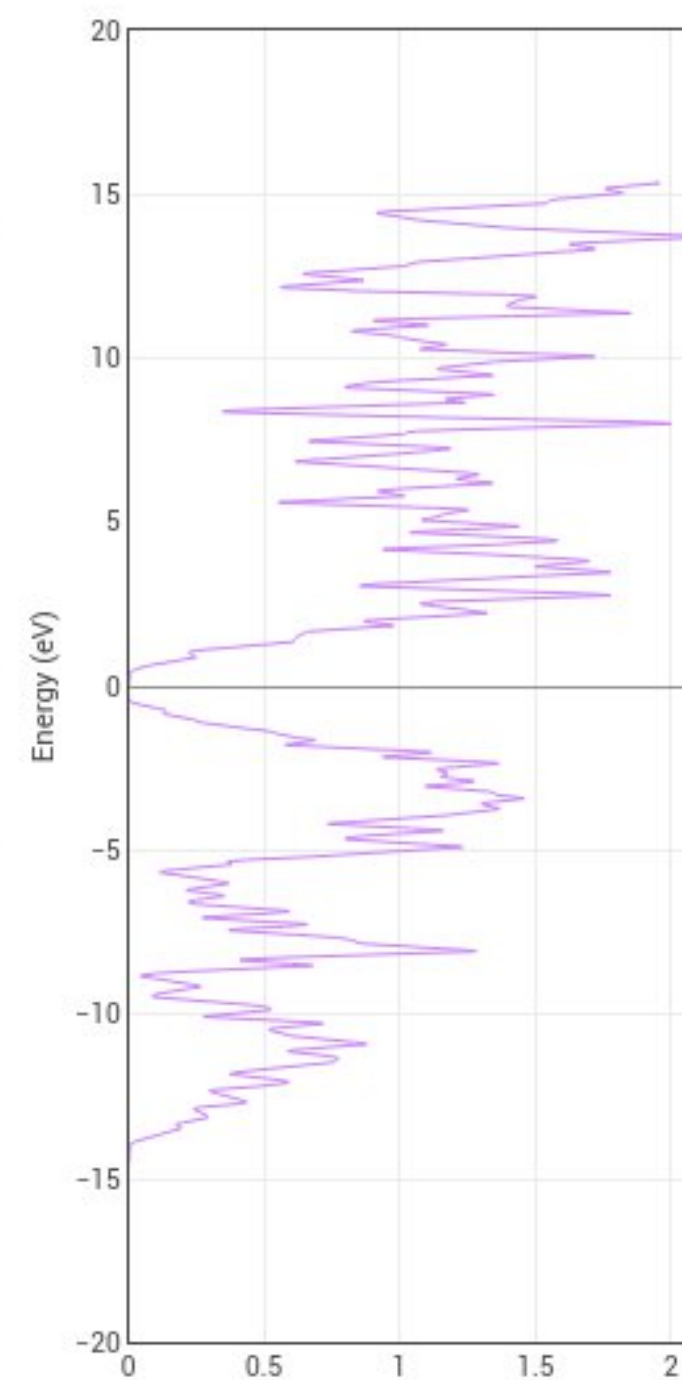
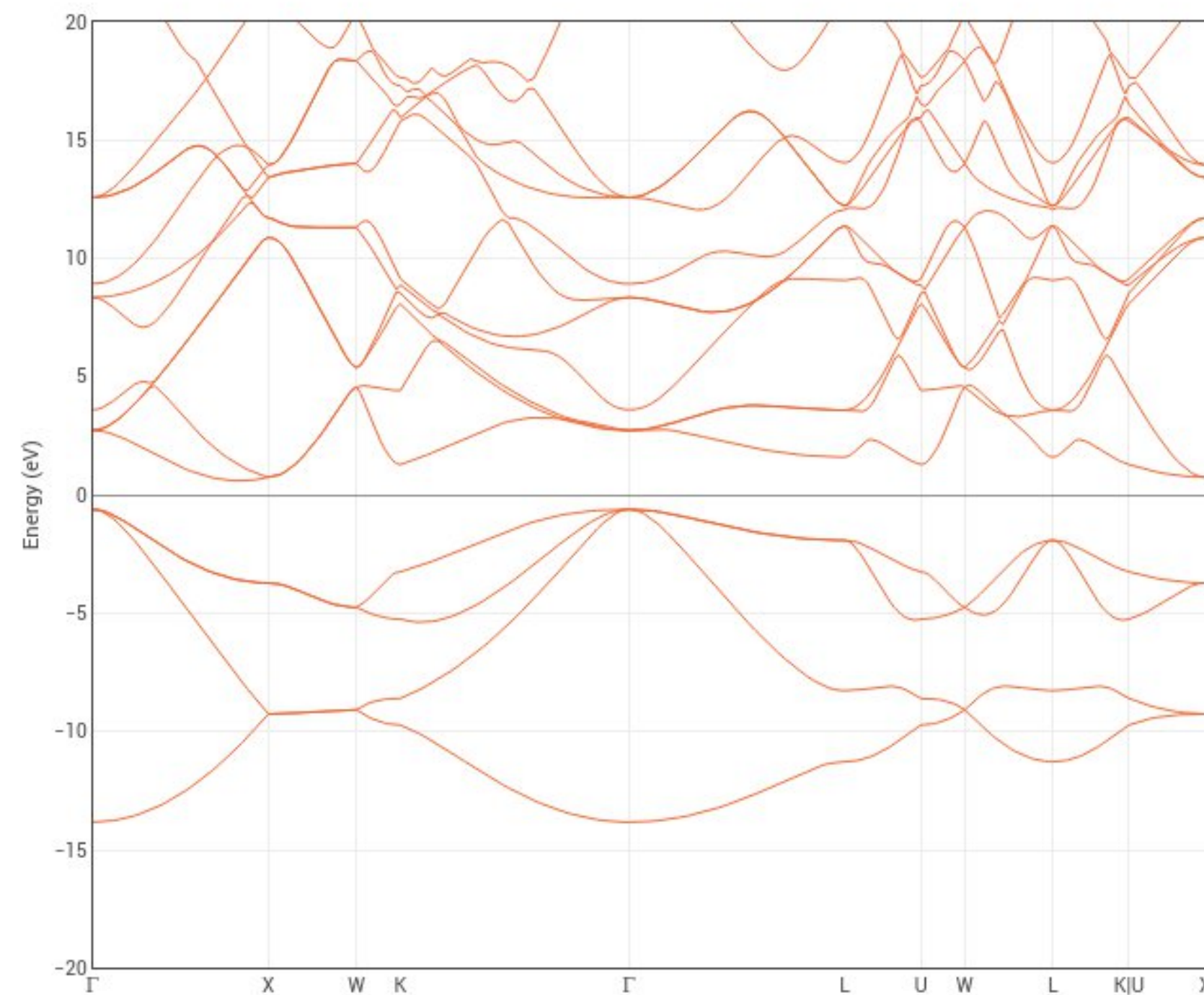
Results

Total Energy (eV)	-15804.83014
Fermi Energy (eV)	-5.36784
Highest occupied state (eV)	-5.97018
Lowest unoccupied state (eV)	-4.76551
Estimated HOMO-LUMO gap (eV)	1.20467
Cell Volume (Å ³)	40.45449

Si

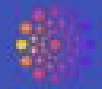


DOS and Band Structure graphs



- Numerical and graphical representation of the output file – geometry, energies, HOMO-LUMO etc
- Graphs: convergence (energy, eigenvalues, density for each ionic step; forces), band structure, DOS, dielectric function

More in the basics of FHI-aims tutorial this afternoon!

 Basics of Running FHI-aims

Search

GitLab
☆ 1 👤 1

Basics of Running FHI-aims

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Part 2: Spin-polarized Systems

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Basics of Running FHI-aims

This tutorial has been updated for FHI-aims version 250822 .

Welcome to this introductory tutorial on how to use the [FHI-aims](#) code for simulations of atoms, molecules, and solids.

In order to successfully execute this tutorial, you should have access to the two primary community resources of the FHI-aims project:

- The FHI-aims development and community server <https://aims-git.rz-berlin.mpg.de>
- The FHI-aims slack workspace <https://fhi-aims.slack.com>

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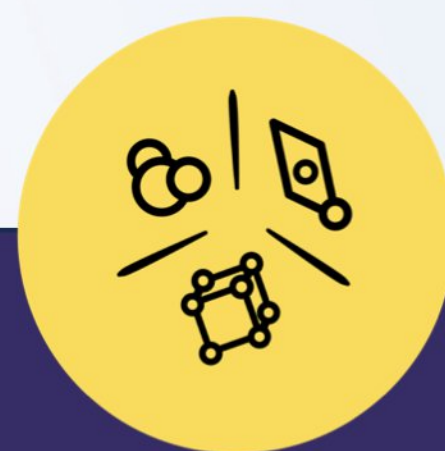


Questions?

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Accurate Dispersion Interactions
Many-body Methods (e.g, GW, RPA)

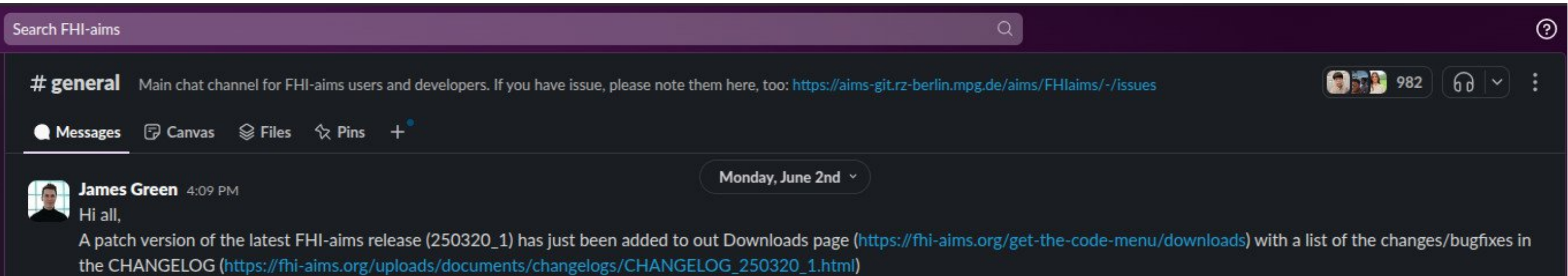
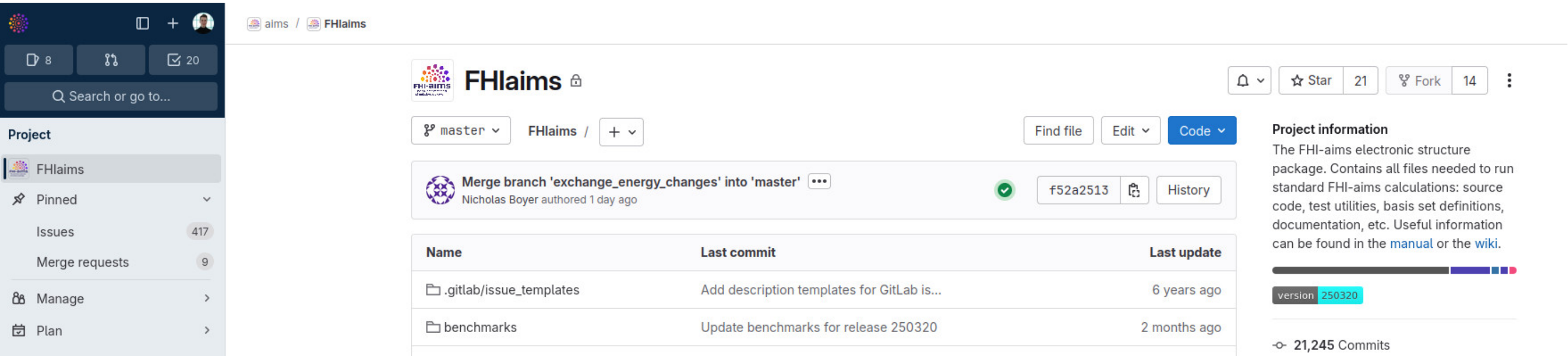


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