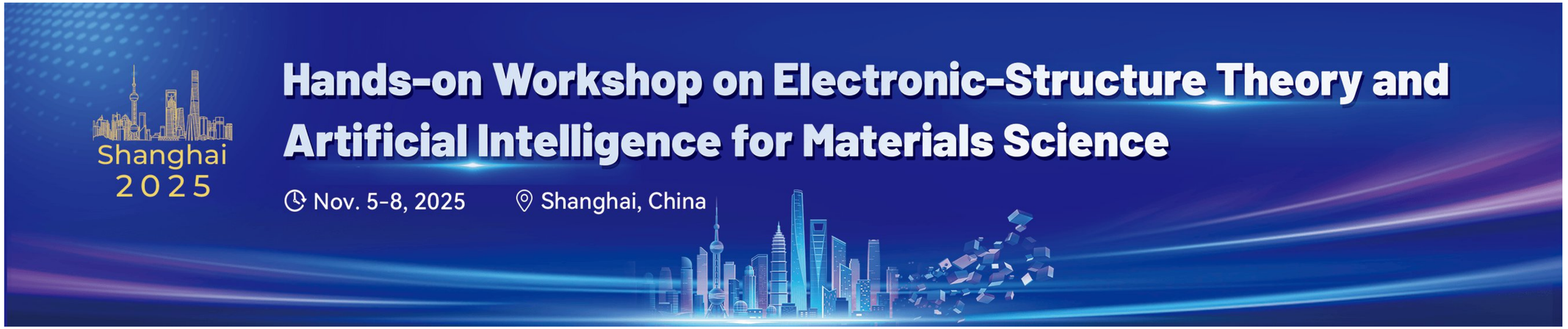
FHI-aims
The ab initio materials simulation package

MS1P
Molecular Simulations from First Principles

The Basics of FHI-aims

James A. Green, Konstantin Lion, and Andrei Sobolev

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



The FHI-aims Code

FHI-aims
The ab initio materials simulation package

- 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, Xinzheng 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 and Roadmap Paper

“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 *

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany

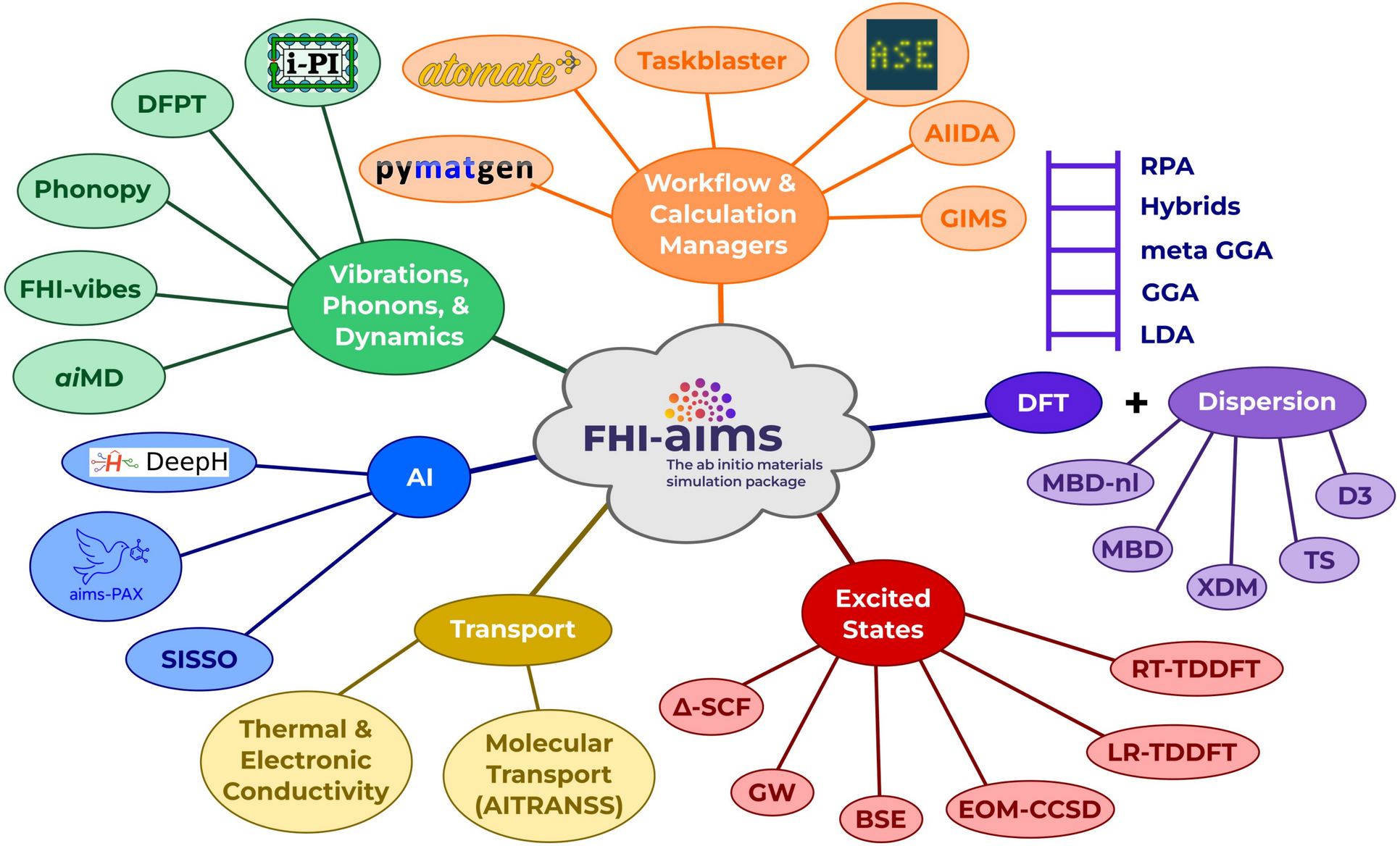
Read the FHI-aims roadmap on arXiv

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

Roadmap on Advancements of the FHI-aims Software Package

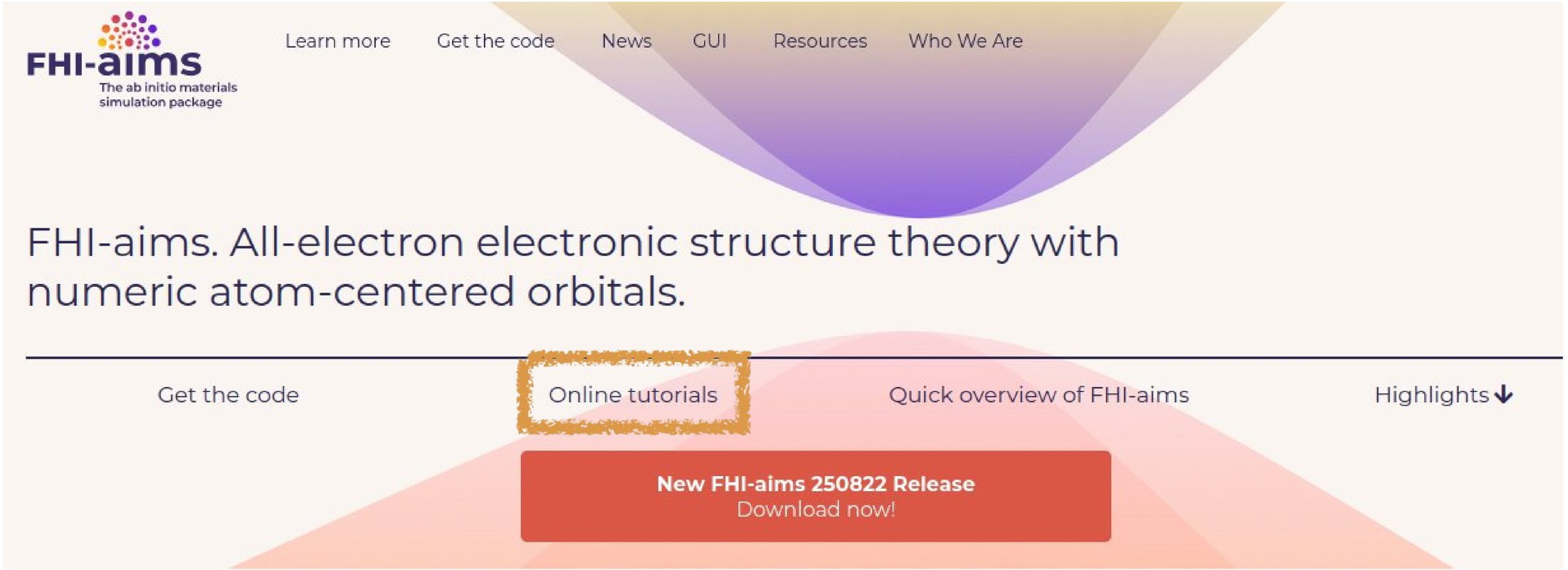
Joseph W. Abbott, Carlos Mera Acosta, Alaa Akkoush, Alberto Ambrosetti, Viktor Atalla, Alexej Bagrets, Jörg Behler, Daniel Berger, Björn Bieniek, Jonas Björk, Volker Blum, Saeed Bohloul, Connor L. Box, Nicholas Boyer, Danilo Simoes Brambila, Gabriel A. Bramley, Kyle R. Bryenton, María Camarasa-Gómez, 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 Hülsberg, 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?



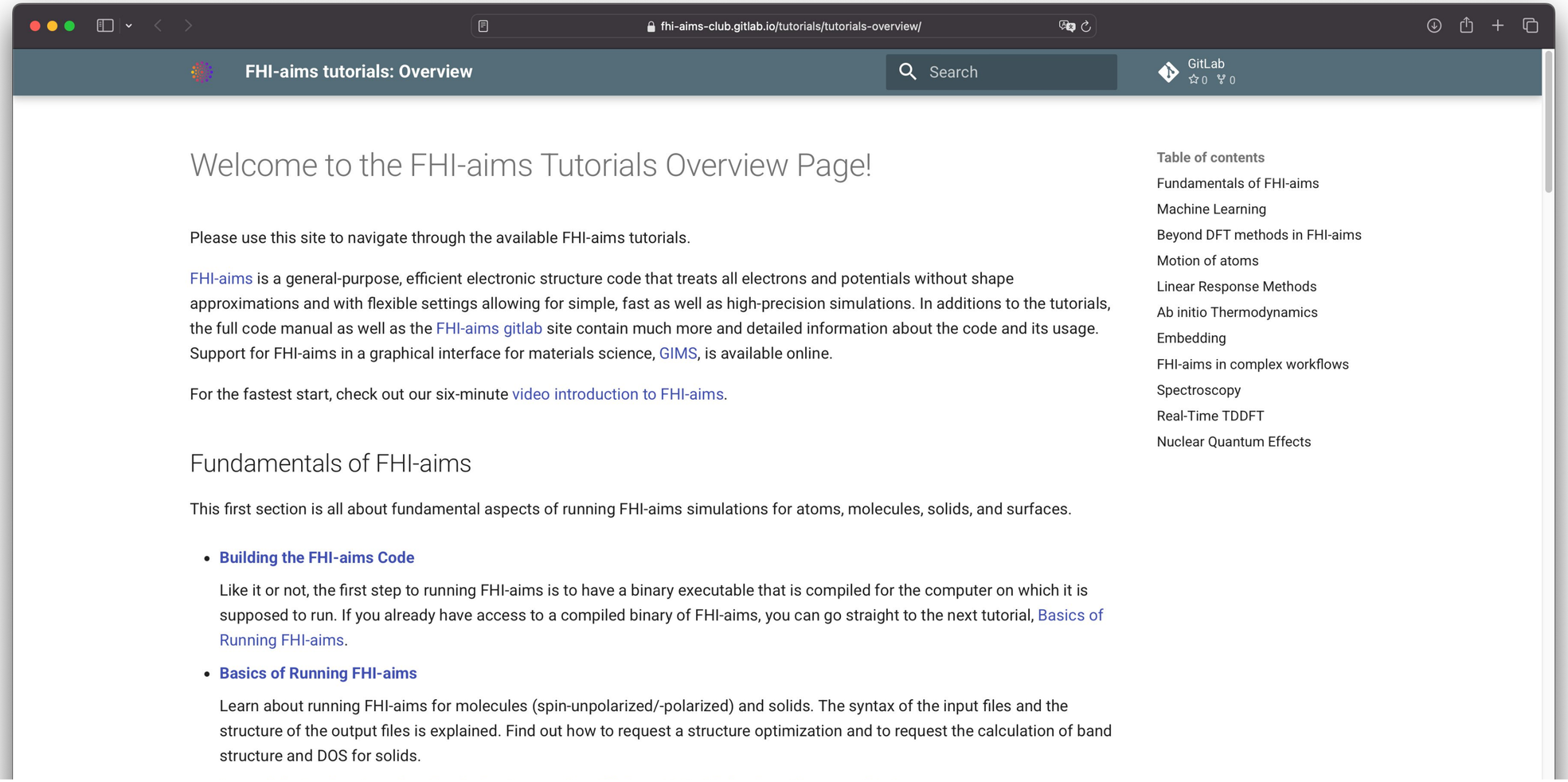
Where Can You Find FHI-aims?

https://fhi-aims.org/



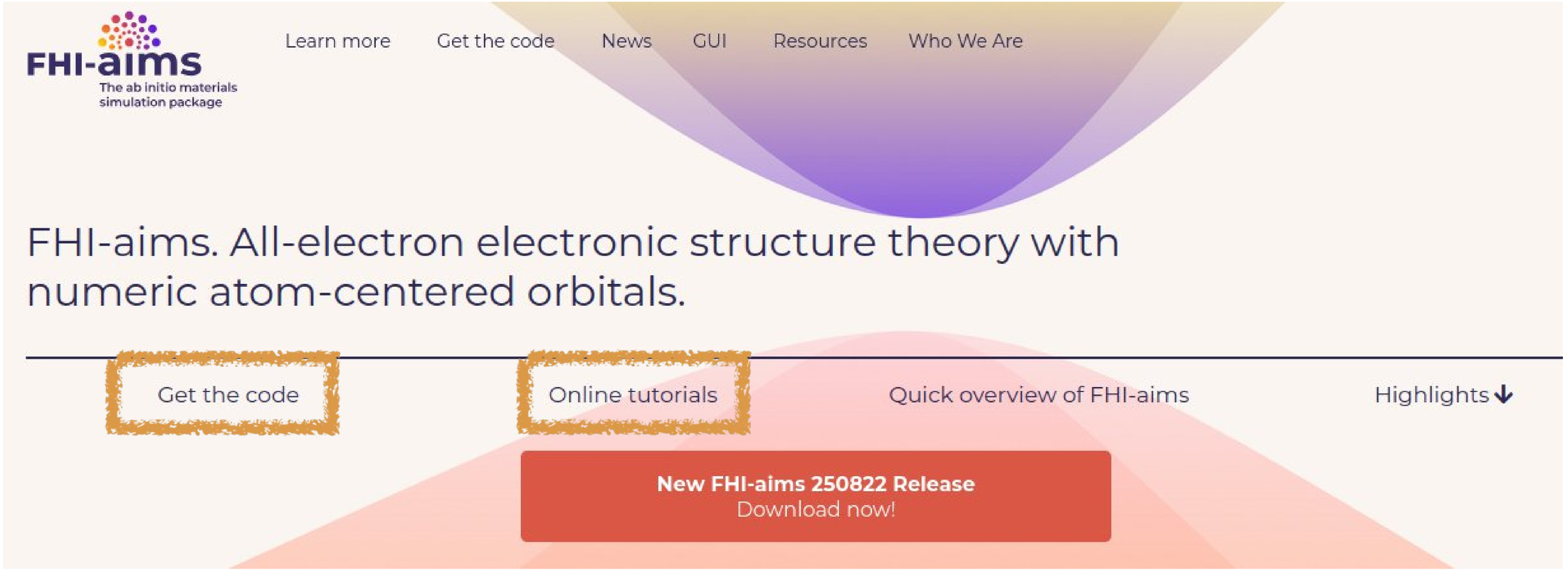
Extensive and Growing List of Tutorials

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



FHI-aims Website

https://fhi-aims.org/



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
```

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@ms1p.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@ms1p.org. In case of questions please contact aims-coordinators@ms1p.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

Gaussian, Inc.

ORCA

TURBOMOLE

Plane Waves/ Pseudopotentials

b-initio VASP ienna ackage imulation

QUANTUMESPRESSO

CASTEP

Numeric Atom-Centered Orbitals

FHI-aims
The ab initio materials simulation package

ABACUS

siesta

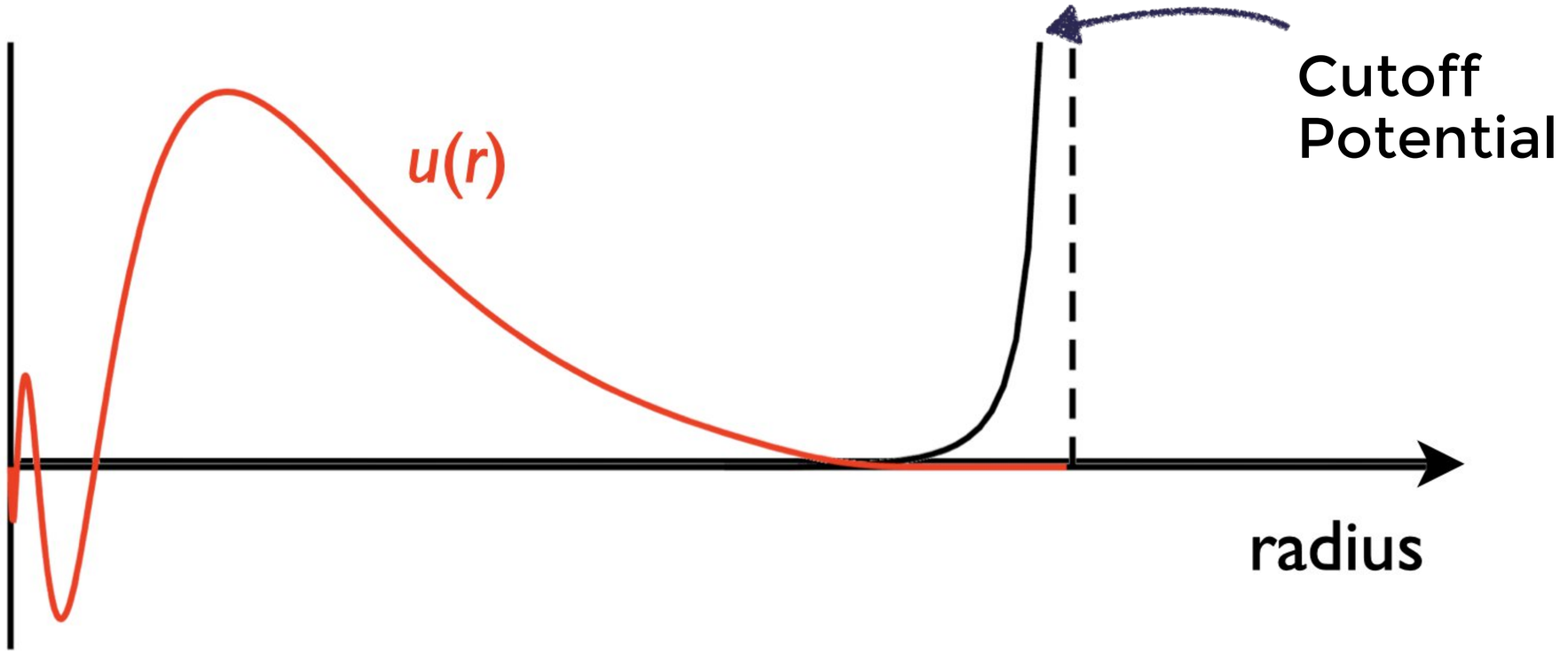
Key Design Choice: Numeric Atom-Centered Orbitals

FHI-aims
The ab initio materials simulation package

Basis Set Expansion

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

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



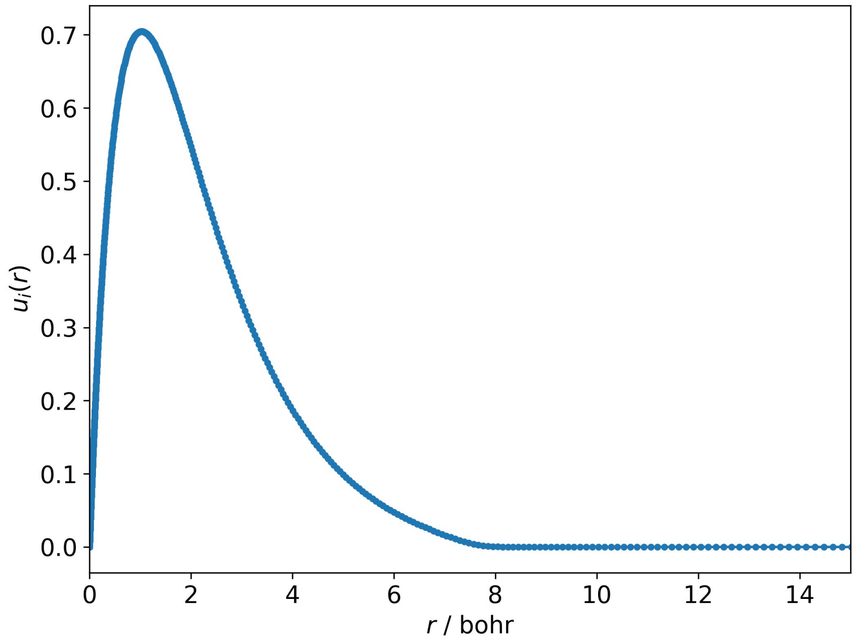
MS1P
Molecular Simulations from First Principles

How is the Basis Set Generated in FHI-aims?

- Solve radial Schrodinger eq on dense 1D logarithmic grid

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

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



Species Defaults in FHI-aims

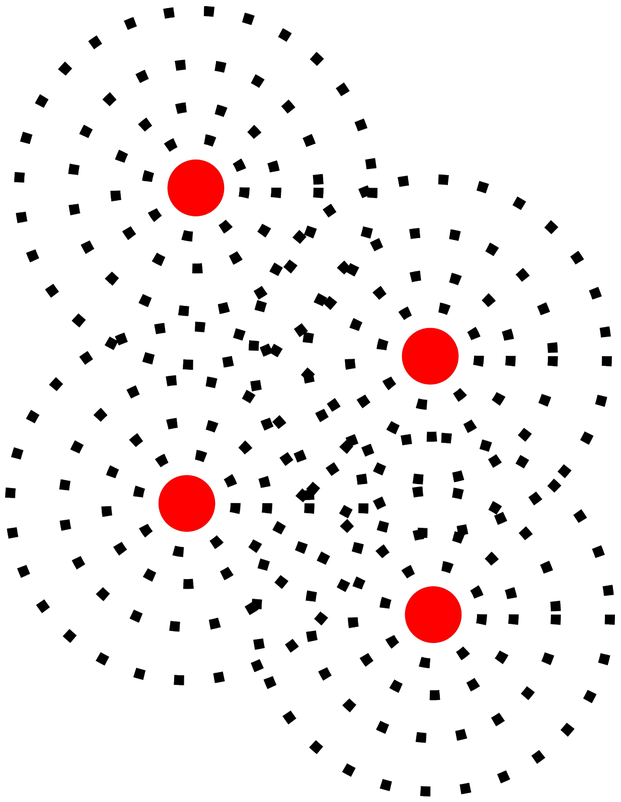
- In FHI-aims there are pre-calculated “species defaults” for elements 1-102 which contain basis functions, but not only…

- Include parameters for: cut-off potential, angular and radial grids, hartree potential, as well as species name, atomic mass, and atomic number

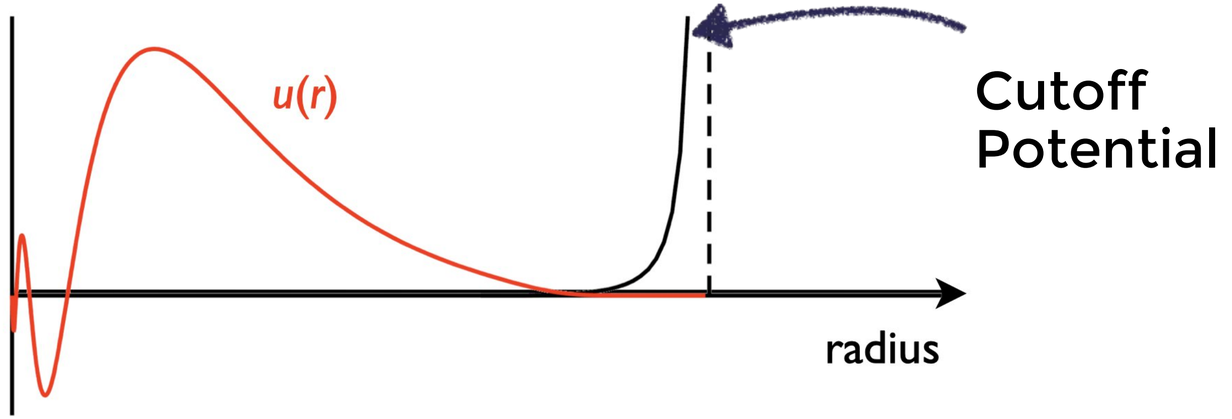
- Pre-calculated defaults, ranging from fast-qualitative to meV-converged calculations (Total energy, DFT)

- Also freely user customizable

- More later in practical aspects…



Why This Choice of NAOs?

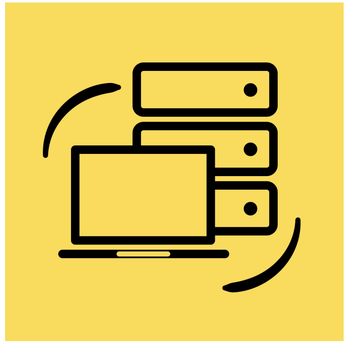


Versatile

Non-periodic and periodic systems on same footing

Precise + Accurate

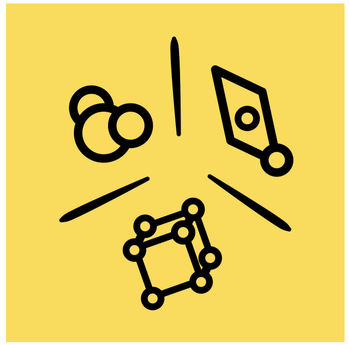
Flexible shape and all-electron description for DFT and correlated methods (RPA, GW, ...)

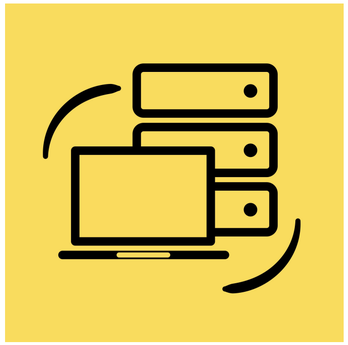


Scalable

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).

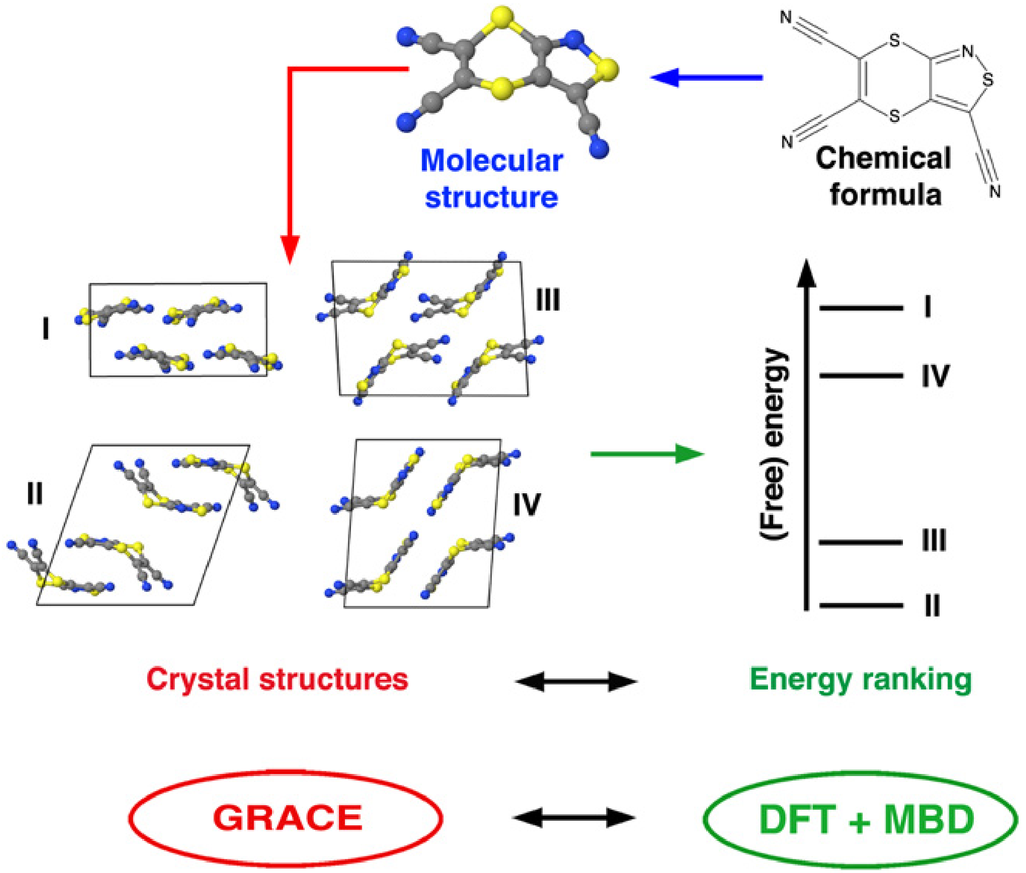
E(V) for 71 elemental solids - 15 codes, all-electron & 40 pseudopotential sets

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

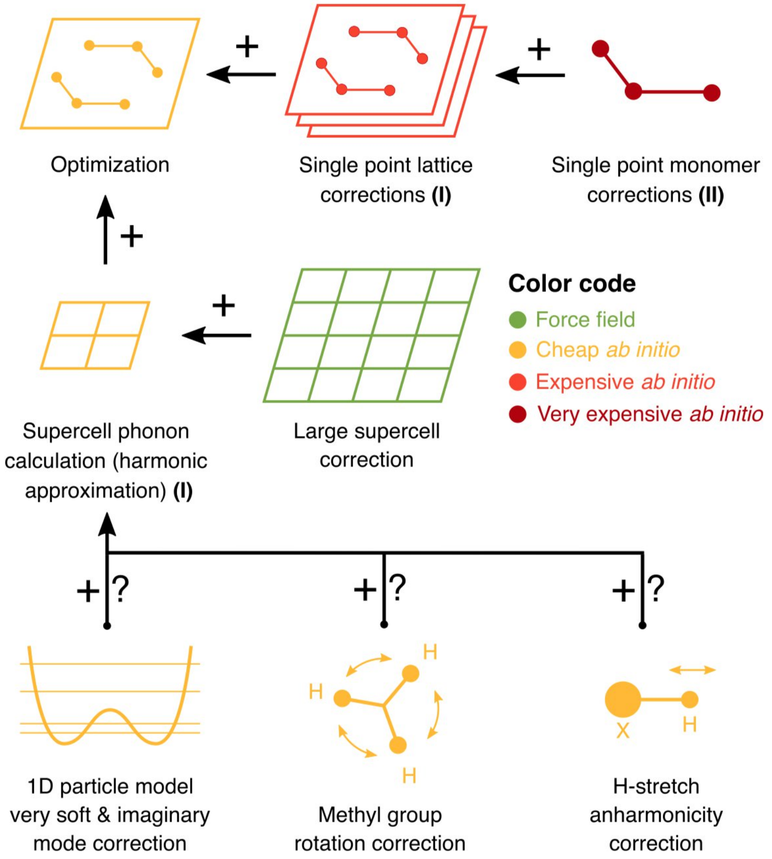
* Results: Marcin Dulak, DTU (Copenhagen)

Slide: Courtesy of V. Blum

High Accuracy in Crystal Structure Prediction



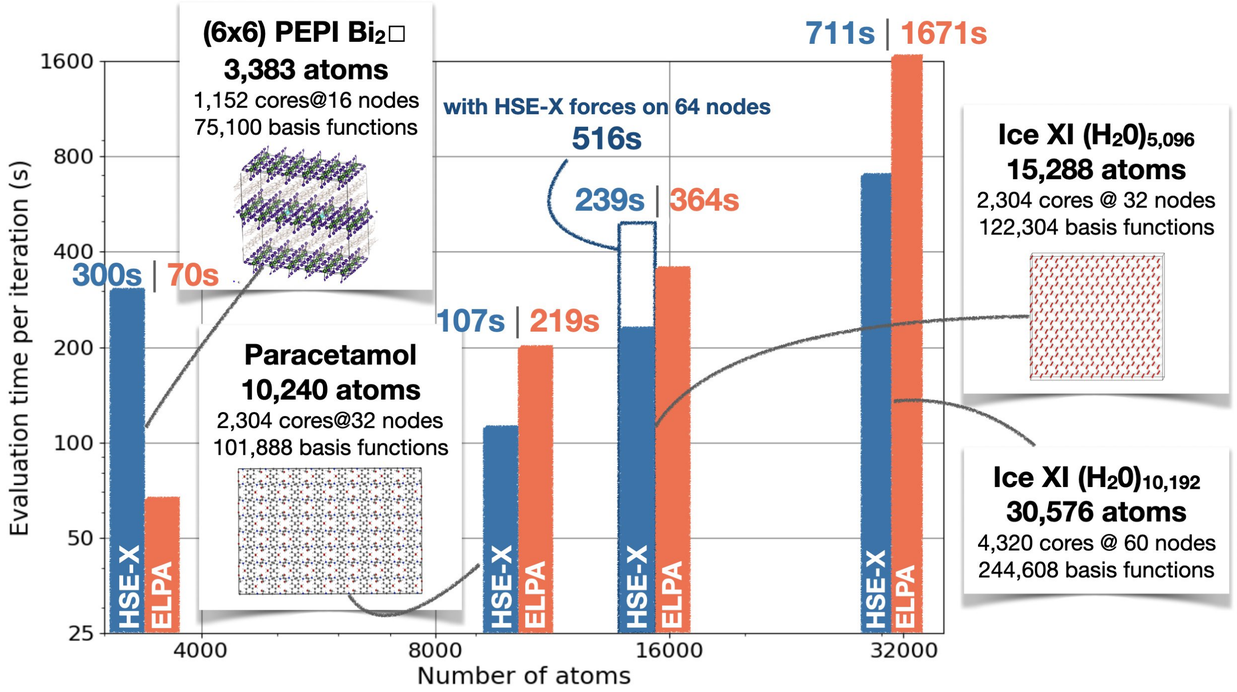
J. Hoja et al., Sci. Adv. 5, eaau3338 (2019)



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



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 Rampp; Matthias Scheffler; Volker Blum

Check for updates

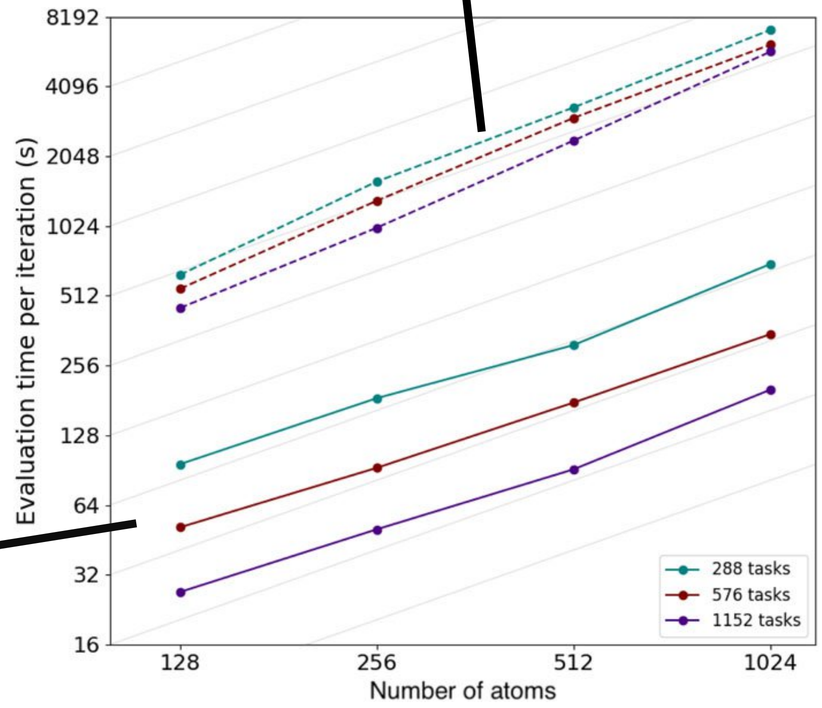
+ Author & Article Information

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

https://doi.org/10.1063/5.0208103 **Article history**

New implementation

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



Efficiency for Creating Machine Learning Datasets

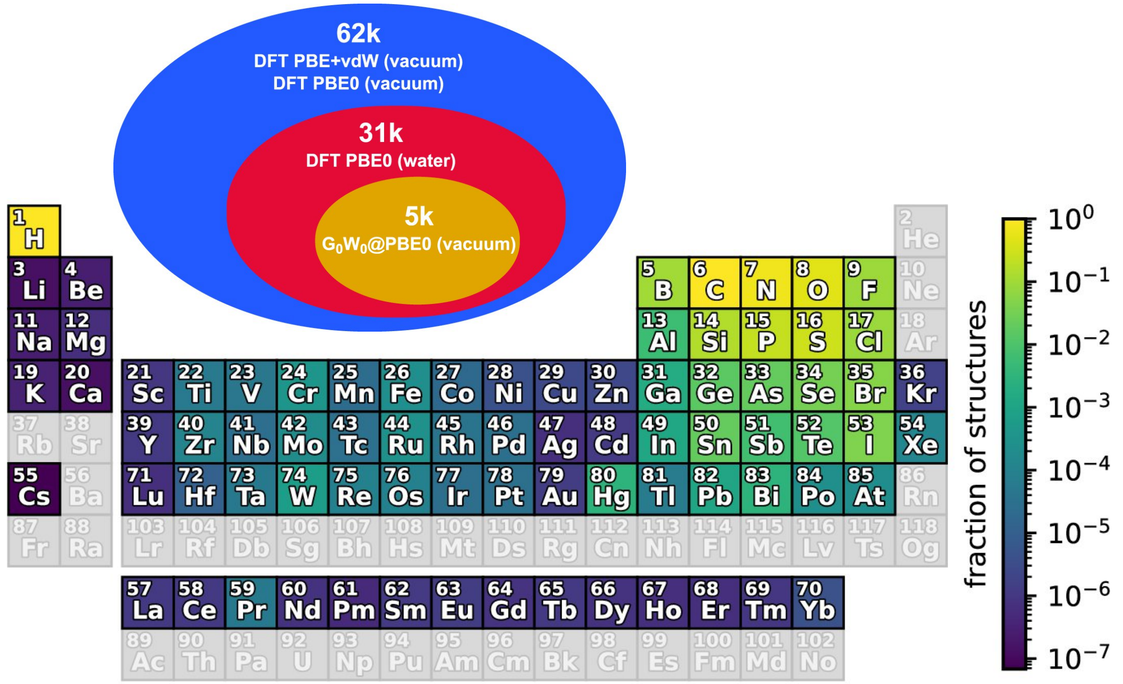
1. OE62 Dataset:

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

2. QCML Dataset:

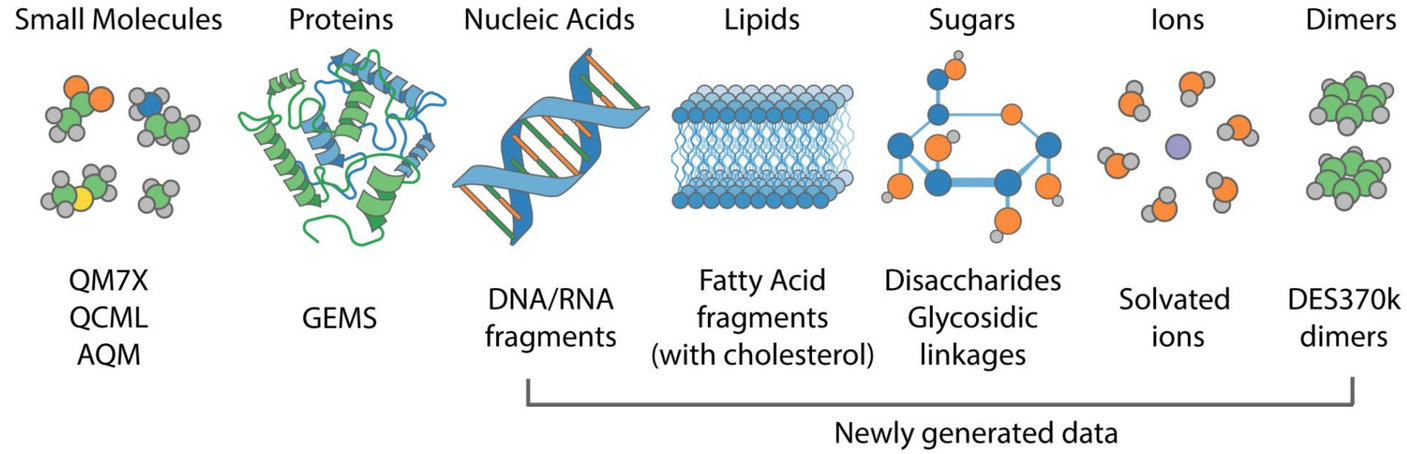
DeepMind

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)

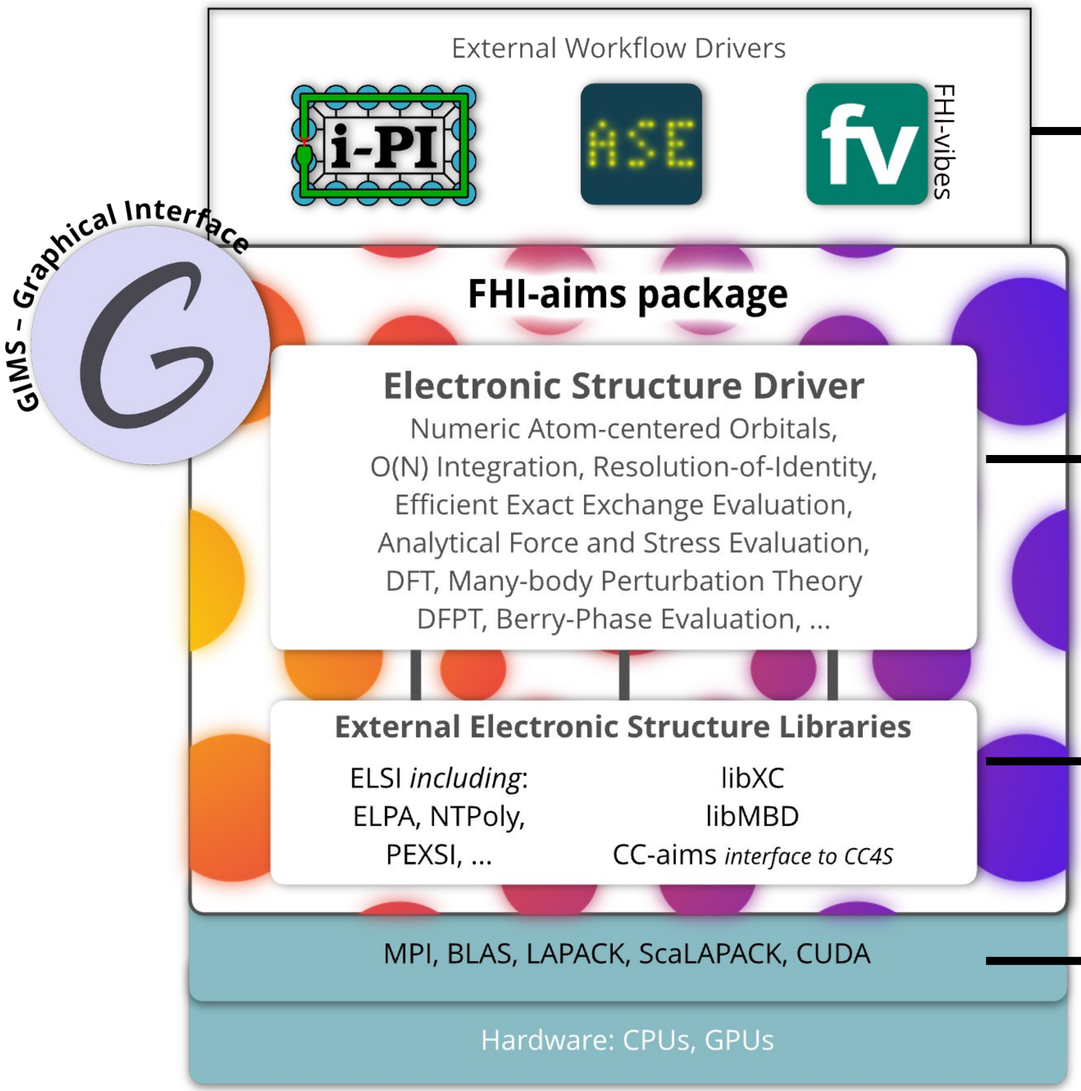


3. QCell Dataset:

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



External drivers for FHI-aims

Main “internal” FHI-aims code

External electronic structure libraries

Linear algebra and hardware libraries

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]
```

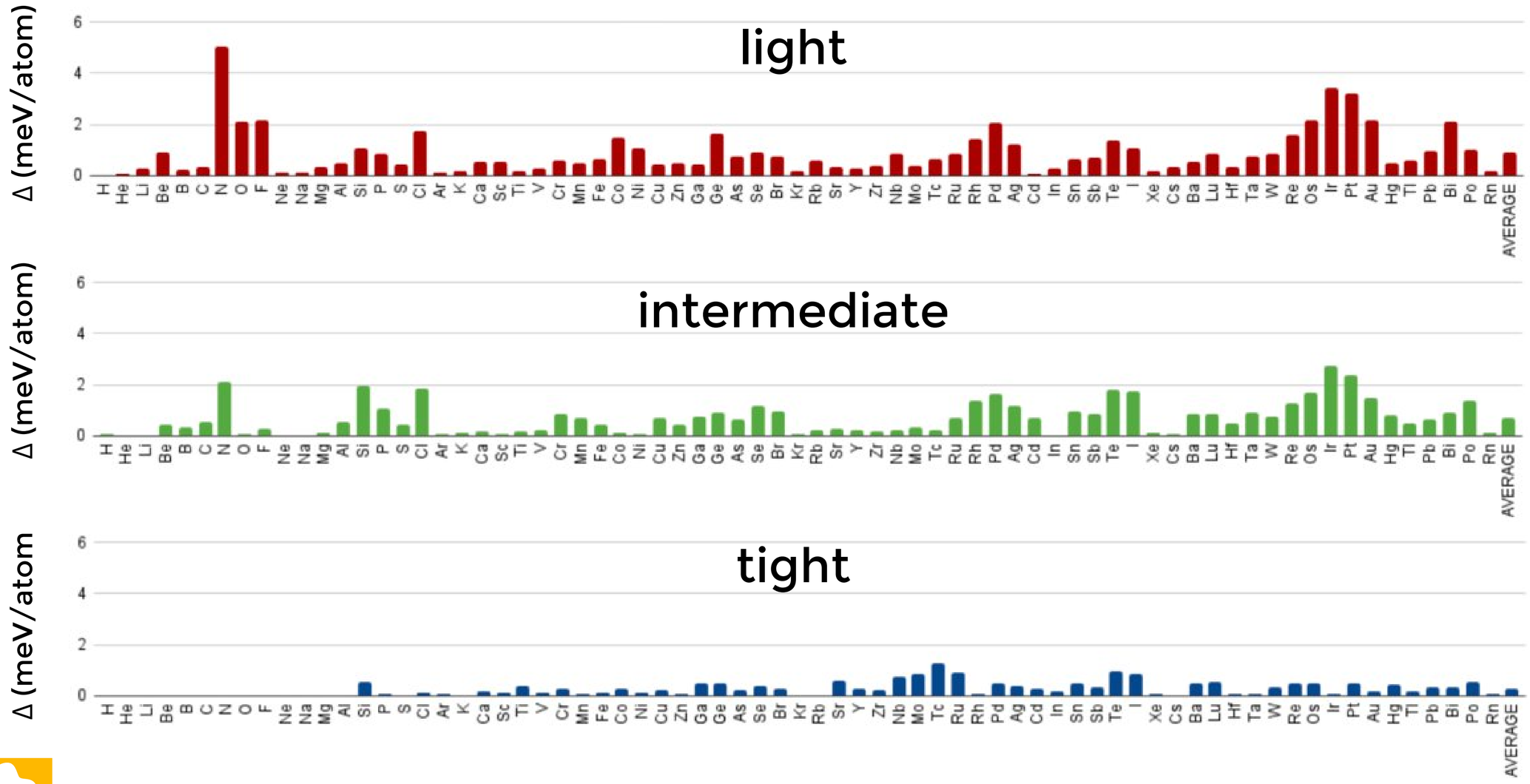
Species Defaults in FHI-aims : The Basics

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

Species Defaults in FHI-aims: Convergence

- 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

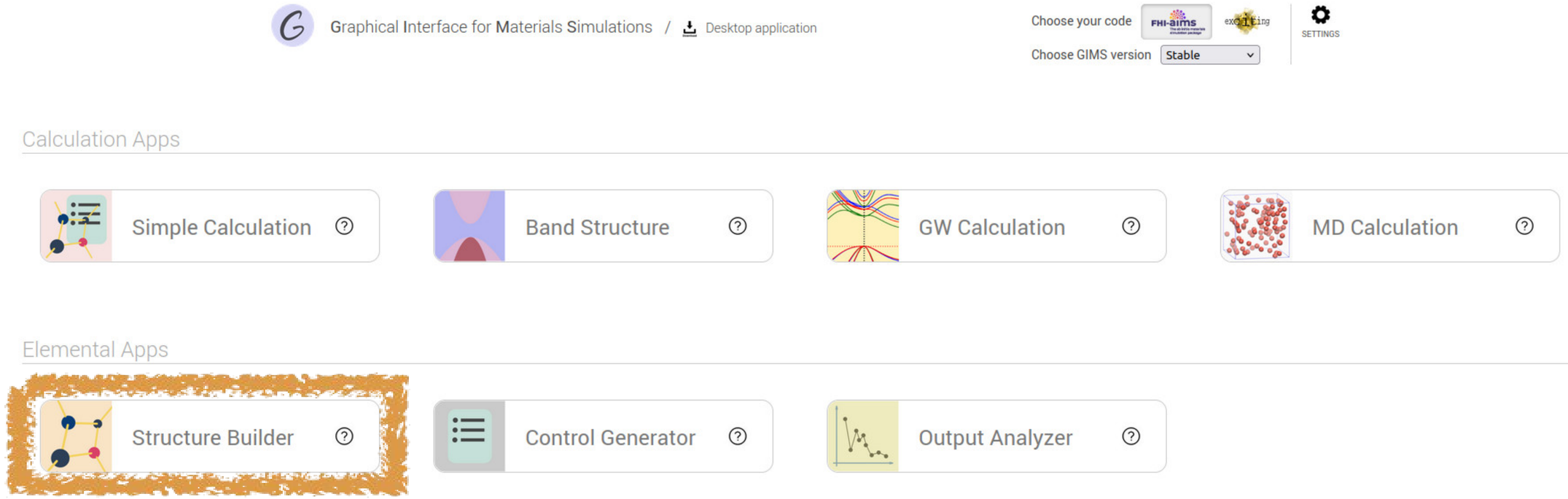
```
mpirun –np N aims.x > aims.out
```

```
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 initalization           :        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.
                                  l be greater.


     Have a nice day.
-----------------------------------------------------------
```

Graphical Interface for Materials Simulations (GIMS)

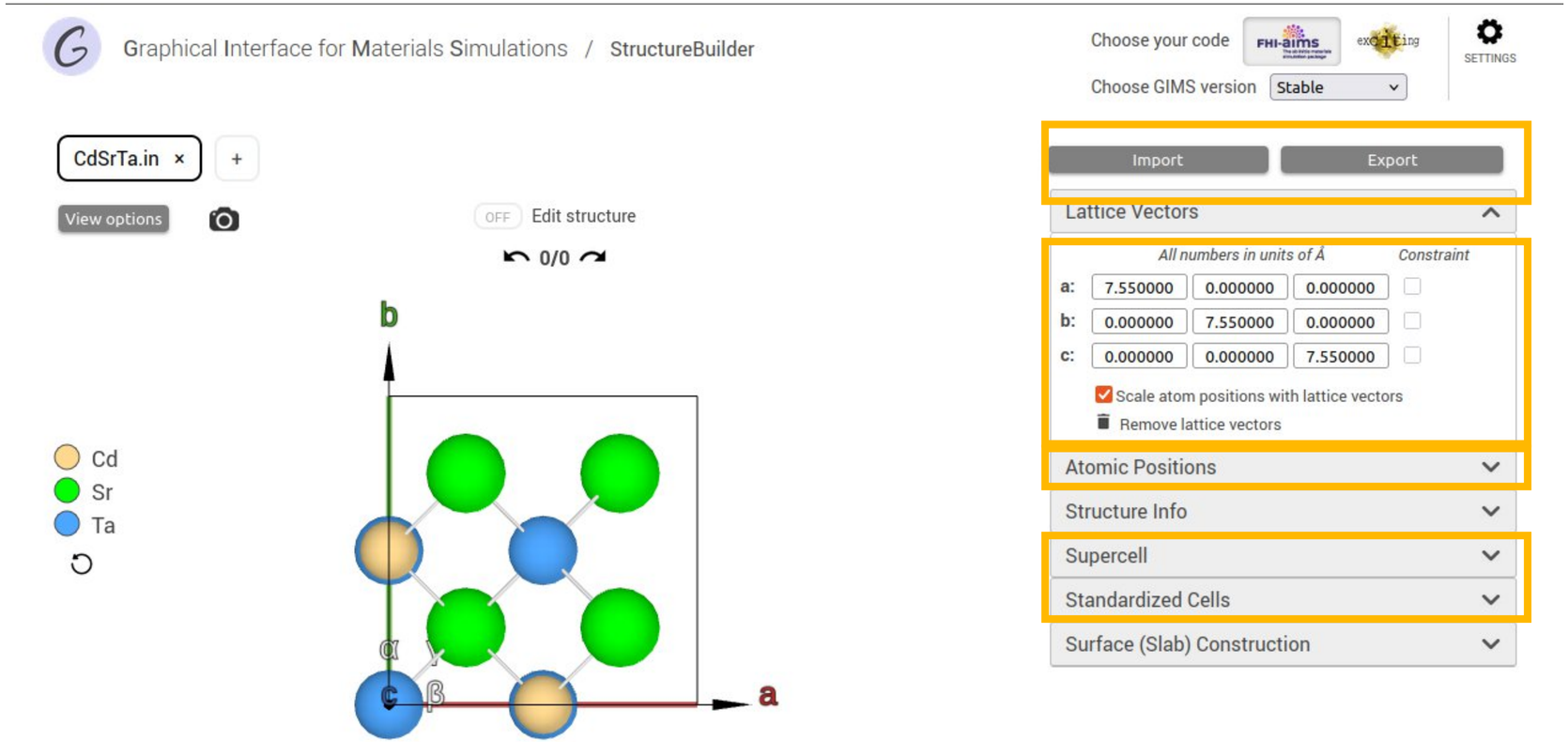
https://gims.ms1p.org

- Create input files, analyse output files



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

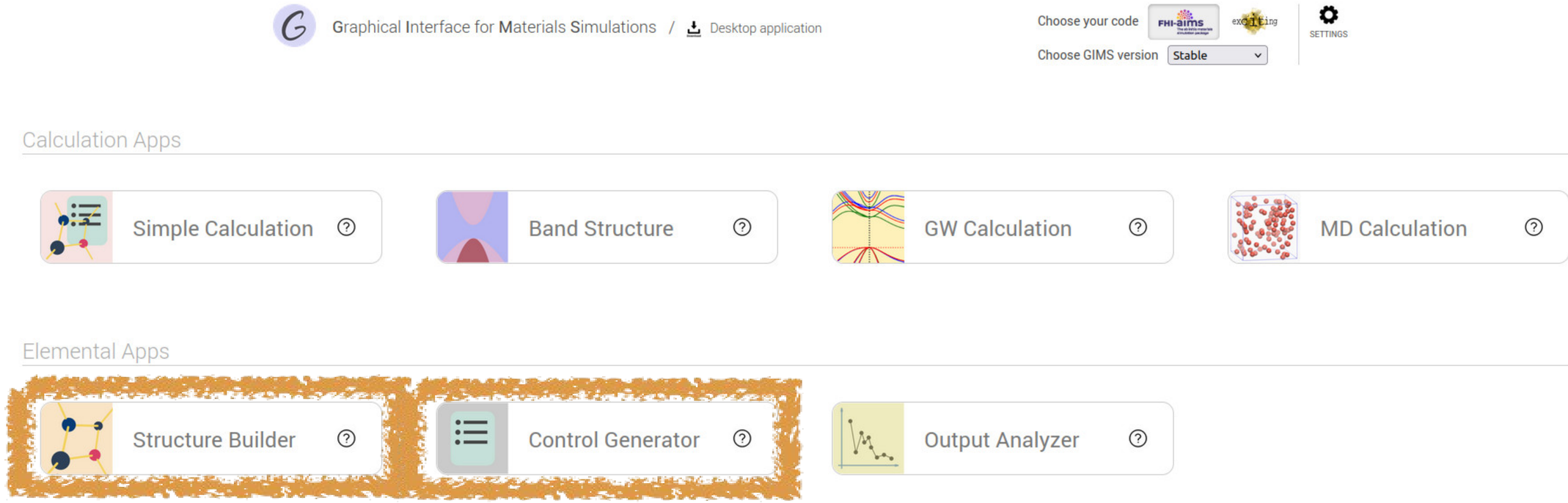


- Import structure from ASE supported formats (e.g. CIF) and export to geometry.in
- Edit / remove lattice vectors
- Add / move / remove atoms, change atomic species
- Simply create supercell / primitive cell
- Plus much more...

Graphical Interface for Materials Simulations (GIMS)

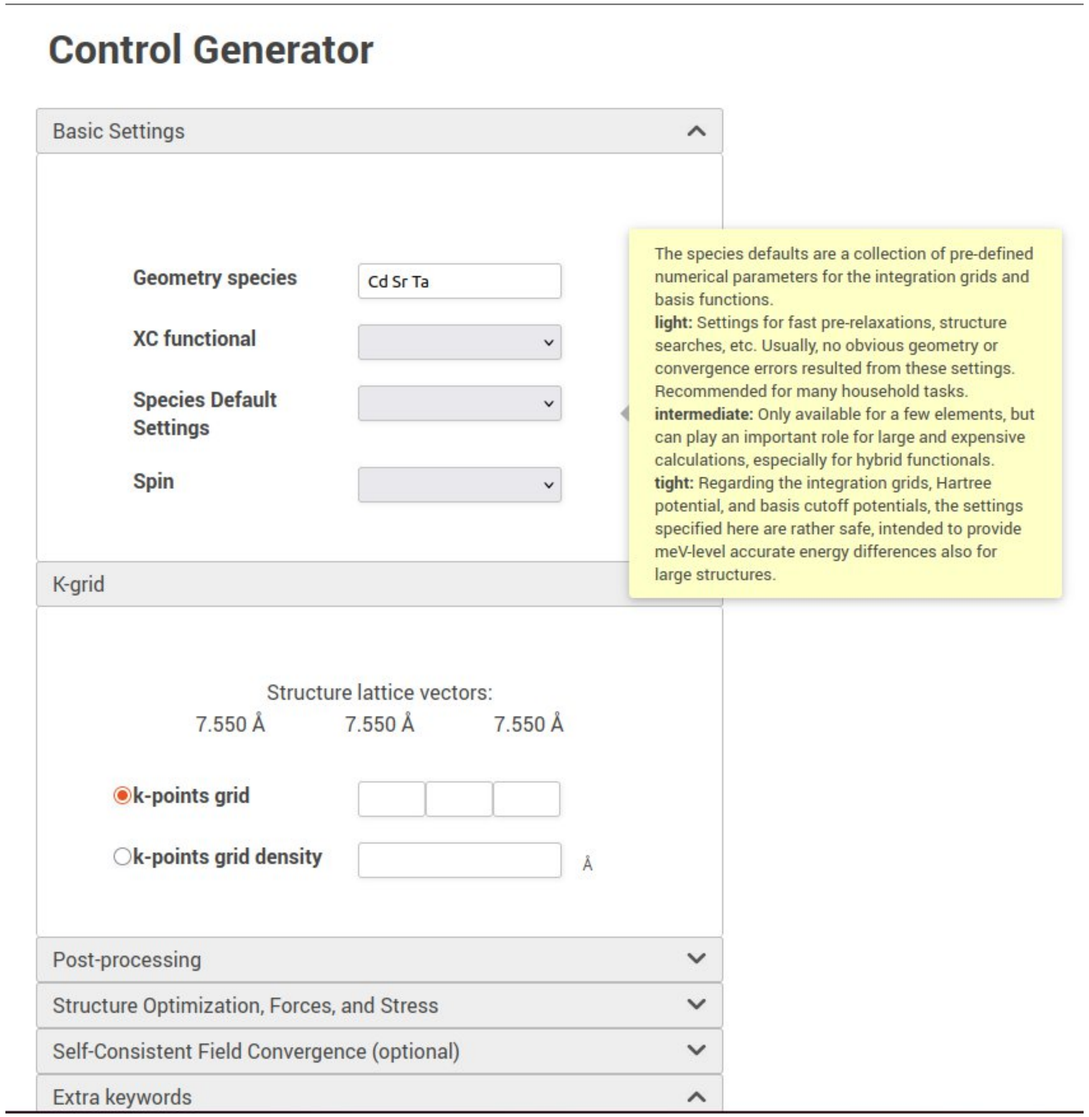
https://gims.ms1p.org

- Create input files, analyse output files



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: Create a control.in File

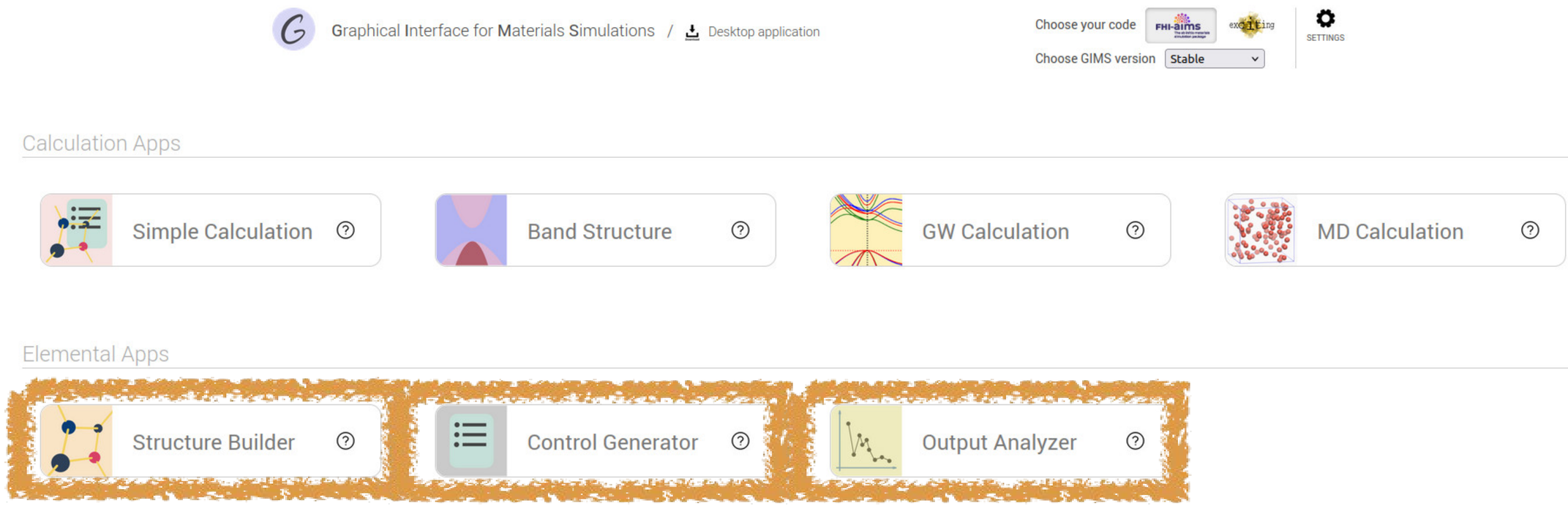


- A set of mostly used input file keywords with explanation
- A simple mechanism of visibility constraints (certain keyword inputs may not be visible based on other inputs' values) and sanity checks of inputs' values based on other inputs and structure
- Extra keywords table allows building complicated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

Graphical Interface for Materials Simulations (GIMS)

https://gims.ms1p.org

- Create input files, analyse output files

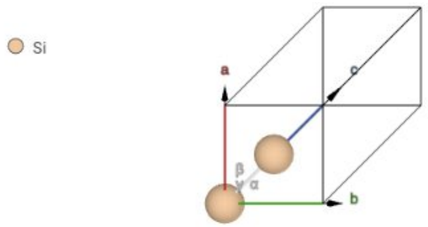


Sebastian Kokott, Iker Hurtado, Christian Vorwerk, Claudia Draxl,Volker Blum, Matthias Scheffler, GIMS: Graphical Interface for Materials Simulations. Journal of Open Source Software, 6(57), 2767. https://doi.org/10.21105/joss.02767

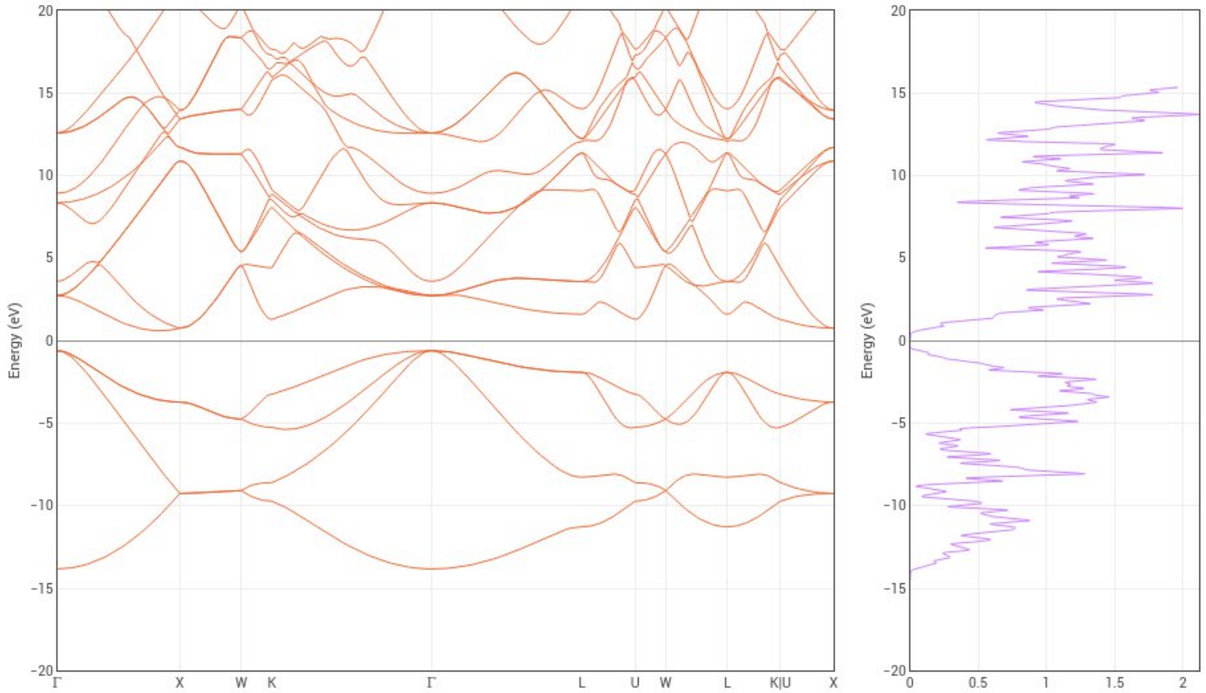
GIMS: Analyse Output

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



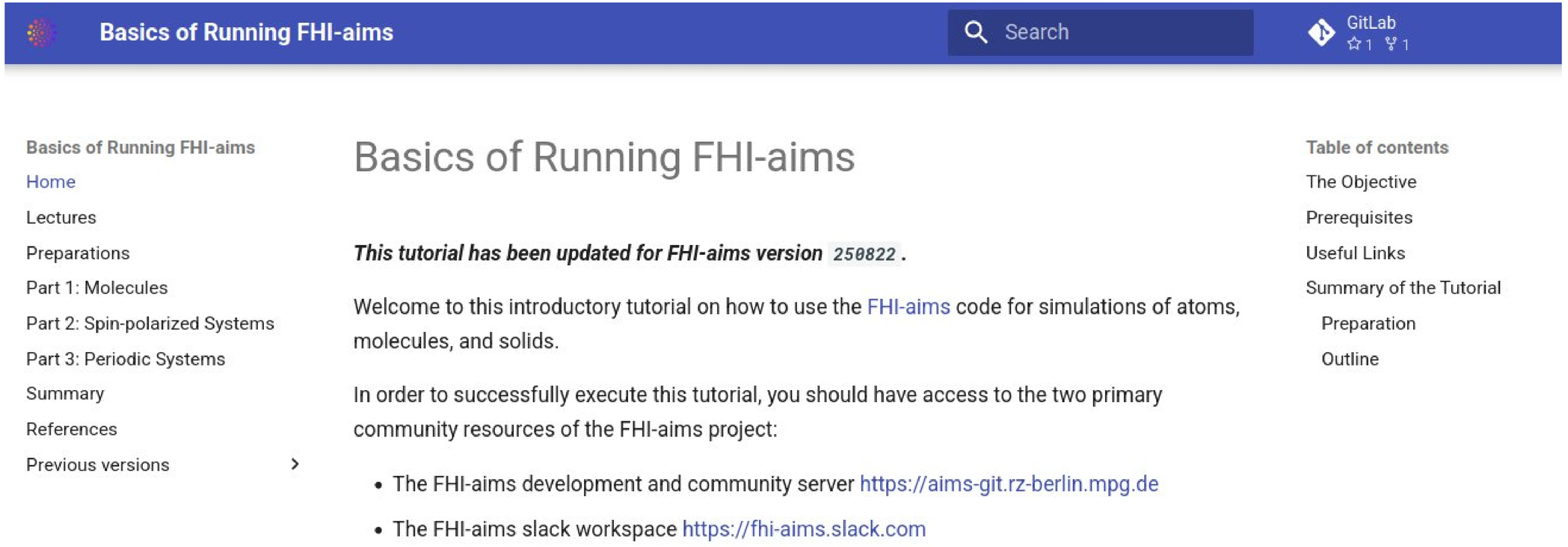
DOS and Band Structure graphs



- 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

Basics Tutorial

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



Questions?

FHI-aims

The ab initio materials simulation package

Efficient **electronic structure theory** with numeric atom-centered orbitals.

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Where Can You Find FHI-aims?

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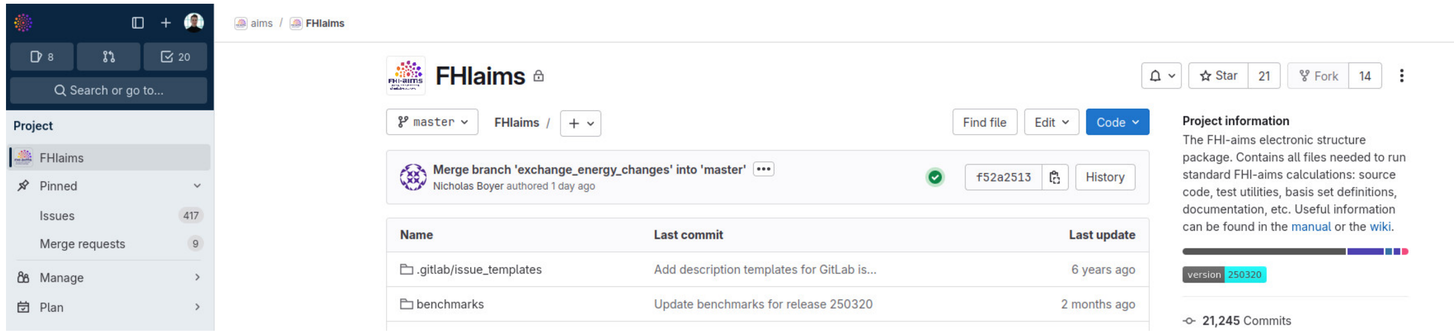
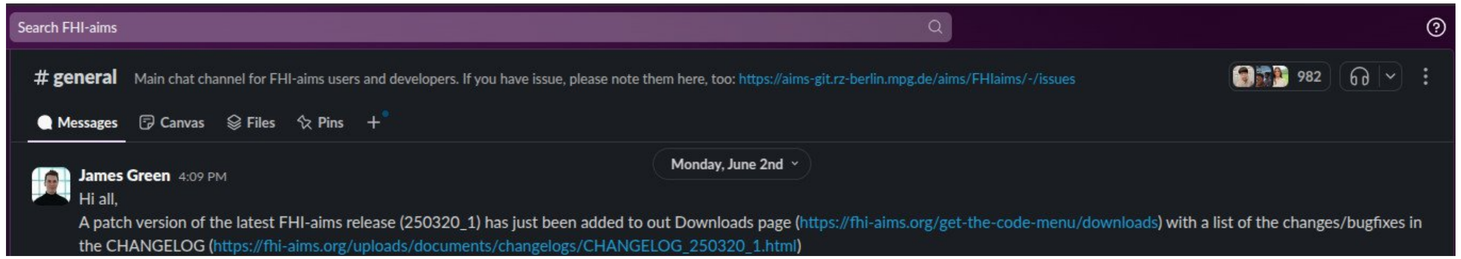
GitLab



slack



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