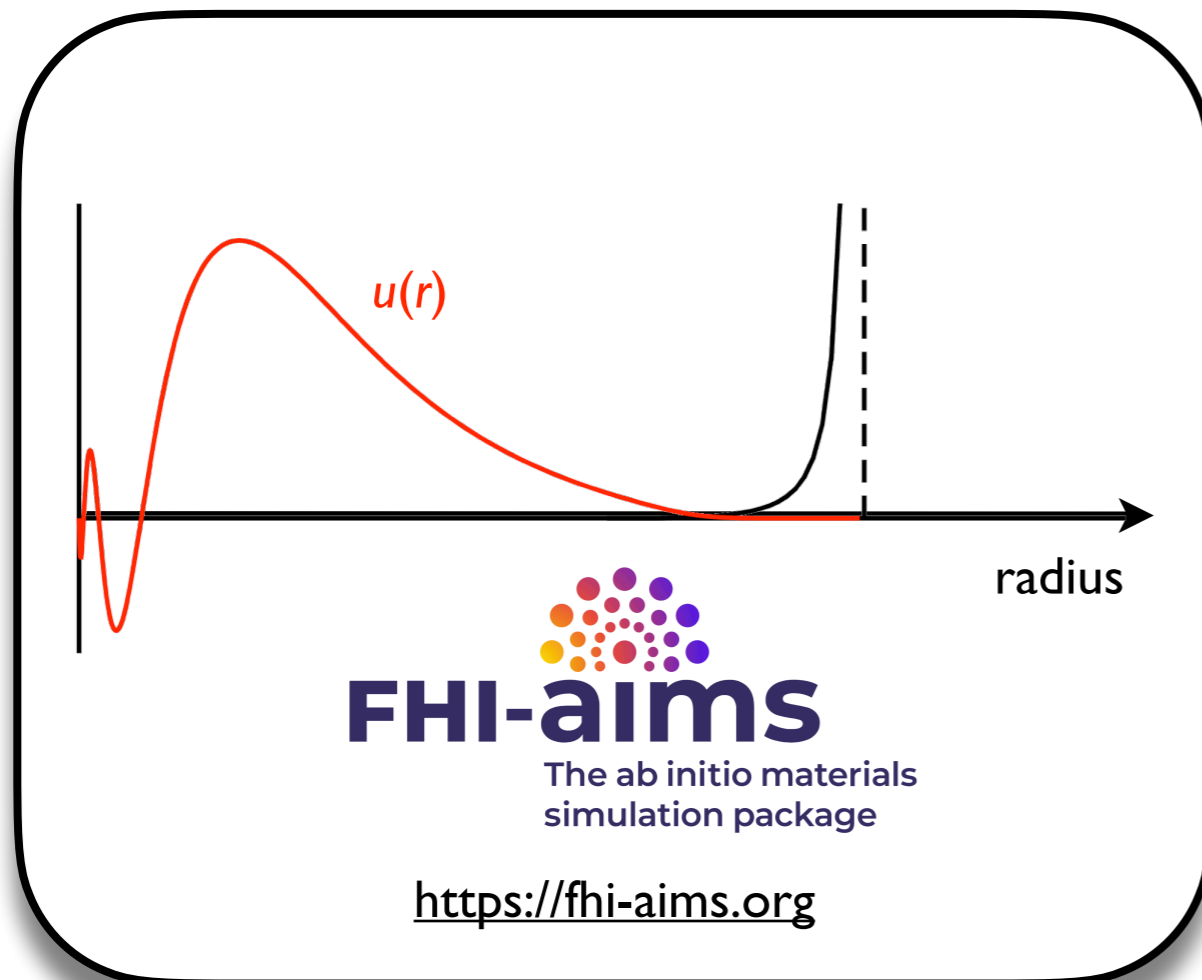


State of FHI-aims (and Its Ecosystem, here: GIMS)

Volker Blum

MEMS Department, Duke University, Durham, NC

<http://aims.pratt.duke.edu>



Andrei Sobolev

MSIP e.V., Berlin

User and Developer
Workshops

2010

2012

2014

2016

2018

2020

2023

We're back!

Organizers Behind this Workshop



Mariana Rossi



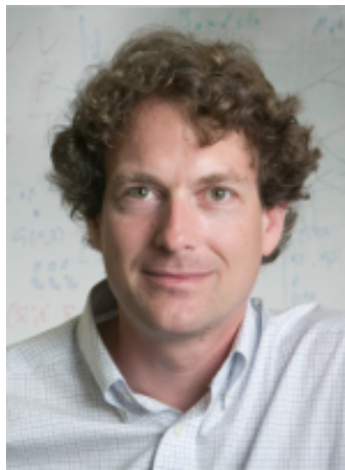
Sebastian Kokott



Uthpala Herath



Konstantin Lion



VB



Christian Carbogno



Ville Havu



Patrick Rinke



Matthias Scheffler

FHI-aims Code

<https://fhi-aims.org>



FHI-aims team and collaborators: **Matthias Scheffler (Berlin), Sebastian Kokott (Berlin), Mariana Rossi (Hamburg), Xinguo Ren (Beijing), Karsten Reuter (Berlin), over 150 individuals** with contributions to the project. Development in Berlin, Duke, UNC, Beijing, Helsinki, Warwick, Cardiff, Dresden, Dalhousie, etc.

Coordinators: Blum, Kokott, Rossi, Scheffler

Alaa Akkoush, Heiko Appel, Victor Atalla, Kurt Baermann, 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, Christian Carbogno, Fabio Caruso, Marco Casadei, Michele Ceriotti, 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, Luca Ghiringhelli, Mark Glass, Vivekanand Gobre, Dorothea Golze, Matthias Gramzow, Patrick Guetlein, Stefan Gutzeit, Volker Haigis, Felix Hanke, Paula Havu, Ville Havu, Joscha Hekele, Olle Hellman, Jan Hermann, Oliver Hofmann, Johannes Hoja, Xiaojuan Hu, William Huhn, Lukas Hörmann, Arvid Ihrig, Timo Jacob, Adam Jackson, Svenja Janke, Ran Jia, Rainer Johanni, Erin Johnson, Werner Jürgens, Matthias Kahk, Yosuke Kanai, Levi Keller, Matthias Kick, Woo Youn Kim, Jan Kloppenburg, Alexander Knoll, Florian Knoop, Franz Knuth, Simone Koecher, Gabrielle Koknat, Sebastian Kokott, Raul Laasner, Lucas Lang, Bjoern Lange, Marvin Lechner, Susi Lehtola, Maja-Olivia Lenz, Sergey Levchenko, Alan Lewis, Jiachen Li, Xinzhen Li, Kailai Lin, Xinyi Lin, Konstantin Lion, Yair Litman, Chi Liu, Andrew Logsdail, Andreas Marek, Thomas Markovich, Reinhard Maurer, Florian Merz, Joerg Meyer, Wenhui Mi, Evgeny Moerman, Christoph Muschielok, Mohammad Nakhaee, Lydia Nemeč, Norbert Nemeč, Kane O'Donnell, Harald Oberhofer, Berk Onat, Alberto Otero de la Rosa, Ramon L. Panades-Barrueta, Eszter Pos, Alastair Price, Thomas Purcell, Nathaniel Raimbault, 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, Ari-Pekka Soikkeli, Ruyi Song, Aloysius Soon, Pavel Stishenko, Muhammad Tahir, Alexandre Tkatchenko, Thomas Theis, Alvaro Vazquez Mayagoitia, 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, Wenxing Zhang, Rundong Zhao, Ruiyi Zhou, Yuanyuan Zhou, Tong Zhu



... and, with absolute certainty, more! Thank you!

FHI-aims Code

<https://fhi-aims.org>



FHI-aims team and collaborators: **Matthias Scheffler (Berlin), Sebastian Kokott (Berlin), Mariana Rossi (Hamburg), Xinguo Ren (Beijing), Karsten Reuter (Berlin), over 150 individuals** with contributions to the project. Development in Berlin, Duke, UNC, Beijing, Helsinki, Warwick, Cardiff, Dresden, Dalhousie, etc.

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Ferdinand Evers, Eduardo Fabia, ...
Ghiringhelli, Mark Glass, Vivekanand, ...
Haigis, Felix Hanke, Paula Havu, ...
Xiaojuan Hu, William Huhn, Luk, ...
Erin Johnson, Werner Jürgens, ...
Alexander Knoll, Florian Knoop, ...
Bjoern Lange, Marvin Lechner, ...
Lin, Xinyi Lin, Konstantin Lion, Y, ...
Florian Merz, Joerg Meyer, Wen, ...
Nemec, Kane O'Donnell, Harald, ...
Alastair Price, Thomas Purcell, N, ...
Patrick Rinke, Herzain Rivera, Mat, ...
Andrea Sanfilippo, Matthias Scheffler, Markus Schneider, Christoph Schober, Franziska Schubert, Honghui Shang, Tonghao Shen, Markus Sinstein, Justin Clifford Smith, Ari-Pekka Soikkeli, Ruyi Song, Aloysius Soon, Pavel Stishenko, Muhammad Tahir, Alexandre Tkatchenko, Thomas Theis, Alvaro Vazquez Mayagoitia, 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, Wenxing Zhang, Rundong Zhao, Ruiyi Zhou, Yuanyuan Zhou, Tong Zhu

**Actually, you know
there are more.**

**Can we use this workshop
to update website,
FHI-aims output citations?**

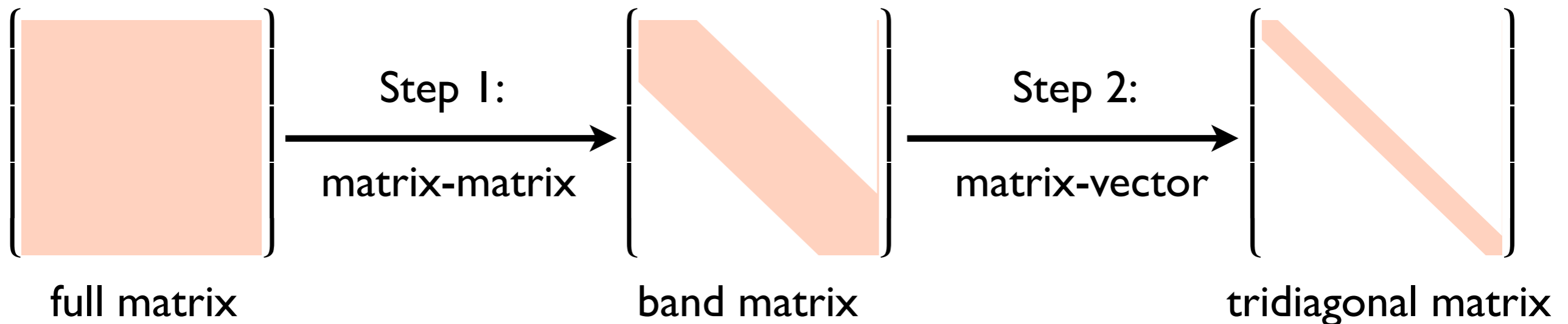
... and, with absolute certainty, more! Thank you!



However, We Have a Whole Ecosystem ... ELPA

Massively parallel eigenvalue solutions,
CPU and GPU ... came from FHI-aims, used far beyond FHI-aims.

$$\underline{\underline{h}} \underline{\underline{c}}_k = \epsilon_k \underline{\underline{S}} \underline{\underline{c}}_k$$



- Auckenthaler et al., Parallel Computing 37, 783 (2011)
Marek et al., J. Phys.: Condens. Matter 26, 213201 (2014)
Kus et al., Parallel Computing 85, 167 (2019)
Yu et al., Comp. Phys. Commun. 262, 107808 (2021)

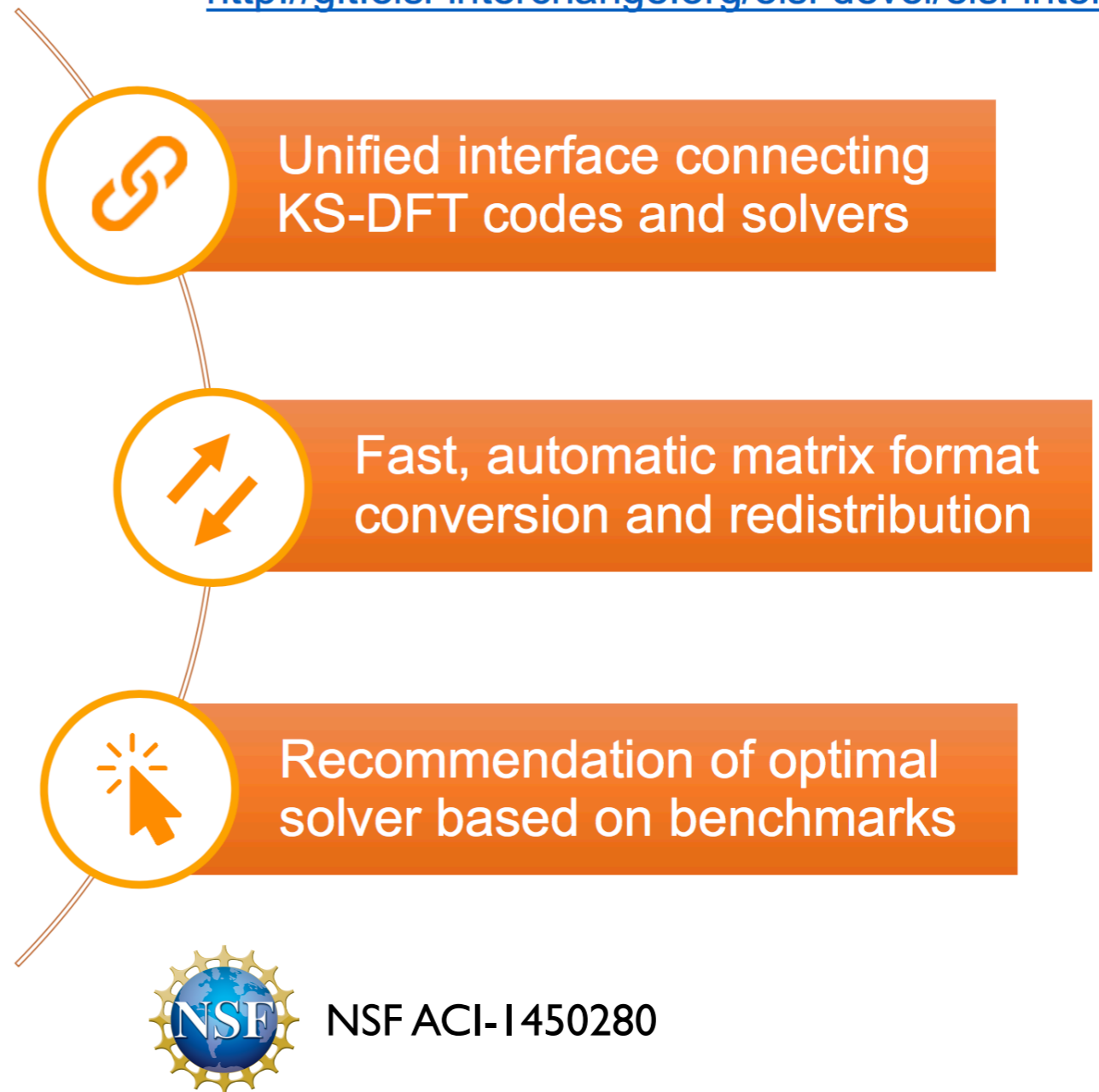
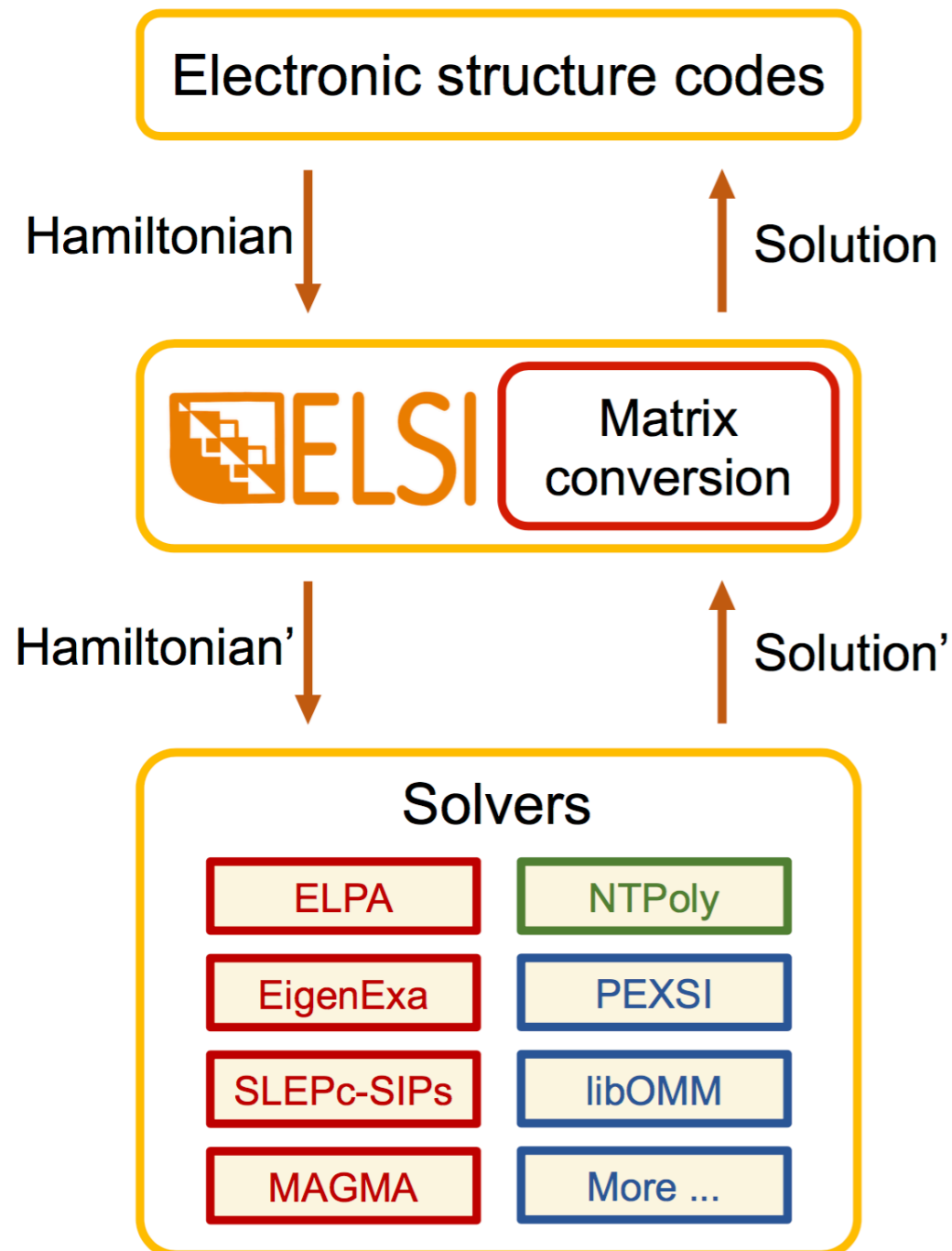
However, We Have a Whole Ecosystem ... ELSI

Yu et al., "ELSI – An Open Infrastructure for Electronic Structure Solvers"
Comp. Phys. Commun. 256, 107459 (2020).

Yu et al., *Comput. Phys. Commun.* 2018

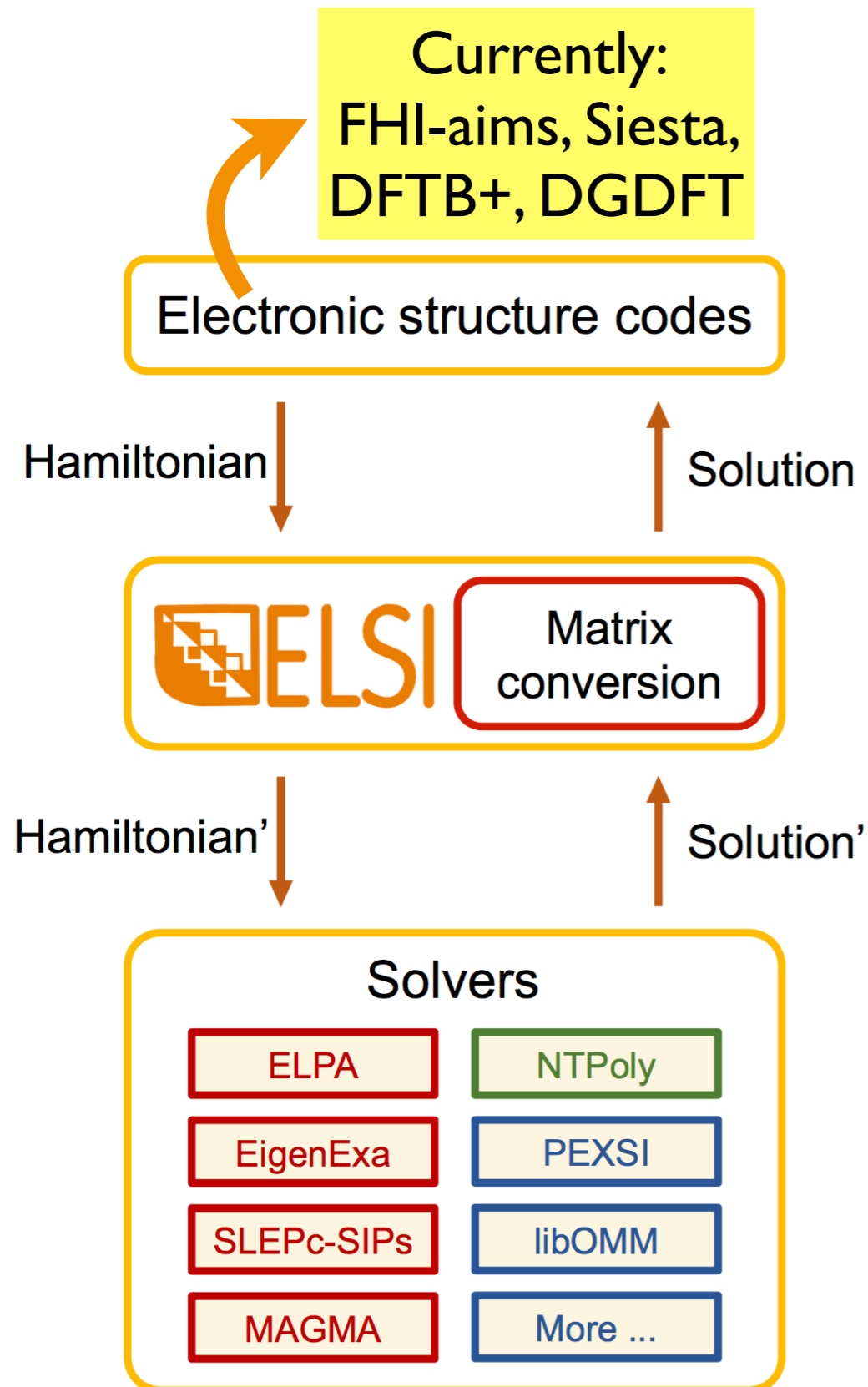
<http://elsi-interchange.org>

<http://git.elsi-interchange.org/elsi-devel/elsi-interface>



NSF ACI-I450280

However, We Have a Whole Ecosystem ... ELSI

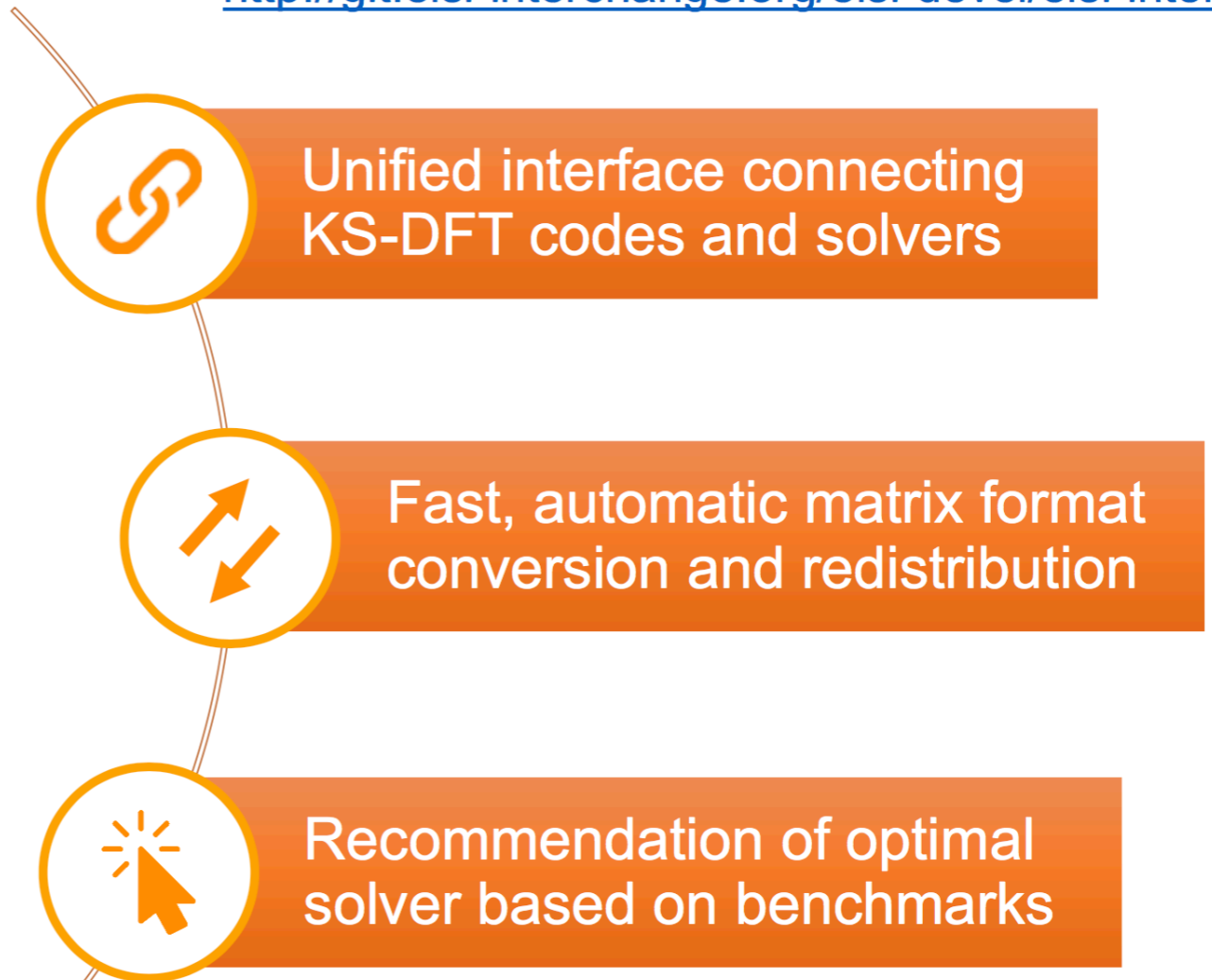


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<http://git.elsi-interchange.org/elsi-devel/elsi-interface>



NSF ACI-I450280

However, We Have a Whole Ecosystem ... GIMS

<https://gims.ms1p.org>

Browser-based graphical interface - no installation, open to more codes.

The screenshot displays the GIMS web interface for a 'Simple Calculation workflow'. The browser address bar shows the URL <https://gims.ms1p.org/static/index.html#SimpleCalculation-workflow#Structure>. The page title is 'Graphical Interface for Materials Simulations / SimpleCalculation workflow'. In the top right, there are options to 'Choose your code' (with 'FHI-aims' and 'exciting' logos) and 'Choose GIMS version' (set to 'Stable'). A 'SETTINGS' gear icon is also present.

The main content area is titled 'Simple Calculation workflow' and 'Step 1. Create or upload geometry'. A 'Save geometry & Go ahead' button is visible. Below this, a file named 'CdSrTa.in' is loaded. There are 'View options' and 'Edit structure' (currently OFF) controls. A central 3D visualization shows a crystal structure with atoms represented by spheres: Cd (orange), Sr (green), and Ta (blue). The structure is plotted in a coordinate system with axes 'a', 'b', and 'c'. A legend on the left identifies the species: Cd (orange), Sr (green), and Ta (blue).

On the right side, there are 'Import' and 'Export' buttons. Below them is a 'Lattice Vectors' section with the following data:

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

Additional options include 'Scale atom positions with lattice vectors' (checked) and 'Remove Lattice Vectors'. Below this are expandable sections for 'Structure Info', 'Supercell', 'Standardized Cells', 'Surface (Slab) Construction', and 'Basis Atoms'. The 'Basis Atoms' section shows a list of atoms with their coordinates:

All numbers in units of Å			
1.	0.000000	3.775000	3.775000

Buttons for 'New atom' and 'Constrain all atoms' are also present. A 'user manual' and 'feedback' sidebar are visible on the left. The bottom status bar shows 'Undo/Redo Ctrl+Z / Ctrl+Y' and 'Atoms selection and measurements'.

Sebastian Kokott, Iker Hurtado, Christian Vorwerk, Claudia Draxl, Volker Blum and Matthias Scheffler, "GIMS: Graphical Interface for Materials Simulations," The Journal of Open Source Software, Vol. 6, No. 57, 2767 (2021). <https://doi.org/10.21105/joss.02767>.

However, We Have a Whole Ecosystem ... Many More

FHI-vibes

(Florian Knoop, Christian Carbogno et al., vibrations & transport)

i-pi

(Michele Ceriotti, Mariana Rossi et al., molecular dynamics)

Atomic Simulation Interface (ASI)

(Pavel Stishenko et al., data exchange)

GAtor / Genarris

(Noa Marom et al., Crystal Structure Prediction)

AvMatSim

(Marcus Neumann et al., Crystal Structure Prediction)

...

Where Do We Need to Grow?

- Documentation / Tutorials!

The image shows a screenshot of the FHI-aims website. The browser address bar shows <https://fhi-aims.org>. The main navigation menu includes: Learn more, Get the code, News, GUI, **Useful Things**, and Who We Are. A dropdown menu for 'Useful Things' is open, listing: Useful Things, Online Tutorials (with an external link icon), FHI-aims Tutorial Series 2021, Hands-on DFT 2017, Logo, and Simulation Tools. The main content area features the text: 'FHI-aims. All-electron electronic structure calculations using numeric atom-centered orbitals.' Below this is a red button that says 'Take a quick tour through FHI-aims'. At the bottom, three key features are highlighted with icons and text:

- Versatile**: Molecules - Clusters, Nanostructures, Surfaces - Solids
- Precise and Accurate**: Density Functional Theory, Many-Body Methods, Quantum Chemistry
- Scalable**: From Laptops to Highest-Performance Computers

Where Do We Need to Grow?

- Documentation / Tutorials!

The image shows a screenshot of a web browser with two tabs. The top tab is titled 'Home - FHI-aims' and shows the main website with a navigation menu including 'Learn more', 'Get the code', 'News', 'GUI', 'Useful Things', and 'Who We Are'. The bottom tab is titled 'FHI-aims tutorials: Overview' and shows the 'FHI-aims tutorials: Overview' page. The page content includes a welcome message, a table of contents, and a list of tutorial topics.

Home - FHI-aims

https://fhi-aims.org

elpa

Learn more Get the code News GUI **Useful Things** Who We Are

Home - FHI-aims FHI-aims tutorials: Overview

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

FHI-aims tutorials: Overview

Search

GitLab

Welcome to the FHI-aims Tutorials Overview Page!

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

Fundamentals of FHI-aims

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

- **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.
- **Charge and Spin Initialization: Complex Materials Simulations**
A tutorial that introduces FHI-aims for complex materials with non-trivial atomic and electronic structure. Key concepts include efficient initialization of ionic and spin-polarized solids and how to construct and simulate clusters, here demonstrated for the transition metal oxide Fe_2O_3 .
- **Slab calculations and surface simulations with FHI-aims**
The basic techniques for surface simulations with FHI-aims are introduced. Learn how to construct, run a slab simulation, and

Table of contents

- Fundamentals of FHI-aims
- Beyond DFT methods in FHI-aims
- Motion of atoms
- Ab initio Thermodynamics
- Data Management

Where Do We Need to Grow?

- Documentation / Tutorials!

The image shows a browser window with two tabs. The first tab is 'Home - FHI-aims' with the URL 'https://fhi-aims.org'. The second tab is 'FHI-aims tutorials: Overview' with the URL 'https://fhi-aims-club.gitlab.io/tutorials/tutorials-overview/'. The main content of the second tab is visible, showing a 'Welcome to the FHI-aims Tutorials Overview Page!' message and a 'Table of contents' sidebar with items like 'Fundamentals of FHI-aims', 'Beyond DFT methods in FHI-aims', 'Motion of atoms', 'Ab initio Thermodynamics', and 'Data Management'. A search bar is also present in the top right of the page.

**Openly accessible on gitlab.com -
in addition to manual, wiki, a trick that Mariana and Sebastian told me, ...
Please grow our tutorials and your work will be seen!**

efficient initialization of ionic and spin-polarized solids and how to construct and simulate clusters, here demonstrated for the transition metal oxide Fe_2O_3 .

- **Slab calculations and surface simulations with FHI-aims**

The basic techniques for surface simulations with FHI-aims are introduced. Learn how to construct, run a slab simulation, and

Where Do We Need to Grow?

- Code, continuous integration, testing

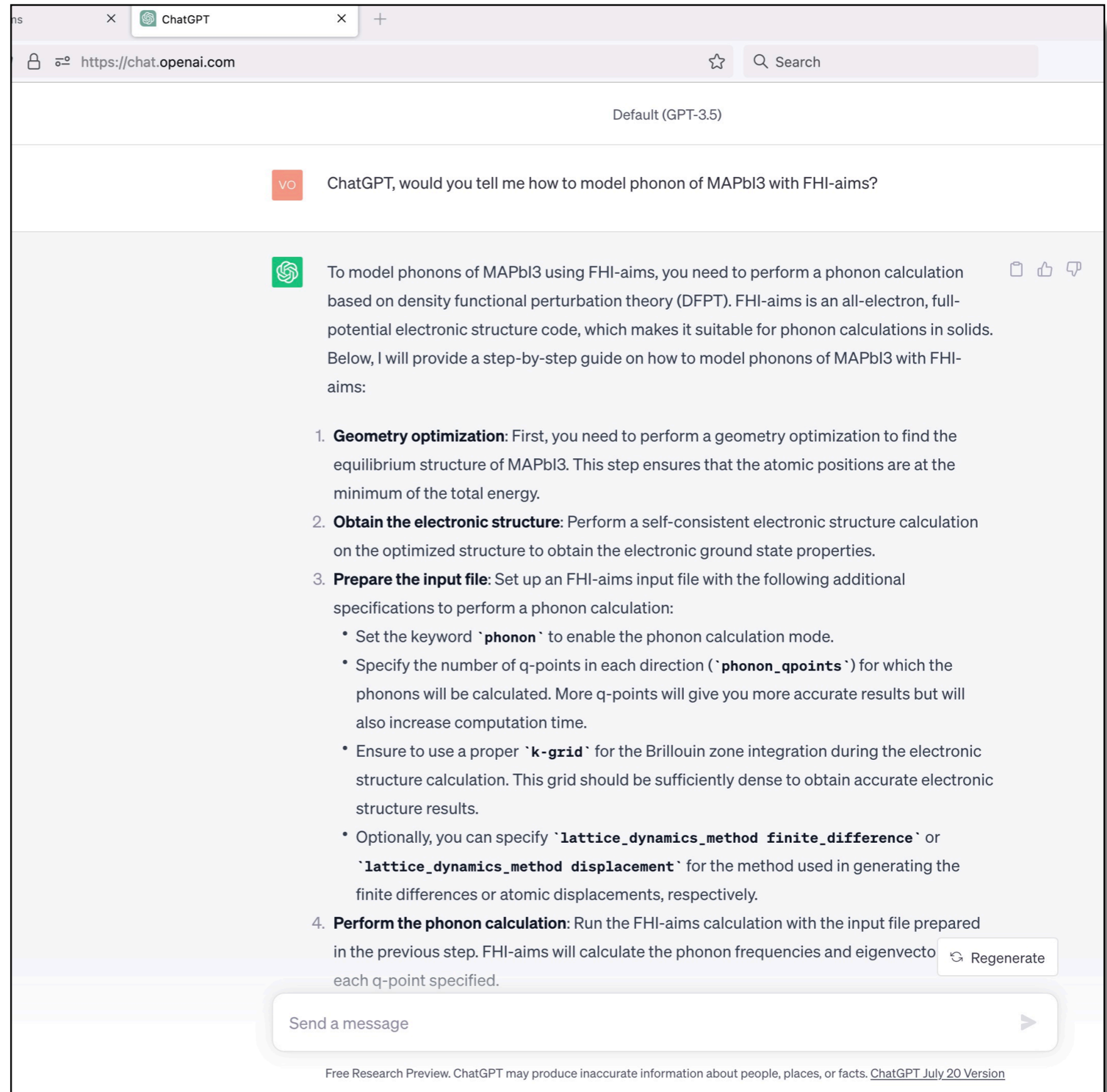
Thorough testing is critical to stable code.
I know we all know this and we are not doing badly,
but consider adding more CI tests, whenever something is amiss!

The screenshot displays the GitLab CI/CD interface for the 'FHlaims' project. The main content area shows a list of pipeline jobs, all of which have passed. A dropdown menu is open for the 'test_more' stage, showing a list of test jobs: test.more.debug.intel, test.more.ext.elsi.in..., test.more.gnu, test.more.gpu.intel, test.more.intel, and test.more.mpi.only.i... Each job has a green checkmark and a refresh icon. The left sidebar contains navigation links for Project information, Repository, Issues (268), Merge requests (12), CI/CD, Pipelines, Editor, Jobs, Artifacts, Schedules, Security and Compliance, Deployments, Infrastructure, and Monitor. The top navigation bar includes a search bar and user profile information.

Where Do We Need to Grow?

- Actually, AI.

Hm. Not quite.
We have some work
cut out for us ... no
way to ignore this.



The screenshot shows a web browser window with the URL <https://chat.openai.com>. The page title is "Default (GPT-3.5)". A user message asks: "ChatGPT, would you tell me how to model phonon of MAPbI3 with FHI-aims?". The AI response provides a step-by-step guide:

- Geometry optimization:** First, you need to perform a geometry optimization to find the equilibrium structure of MAPbI3. This step ensures that the atomic positions are at the minimum of the total energy.
- Obtain the electronic structure:** Perform a self-consistent electronic structure calculation on the optimized structure to obtain the electronic ground state properties.
- Prepare the input file:** Set up an FHI-aims input file with the following additional specifications to perform a phonon calculation:
 - Set the keyword ``phonon`` to enable the phonon calculation mode.
 - Specify the number of q-points in each direction (``phonon_qpoints``) for which the phonons will be calculated. More q-points will give you more accurate results but will also increase computation time.
 - Ensure to use a proper ``k-grid`` for the Brillouin zone integration during the electronic structure calculation. This grid should be sufficiently dense to obtain accurate electronic structure results.
 - Optionally, you can specify ``lattice_dynamics_method finite_difference`` or ``lattice_dynamics_method displacement`` for the method used in generating the finite differences or atomic displacements, respectively.
- Perform the phonon calculation:** Run the FHI-aims calculation with the input file prepared in the previous step. FHI-aims will calculate the phonon frequencies and eigenvectors for each q-point specified.

At the bottom of the chat window, there is a "Send a message" input field and a "Regenerate" button. A footer note reads: "Free Research Preview. ChatGPT may produce inaccurate information about people, places, or facts. [ChatGPT July 20 Version](#)".

What Can We Do? (This Workshop.)



Vision:

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

→ Algorithmic choices and priorities:

- All-electron
- Non-periodic and periodic systems on equal footing
- Scalability to large systems (thousands of atoms) without precision limitations
- Seamless scalability from laptop to massively parallel and/or new HPC architectures
- Density functional theory and correlated methods (RPA, GW, CC via CC4S...)

Critical choice

- **Numeric atom-centered basis functions (accurate representation of occupied orbitals and densities)**

Stewardship: MSIP e.V. (non-profit organization, purpose: basic science)
Advisory board, very active community

Example - Bi-Doping of Layered HOIS, Hybrid DFT

Predicted
Observable

High-precision atomic structure,
energies and energy differences

Energy band structures for
large, complex systems

Example - Bi-Doping of Layered HOIS, Hybrid DFT

Predicted
Observable

High-precision atomic structure,
energies and energy differences

Energy band structures for
large, complex systems

Level of
Theory

Semilocal density functional theory
with van der Waals corrections

Hybrid density functional theory
including spin-orbit coupling

Example - Bi-Doping of Layered HOIS, Hybrid DFT

Predicted
Observable

High-precision atomic structure,
energies and energy differences

Energy band structures for
large, complex systems

Level of
Theory

Semilocal density functional theory
with van der Waals corrections

Hybrid density functional theory
including spin-orbit coupling



Dr. Yi Yao



Gabrielle
Koknat

Example:

Bi-doped $(\text{PEA})_2\text{PbI}_4$

1,504 atoms

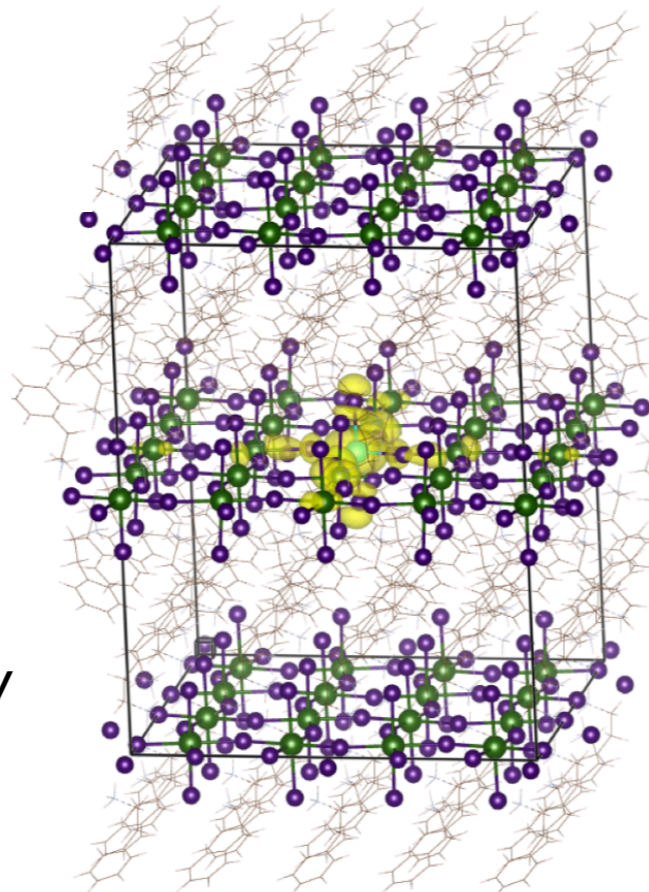
HSE06+SOC,

all-electron

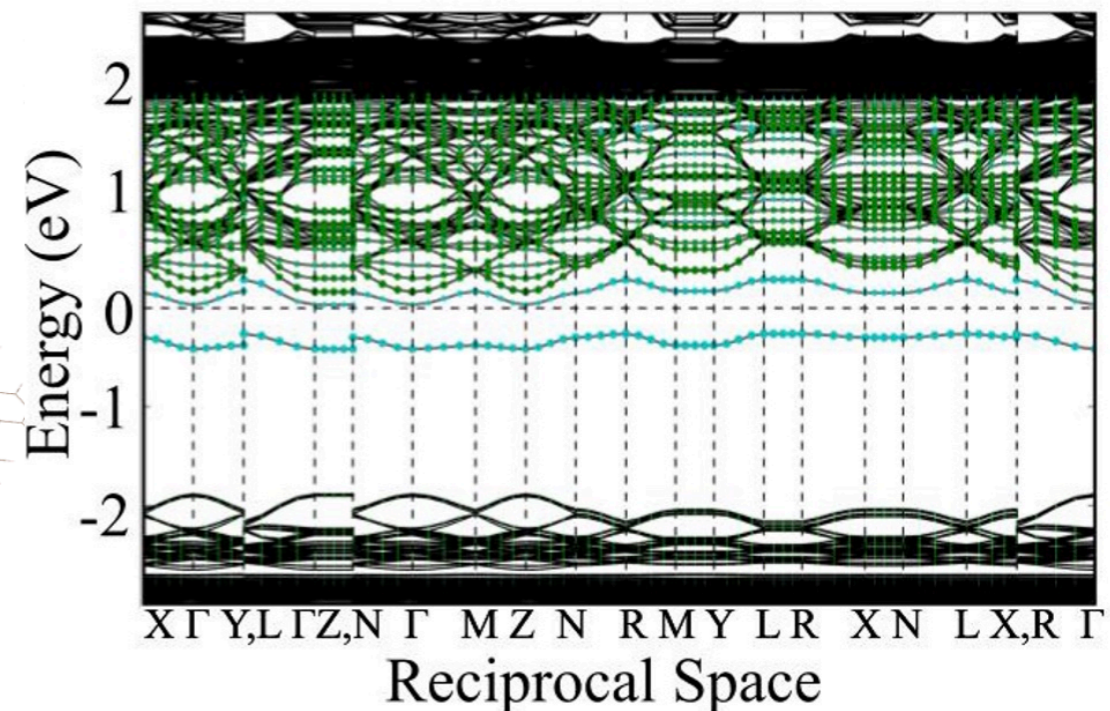
High precision -

no tricks!

Lu et al., PRX Energy
2, 023010 (2023).



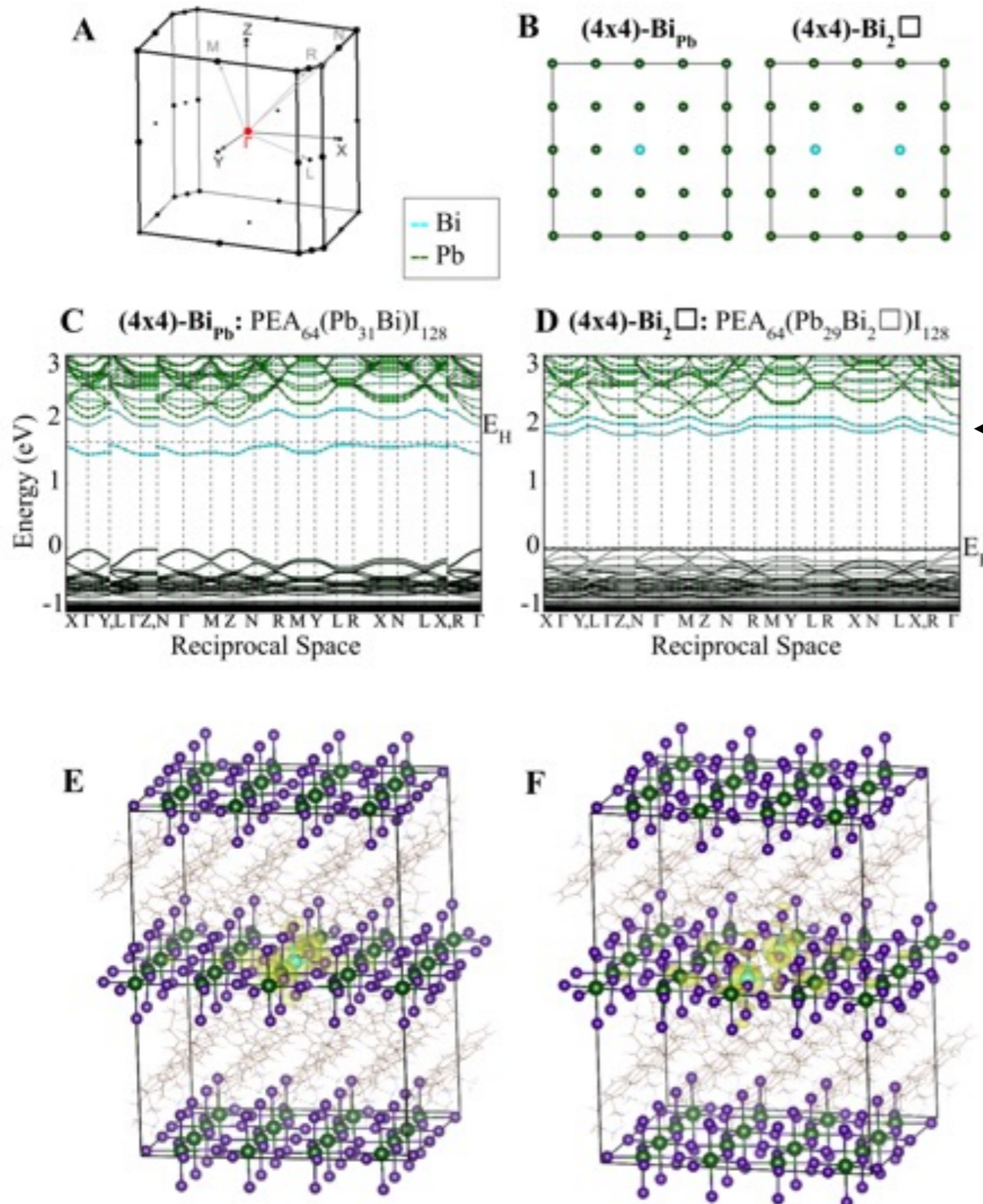
DFT-HSE06+SOC Band Structure



So Are We There Yet?

HSE06+SOC. No tricks.

Lu, Koknat et al., PRX Energy 2, 023010 (2023).



Anonymous reviewer:

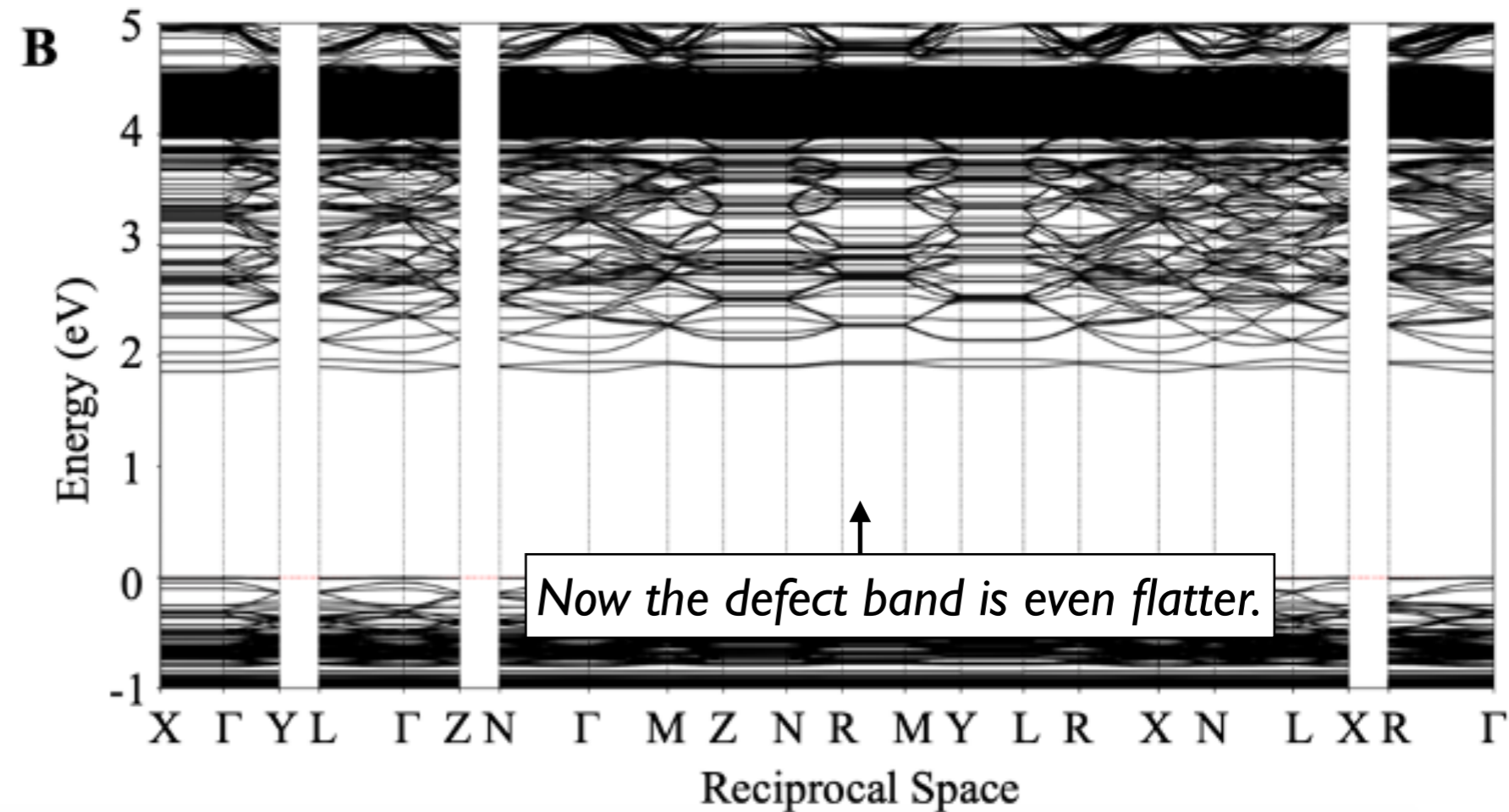
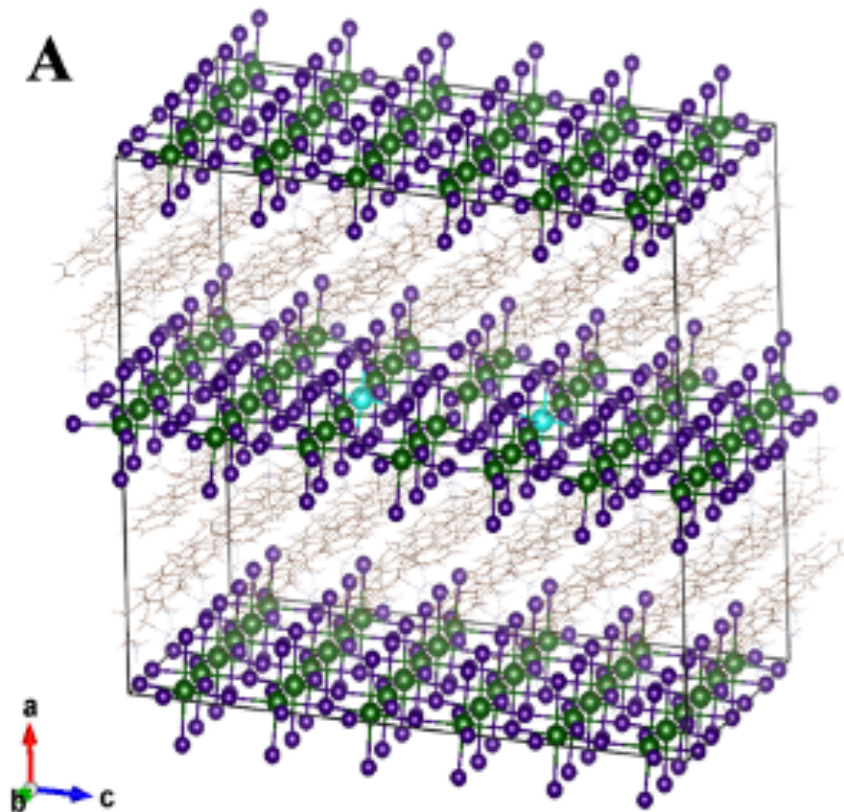
“Finally, I actually worry that in some cases the supercell is not large enough despite its large number of atoms. In particular, for the Bi₂ case shown in Fig. 3B, within the utilized supercell the Bi atoms are actually second-nearest neighbors with each other, likely indicating that the supercell is too small. A hint of this can be seen in Fig. 3D, which shows that the defect orbitals are not flat as expected but show some dispersion.”

I'm not sure what to say.

So How About 3,383 Atoms.

Lu, Koknat et al., PRX Energy 2, 023010 (2023).

HSE06+SOC. Still no tricks.



Electronic structure of the (6x6)-Bi₂O structure.

3,383 atoms, 30,736 electrons, 75,100 basis functions, 24,076 KS orbitals (closed shell system).

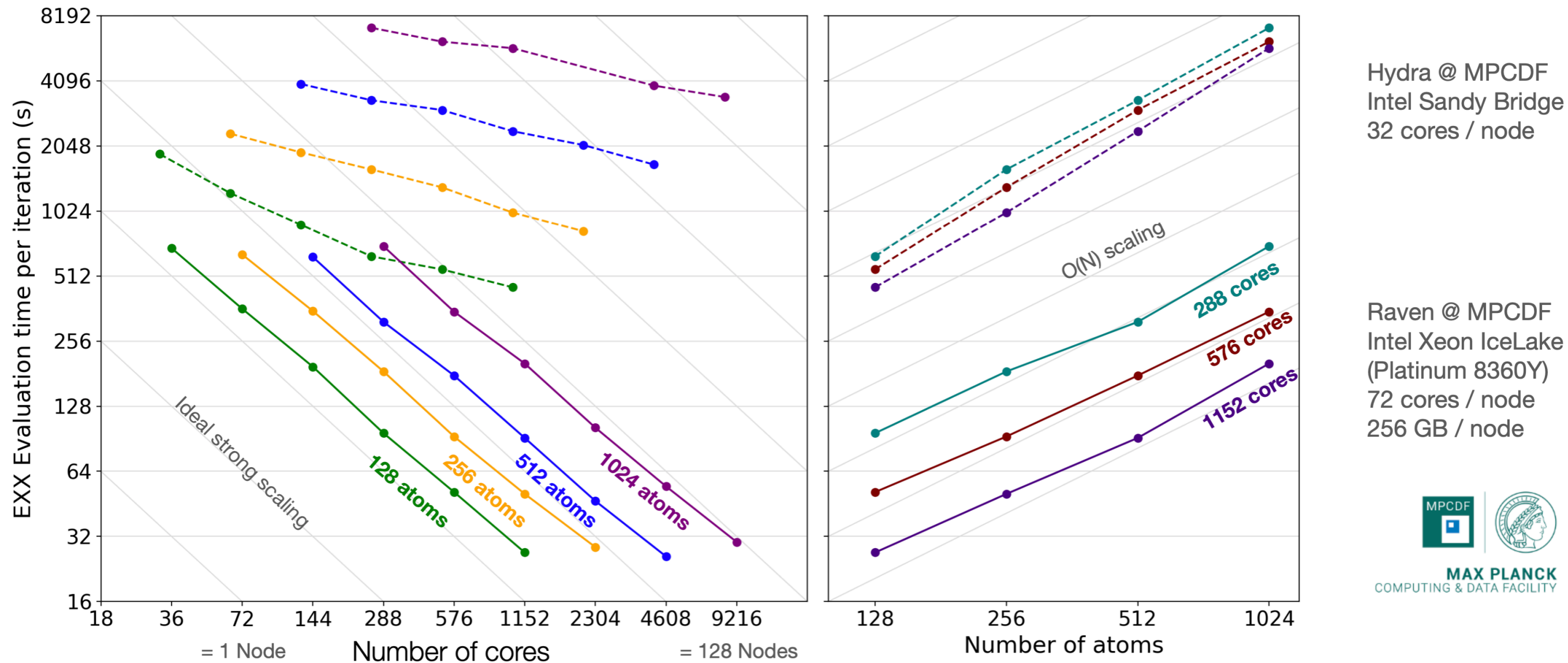
3x3x3 s.c.f. k-space grid, i.e., Born-von Karman cell.

12,096 Intel IceLake cores. SCF: 1 EXX matrix evaluation - 490s, 14 Eigenvalue problems - 225s

Hybrid DFT: Drastic Scalability Improvements*

Florian Merz¹, Andreas Marek², **Sebastian Kokott**³, Christian Carbogno³, Yi Yao^{3,5}, Mariana Rossi⁴, Markus Rampp², Matthias Scheffler³, and Volker Blum⁵

GaAs supercells: HSE06, tight settings



*Not so simple. Our 2015 implementation had already seen some years of work by several very smart and focused individuals.

Summary

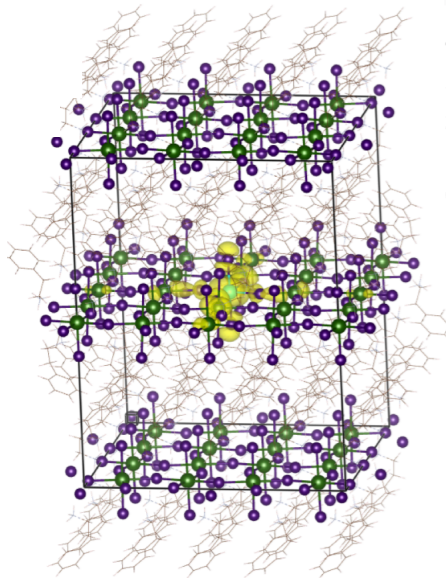


Efficient, scalable first-principles approach to structure, electron band structure, relativity in complex materials.



Great ecosystem of library infrastructure, software tools for electronic structure theory (not just FHI-aims)

We can do some remarkable science.



Tutorials, stability, infrastructure, constant care matter.
Our VERY LARGE community makes all of this possible.
Thank you all for being here!