

PSI Center for Scientific Computing,
Theory and Data

Scientific software, modelling and analysis

PSI overview

(for the Laboratory for Materials Simulations LMS)

Giovanni Pizzi, PSI/CSD
STFC-PSI meeting, 17 March 2026

Introduction



- Laboratory for Materials Simulations (LMS) [*lab head: prof. Nicola Marzari*], from **mission statement**:
 - **develop, integrate, and disseminate**[...] the **computational capabilities required to understand, predict, and characterize materials** as studied at PSI research facilities **with photons, neutrons, muons, and electrons**
 - **provide support and access to these computational capabilities** for the PSI science and user program
 - [...]



www.quantum-espresso.org

WANNIER90

www.wannier.org



www.aiida.net

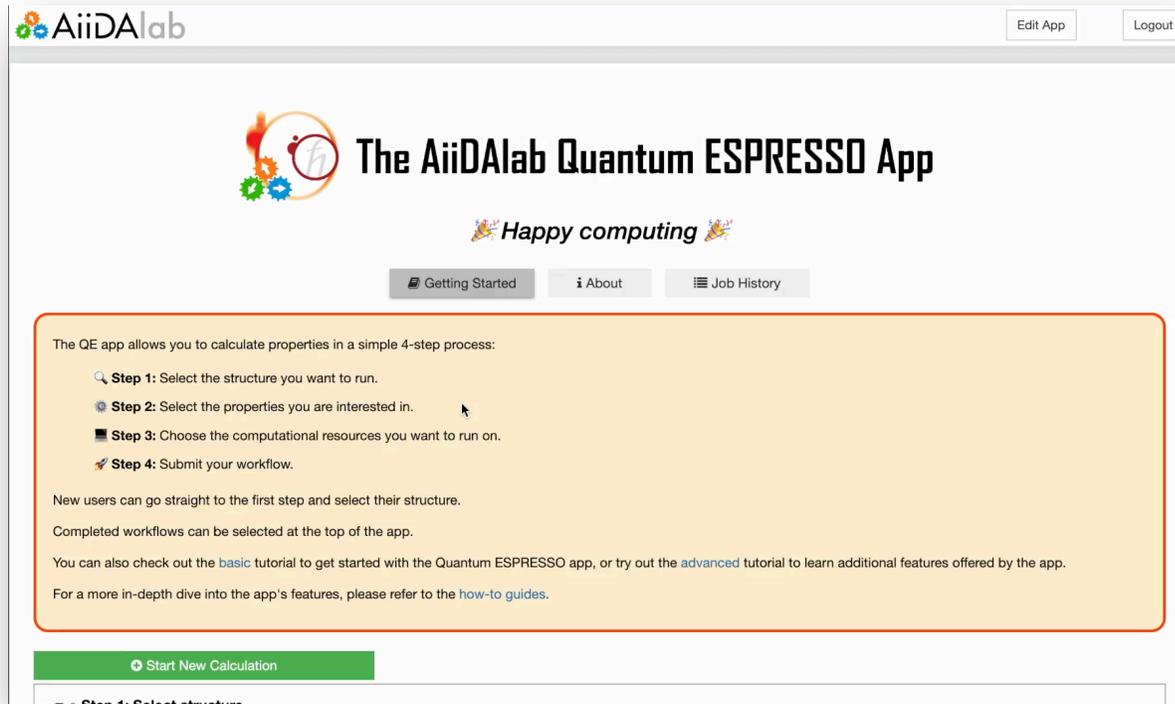


www.aiidalab.net

Making advanced simulation capabilities accessible



AiiDALab Quantum ESPRESSO app



<https://aiidalab-qe.readthedocs.io/>

- Provide immediate, **intuitive access to simulation capabilities**
- Plugin interface, **focus on key properties of interest to PSI**
- Easily redeployable, e.g.:
 - **Instance for PSI staff (inside VPN):** <https://aiidalab.psi.ch>
 - **Instance for PSI experiments (see later):** <https://aiidalab-lns.psi.ch>
 - **Demo server:** <https://demo.aiidalab.io>
- Paper now out: X. Wang et al., npj Comput. Mater. 12, 72 (2026)



Xing
Wang



Jusong
Yu



Edan
Bainglass



Miki
Bonacci

and: A. Ortega-Guerrero, L. Bastonero, M. Bercx, P. Bonfà, R. De Renzi, D. Du, P. N. O. Gillespie, M. A. Hernández-Bertrán, D. Hollas, S. P. Huber, E. Molinari, I. J. Onuorah, N. Paulish, D. Prezzi, J. Qiao, T. Reents, C. J. Sewell, I. Timrov, A. V. Yakutovich, N. Marzari, C. A. Pignedoli

QE app plugin for phonons and inelastic neutron scattering (INS)



- Robust **phonon** workflows (finite differences with *AiiDA+phonopy*) developed by collaborators [1]
- Support phonon **bands and DOS**, **IR/Raman** spectra with intensities, **thermal** properties, ...
- Extended (using *Euphonic* code) to **INS spectra**
- Testing+feedback by **Stas Nikitin** and **Tom Fennell (CNM/LNS)**



Lorenzo Bastonero
(Uni Bremen)



Miki Bonacci
(PSI LMS)

The screenshot displays the AiiDALab Quantum ESPRESSO App interface. At the top, the AiiDALab logo and the app title are visible. Below the title, there are navigation buttons for 'Getting started', 'About', 'Calculation history', 'Setup resources', 'Download examples', and 'New calculation'. The main content area shows a progress bar with four steps: 'Step 1: Select structure', 'Step 2: Configure workflow', 'Step 3: Choose computational resources', and 'Step 4: Status & results'. The 'Step 4' section is expanded, showing a message 'Workflow completed successfully!' and a 'Clean remote data' button. Below this, there are buttons for 'Summary', 'Status', and 'Results'. The 'Structure' tab is selected, showing details for a 'C4 Initial' structure: PK: 2865, Label: C4, Description: Number of atoms: 4, and Creation time: 2024-04-30 13:43:50 (9 months ago). There is also a 'View relaxed' button. On the right side, there are tabs for 'Selection', 'Appearance', 'Cell', and 'Download', with 'Cell' selected, showing 'Length unit: angstrom (Å)' and 'Cell vectors length:'.

*Computing phonons and INS with the AiiDALab QE app:
excellent comparison with experiments for graphite*

[1] L. Bastonero and N. Marzari, [Automated all-functionals infrared and Raman spectra](#), npj Comput. Mater. 10, 55 (2024)

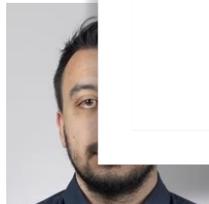
QE app plugin for phonons and inelastic neutron scattering (INS)



- Robust **phonon** workflows (finite differences with *AiiDA*+ developed by collabora
- Support phonon **bands** **IR/Raman** spectra with **thermal** properties, ...
- Extended (using *Eupho*) **INS spectra**
- Testing+feedback by **St** and **Tom Fennell (CNN**

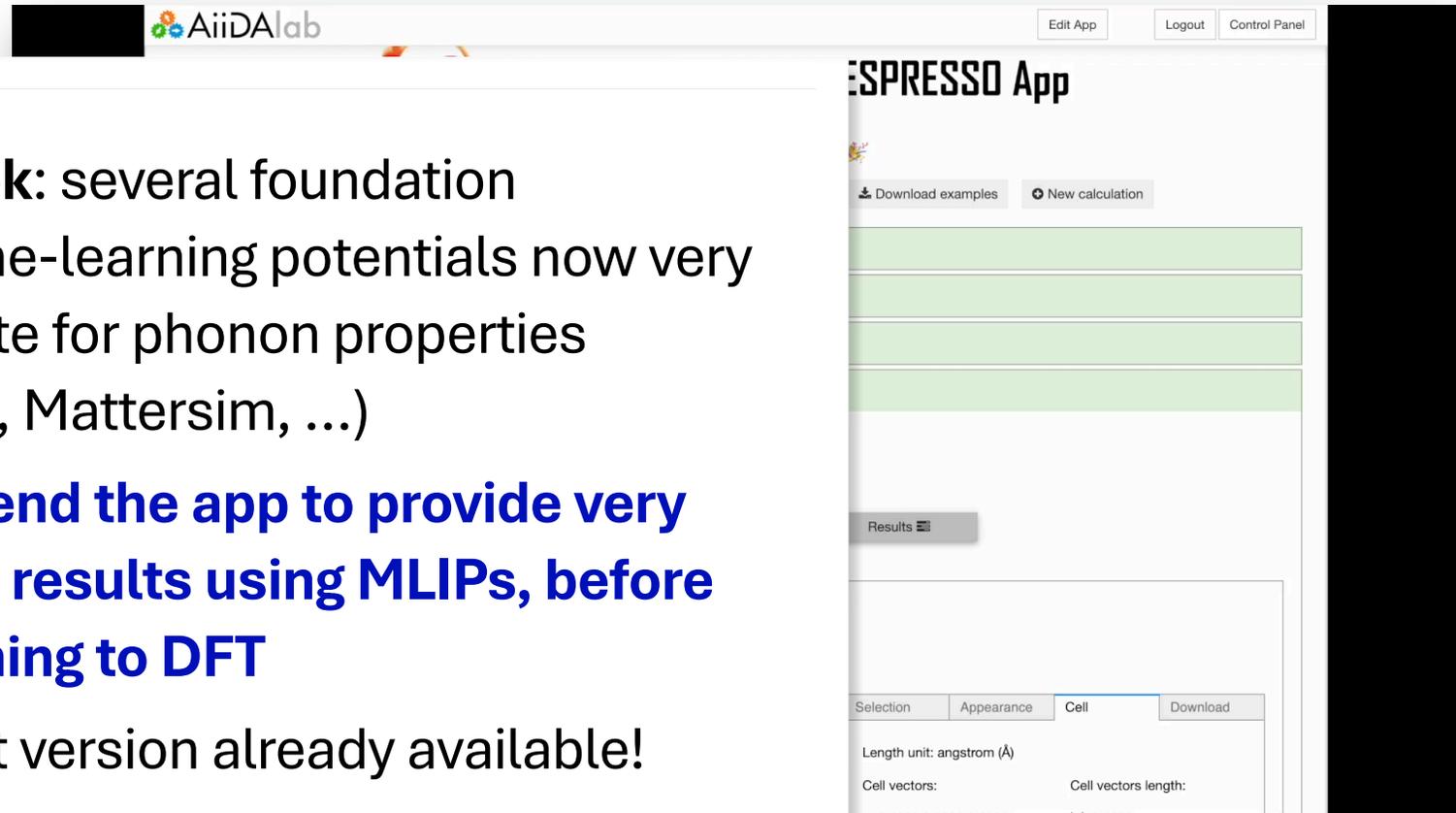


Lorenzo Bastonero
(Uni Bremen)



Miki Bonacci
(PSI LMS)

- **Outlook:** several foundation machine-learning potentials now very accurate for phonon properties (MACE, Mattersim, ...)
 - **Extend the app to provide very fast results using MLIPs, before turning to DFT**
 - First version already available!



Computing phonons and INS with the AiiDALab QE app: excellent comparison with experiments for graphite

[1] L. Bastonero and N. Marzari, [Automated all-functionals infrared and Raman spectra](#), npj Comput. Mater. 10, 55 (2024)

QE app plugin for muon spectroscopy with DFT+ μ



- Muon spectroscopy: extensively used to characterize magnetic and superconducting states in materials
- We developed **AiiDA workflows to identify muon stopping sites [1] using DFT+ μ [2]**



Ifeanyi J. Onuorah
(Uni Parma)



Miki Bonacci
(PSI LMS)



Pietro Bonfà
(Uni Modena)



Roberto De Renzi
(Uni Parma)

- We also developed a plugin for a **GUI in AiiDALab QE [3]**

The screenshot shows the AiiDALab interface. At the top, it says 'AiiDALab' with 'Edit App', 'Logout', and 'Control Panel' buttons. Below that, a green bar indicates 'Step 3: Choose computational resources' and another green bar indicates 'Step 4: Status & results'. A message states 'Workflow completed successfully!' with a 'Clean remote data' button. There are buttons for 'Summary', 'Status', and 'Results'. The 'Structure' tab is active, showing 'F₄Li₄ Initial' with details: PK: 1117, Label: F4Li4, Description: Number of atoms: 8, Creation time: 2025-02-07 16:06:16 (8 days ago). A 3D visualization of the structure is shown. On the right, a table provides cell vectors and symmetry information.

Selection	Appearance	Cell	Download
Length unit: angstrom (Å)			
Cell vectors:		Cell vectors length:	
a:	4.0834 0.0000 0.0000	a :	4.0834
b:	0.0000 4.0834 0.0000	b :	4.0834
c:	0.0000 0.0000 4.0834	c :	4.0834
Angles:		Symmetry information:	
α:	90.0000	Spacegroup:	Fm-3m (No.225)
β:	90.0000	Hall:	-F 4 2 3 (No.523)
γ:	90.0000	Periodicity:	xyz

[1] I. J. Onourah, GP, et al., Digital Discovery, 4, 523 (2025)

[2] J. S. Moller et al., Phys. Rev. B 87, 121108 (2013); F. Bernardini et al., Phys. Rev. B 87, 115148 (2013)

[3] <https://aiidalab-qe.readthedocs.io/tutorials/muons.html>

QE app plugin for muon spectroscopy with DFT+ μ

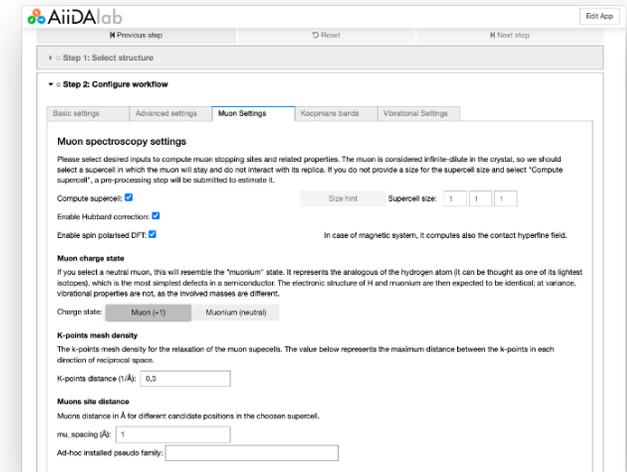


• Available workflow features:

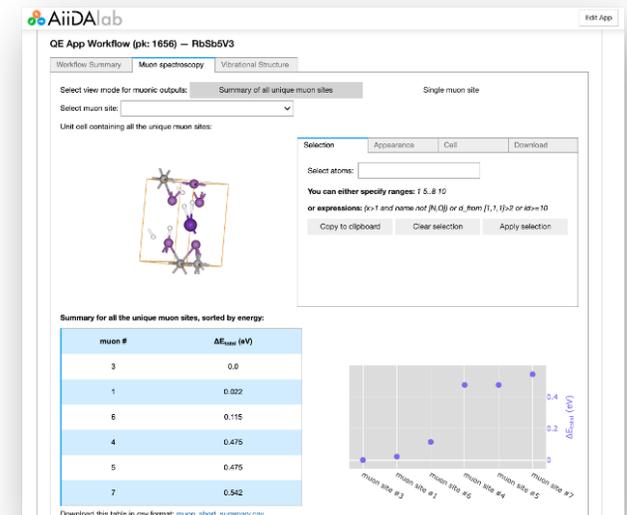
- **muon stopping sites** (with DFT+U, collinear&non-collinear magnetism, SOC, ...)
- **contact hyperfine field B** (difference of spin charge densities at muon site)
- **classical dipolar contribution** (via MuESR using input magnetic moments)
- **Kubo-Toyabe approximation for μ polarization** (for randomly oriented static/fluctuating local fields)
- **time evolution of μ polarization with explicit muon-nuclear dipolar interaction** for given external B value and sample orientation (via UNDI, when no electronic contribution present)

• Work-in-progress features:

- **quadrupolar-interaction** for electric field gradient estimation (to be used in UNDI for the contribution to contact field B , using GIPAW)
- **Efficient reciprocal-space Ewald sums** instead of real space ones (new optimized pylocfield code replacing MuESR (still private, developed by P. Bonfà, University of Modena))



Settings panel



Results panel

[1] I. J. Onourah, GP, et al., Digital Discovery, 4, 523 (2025)

[2] J. S. Moller et al., Phys. Rev. B 87, 121108 (2013); F. Bernardini et al., Phys. Rev. B 87, 115148 (2013)

[3] <https://aiidalab-qe.readthedocs.io/tutorials/muons.html>

QE app

- Available

- muon SOC,
- contact
- class
- Kubo static
- time intera
- (via U

- Work-in-

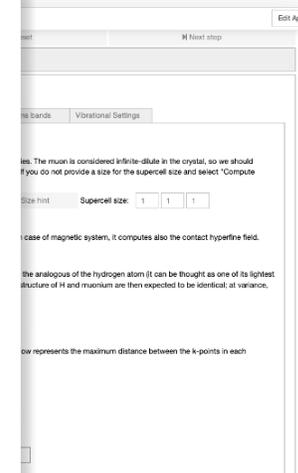
- quad UNDI
- Effici optim
- Bonfà

- Outlook:

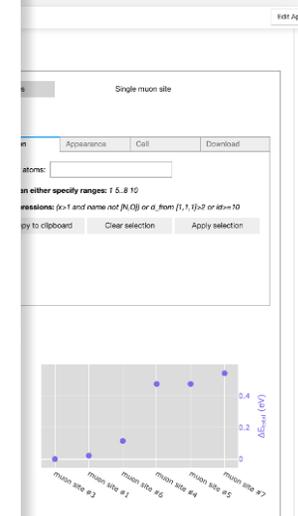
- **MLIPs** for accelerated predictions
- **Generative AI** (*in-painting techniques* on top of MatterGen's score-based diffusion AI model) to identify muon positions (see method in [1])
- **Speed-ups within DFT**: pre-relaxations at Γ , new error handlers, live calculation monitors, ...
- New **NCCR Muoniverse funded!** <https://www.muoniverse.ch> (4 years, potentially extending up to 12)
 - In PSI LMS: 4-year PhD student to implement NEB for assessing barriers and quantum treatment of muons (SSCHA, path integrals, ...)

[3] T. Reents et al., arXiv:2601.01959 (2026)

[1] I. J. Onourah, G
[2] J. S. Moller et al.
[3] <https://aiidalab-qe.readthedocs.io/tutorials/muons.html>

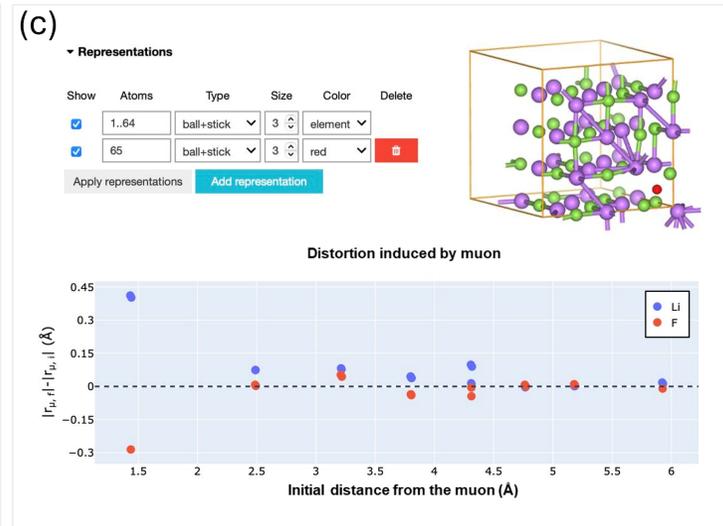
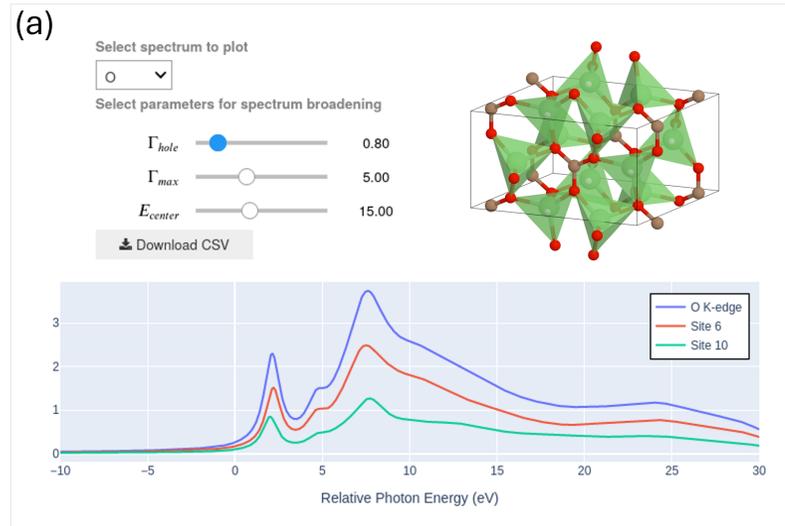


s panel

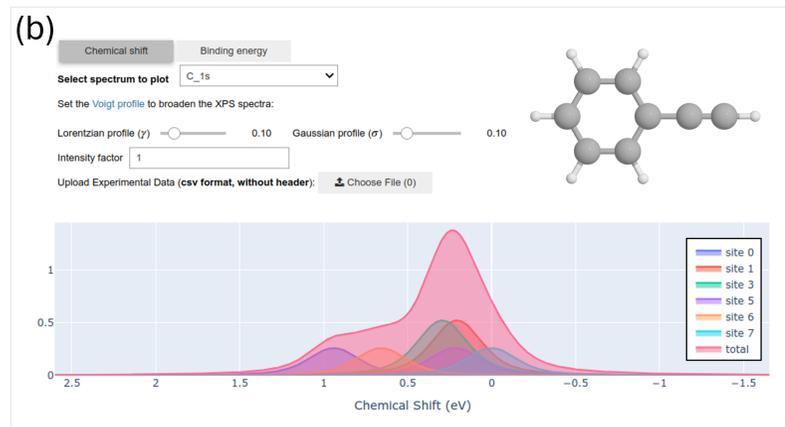


s panel

Many more robust workflows developed (and GUIs to drive them)

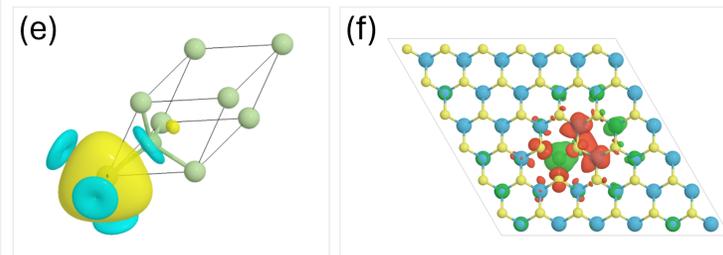


see X. Wang et al., *npj Comput. Mater.* 12, 72 (2026)



(d)

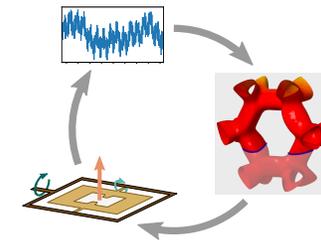
Hubbard	Kind-Manifold (I)	Kind-Neighbour(J)	Index (I)	Index (J)	Value (eV)	Translation	Distance (Å)
V	Co-3d	Co-3d	1	1	6.23	0,0,0	0
V	Co-3d	O-2p	1	11	0.39	-1,-1,0	1.92
V	Co-3d	O-2p	1	22	0.39	-1,0,0	1.92



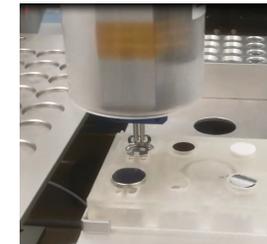
Additional workflows with GUIs (and more in the future thanks to plugin interface) for: electronic band structure with (P)DOS and fat bands, charge density, Bader charge analysis, infrared and Raman spectroscopy, XPS, XAS, fully self-consistent DFT+U+V, Wannier functions, Fermi surfaces, dHvA oscillations, ...

Agentic AI and autonomous labs

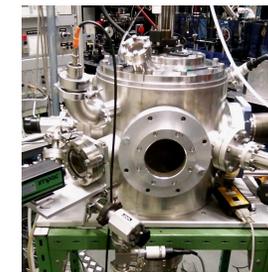
- Active investigation of using **AiiDA as part of Agentic AI workflows**
 - AI tool
 - Active learning workflows
 - ...
- Working toward **autonomous workflows in collaboration with experiments**
 - Ongoing or completed projects on **battery assembly and testing**, and on **Fermi surface** characterization
 - **Active PSI project** (4 years, 1 PhD student: Pietro Mani, shared by Nikita Shepelin PSI/CNM and Giovanni Pizzi PSI/LMS) on **autonomous optimization of pulsed-laser deposition (PLD) growth**
 - Supporting PSI goal to provide a facility also for sample growth and characterization



*Accurate Fermi-surface mapping
(Shubnikov-de Haas)*



*Battery assembly
and testing*



*Pulsed laser deposition
(autonomous crystal growth)*



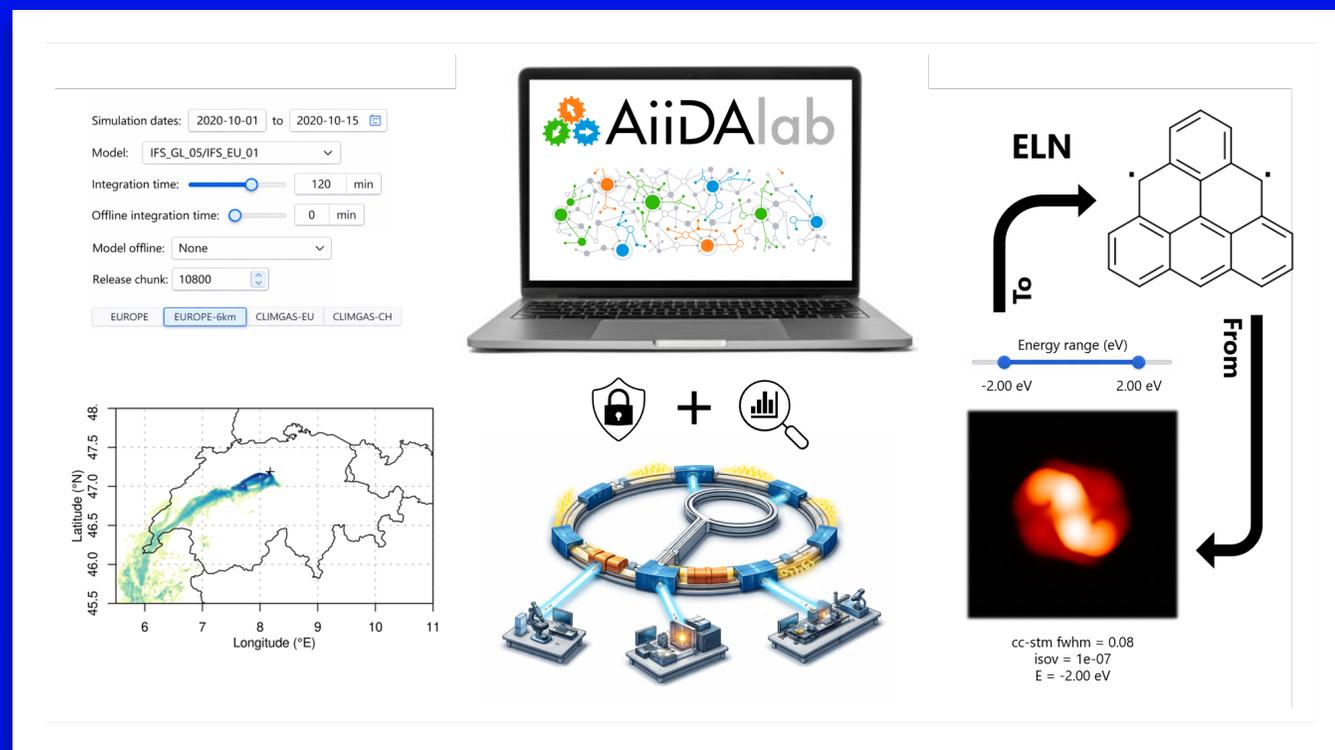
Nikita
Shepelin



Pietro
Mani

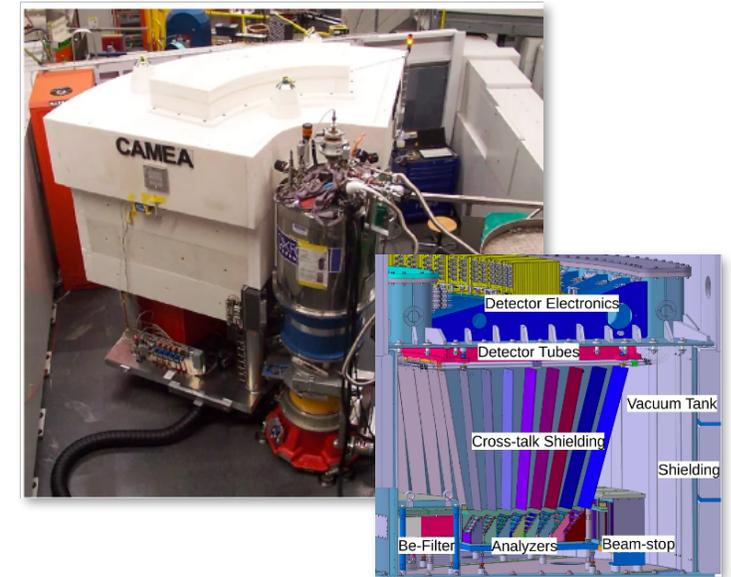
Beyond DFT and AiiDA: AiiDAlab as a data-analysis platform

A. Yakutovich et al., arXiv:2512.22173 (2025)



AiiDALab beyond DFT and AiiDA: the LNS apps

- In collaboration with M. Kenzelmann's lab (CNM/LNS):
AiiDALab as a data analysis platform, beyond DFT
- **First use case: CAMEA** (Daniel Mazzone, Jakob Lass)
 - **ISSUE 1:** LNS developed MJOLNIR, python tool for raw data analysis.
 - **BUT:** users visiting PSI spent a lot of time just to install and learn it: *dependency installation, different OS, different language and keyboard layout, ...*
 - **ISSUE 2:** Data goes on the instrument computer; retrieved by users with USB sticks (unsafe!), and all data visible to all users



CAMEA spectrometer

<https://www.psi.ch/en/sinq/comea>

(q, E) mapping of neutron excitations



Daniel
Mazzone

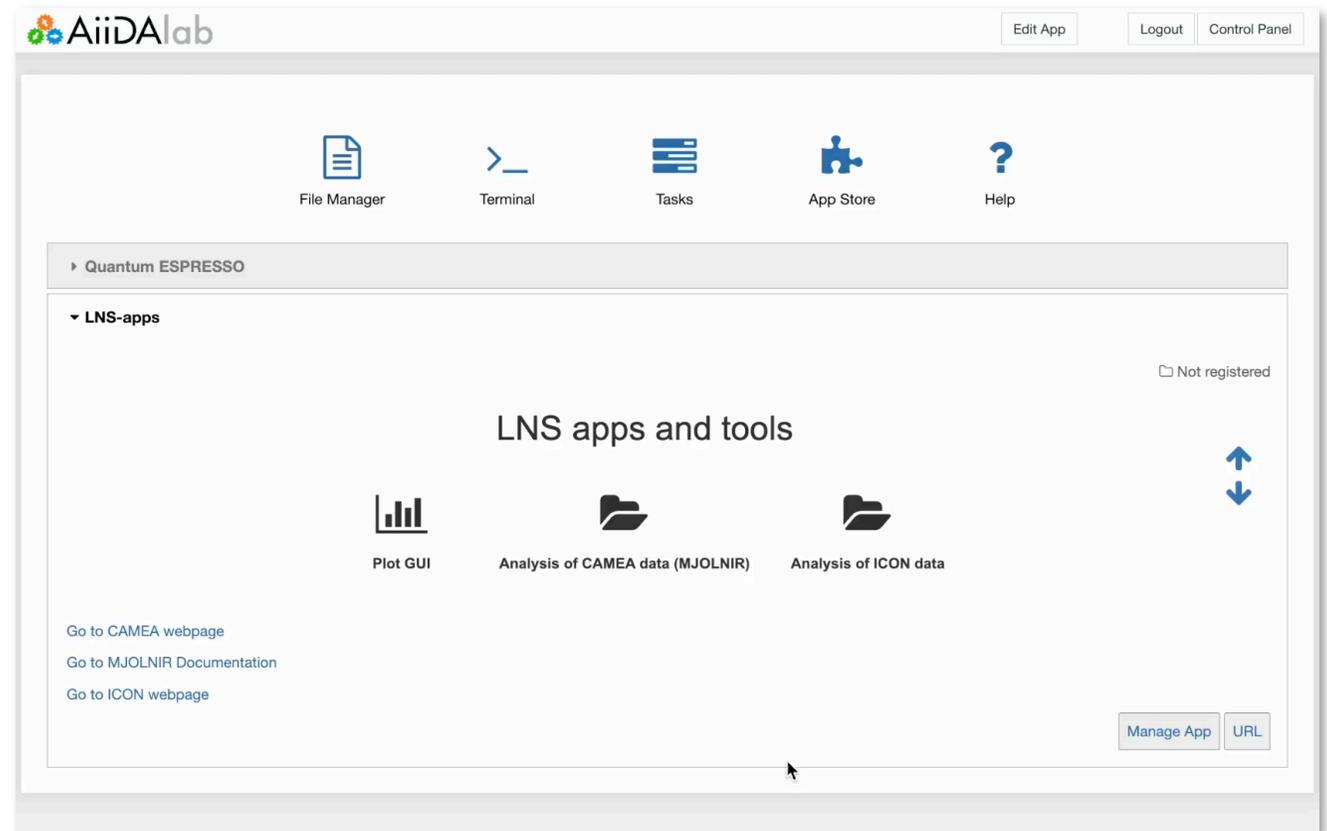


Jakob
Lass

Our proposed solution: The AiiDALab LNS app



- **Environment pre-configured** with MJOLNIR and all dependencies, ...
 - Tested with real user in July:
1 min startup vs. 1+ hours local installation
- **Direct secure access** to experimental data from CAMEA in the app, and **ONLY for the proposals one has access to**
- **Notebooks autogenerated from template**
 - Working in app-mode for quick analysis; working as notebook for more detailed analysis

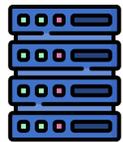


<https://github.com/mikibonacci/LNS-app>

Secure data connection



HPC (Merlin, Ra, CSCS, ...) (Optional)



SSH via AiiDA

Login with PSI credentials (authentication via Azure AD)



Web browser

AiiDA lab frontend

/camea/20201923/



User 1

Live data storage



NFS mount

New aiidalab-lns.psi.ch deployed in the DMZ network



HTTPS

HTTPS

Web browser

AiiDA lab frontend

/camea/20242013/



User 2

NFS mount

HTTPS

PSI NFS mount for CAMEA data

Correct folders mounted in the K8S container of each user, using authorization information from the PSI DUO database

Web browser

AiiDA lab frontend

/camea/20246188/

/camea/20242013/



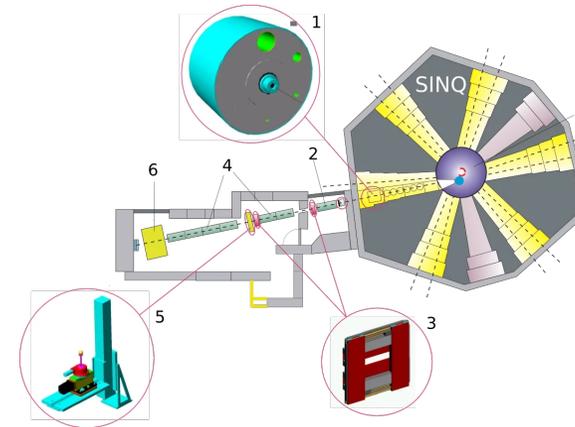
User 3

...

AiiDALab beyond DFT and AiiDA: the LNS apps

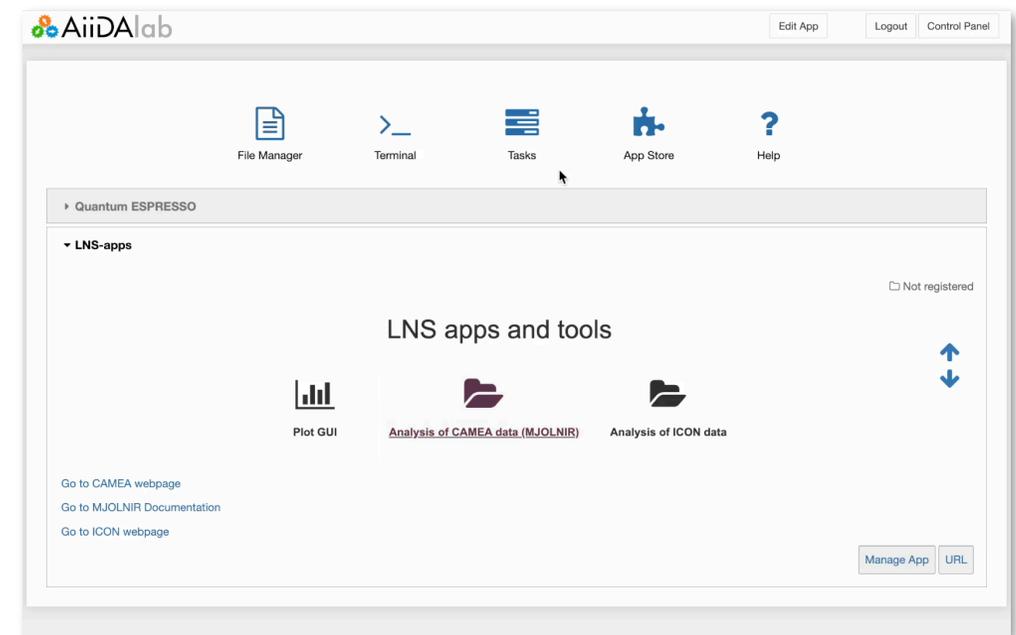


- **Second use case: ICON**
(collaboration with Anders Kaestner)
 - Proof-of-concept app implemented to demonstrate functionality
- **Joint 2-year position** (project scientist, Edan Bainglass) **funded at PSI** (CSD+CNM centers) to onboard all SINQ instruments
 - Support of VM-like interface (VNC via browser) still on JupyterHub
 - Focus on HPC integration, data flow standardization, large datasets, ...



ICON: Imaging with cold neutrons at SINQ

<https://www.psi.ch/en/sinq/icon>



<https://github.com/mikibonacci/LNS-app>

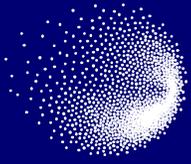
Vision for a computational facility



- **Mid-term plan:** Offer access to simulation capabilities when applying for a proposal at PSI
- Goals:
 - Extend experimental facilities with a **cutting-edge computational facility**
 - **Provide same (AiiDA) interface to users**, both those interested in materials simulations, or only in data analysis and pre-/post-processing

The screenshot displays the PSI Digital User Office (DUO) portal. The top navigation bar includes links for 'User Office', 'Guesthouse', 'Research Facilities', and 'Experiment Schedule' for various facilities like SLS, SINQ, SpS, SwissFEL, and HIPA. A 'User Menu' on the left lists options such as 'New Proposal', 'Edit Proposals' (with a '1 recently...' indicator), 'SLS Continuation Proposals', 'View all Proposals (PDF)', and 'Resubmit Proposals'. The main content area is titled 'Submission of proposal 20250844, Step #1: General Information' and features a progress bar with six steps: 1. General Information (active), 2. Sample Declaration, 3. Instrumental part, 4. Additional instruments, 5. Related Proposals, and 6. Submit Proposal. The form includes a 'Title (*)' field, a section for 'Proposers with DUO account' (listing 'Main Proposer: Dr. Giovanni Pizzi (Paul Scherrer Institute PSI)' with an 'Append Co-Proposer to this proposal' button), a section for 'Co-Proposers without DUO account' with instructions and a text area, and a section for 'Planned experimental team (*)' with a dropdown for team size and a checkbox for travel to PSI.

PSI's Digital User Office (DUO) portal



PSI Center for Scientific Computing,
Theory and Data

Electronic structure simulations for large-scale facilities

Nicola Colonna
STFC-PSI Meeting – on-line, 17 March 2026

Density functional theory

- **Density-functional theory** (DFT): functional theory for the ground state

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) \longleftrightarrow \rho(\mathbf{r})$$

- From the ground-state energy:
 - Cohesive energy
 - Equilibrium geometry
 - Elastic properties
 - Thermomechanical properties
 - Static susceptibilities
 - Nuclear vibrations
 - Vibrational spectroscopies
 - ...
- **BUT**
 - **Current approximations not always enough**
 - **Excitations outside of the realm of the theory**

The most-cited research papers of all time



Nature **640**, 591 (2025)
3 papers about DFT in the top 10

Advanced electronic structure: ground state

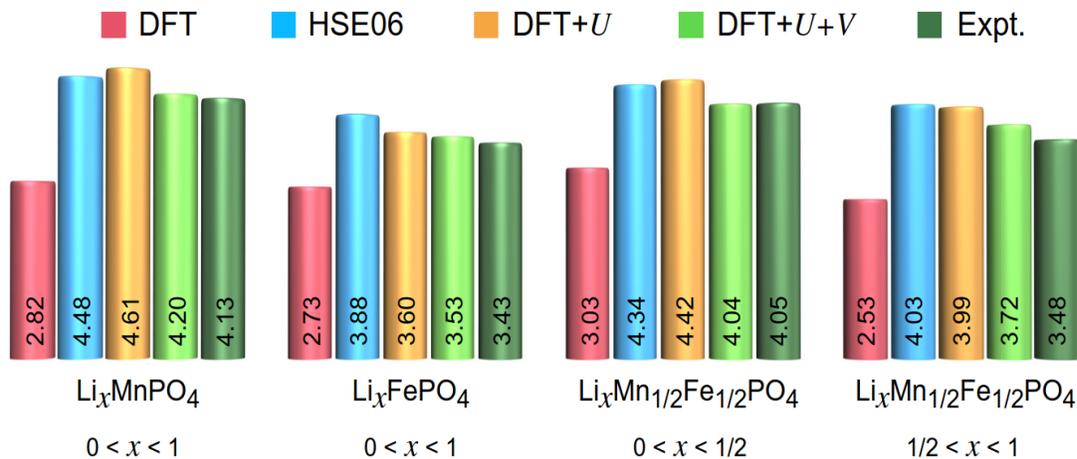
- Extended **Hubbard functionals** (DFT+U, DFT+U+V) for **complex materials** (d/f electrons)

$$E^{\text{DFT+U+V}} = E^{\text{DFT}} + \sum_I \frac{U_I}{2} \text{Tr} [\mathbf{n}^I (1 - \mathbf{n}^I)] - \sum_{I,J} \frac{V_{IJ}}{2} \text{Tr} [\mathbf{n}^{IJ} \mathbf{n}^{JI}]$$



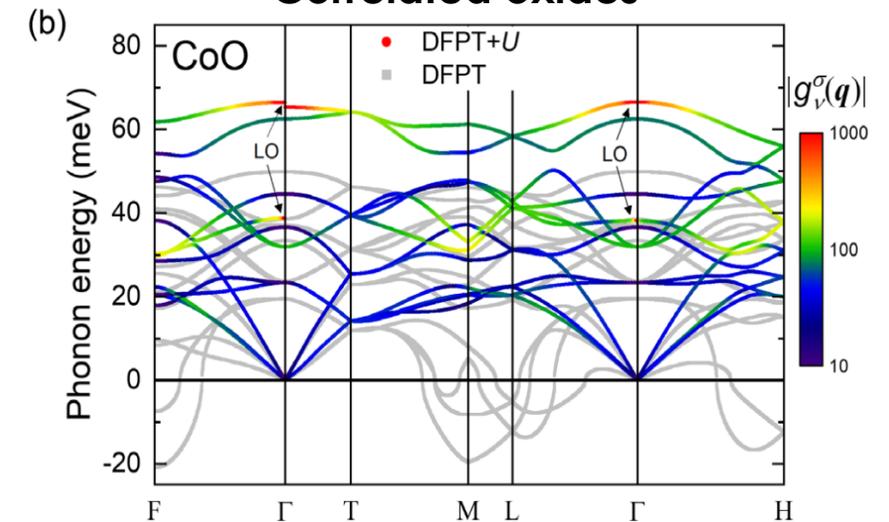
Iurii Timrov
PSI LMS

Li-ion batteries



I. Timrov *et al.* PRX ENERGY **1**, 033003 (2022)

Correlated oxides



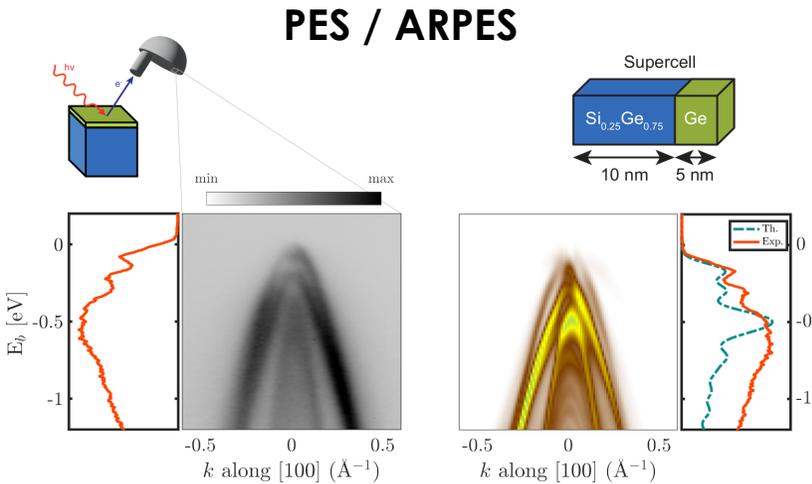
J. Zhou *et al.*, Phys. Rev. Lett. **127**, 12640 (2021)

DFT+U+V calculations with QE and **automated Hubbard U(&V)**
workflow already **available in the AiiDA lab QE app**

Advanced electronic structure: excited states

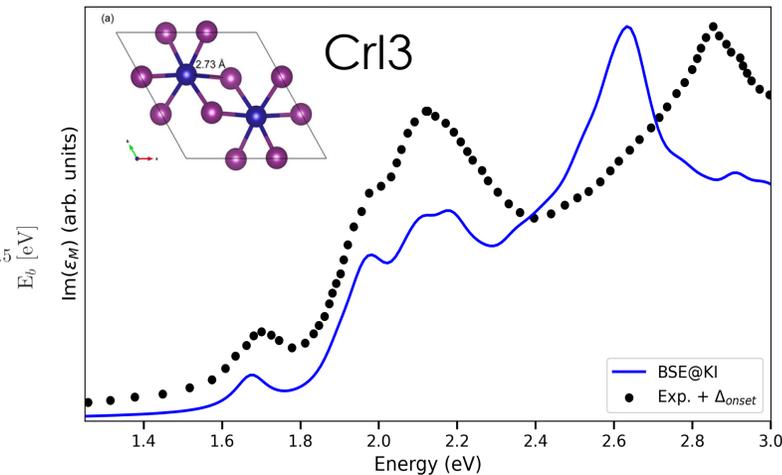
- **Koopmans-compliant spectral functionals** for **complex** (beyond DFT) **properties**

$$E^{\text{K}^{\text{C}}}[\rho, \{\rho_i\}] = E^{\text{DFT}}[\rho] + \sum_i \alpha_i \Pi_i^{\text{K}^{\text{C}}}[\rho_i]$$



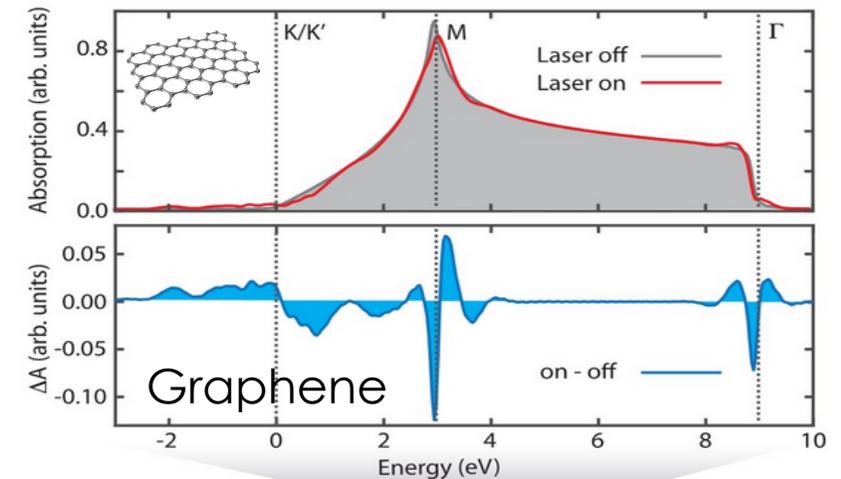
E. della Valle et al. submitted (2026)

Optical/Xray ABS, EELS, IXS, ...



M. Bonacci et al. in preparation (2026)

Time-resolved and ultrafast



G. Cistaro et al. in preparation (2026)



Michael Schuler
PSI LMS



Miki Bonacci
PSI LMS



Giovanni Cistaro
CNR Milano

Open source



<https://www.quantum-espresso.org/>



<https://wannier.org/>

EDUS

https://github.com/gcistaro/EDUS_2.0

koopmans-functionals.org

A screenshot of the website for 'koopmans-functionals.org'. The page has a blue header with the 'k' logo and a search bar. A dark sidebar on the left contains a navigation menu with items like 'About', 'Quick start', 'Theory', 'Installation', etc. The main content area features the title 'koopmans' and a subtitle 'a package for performing and automating Koopmans functional calculations'. Below this is a 'Contents' section with a list of links: 'About', 'Quick start', 'Theory' (with sub-links for 'Quasiparticle energies, piecewise linearity, and Koopmans' theorem', 'Koopmans functionals', 'The key ingredients in a Koopmans calculation', 'The Koopmans workflows', 'Limitations', and 'Related methods'), 'Installation' (with sub-links for 'Downloading' and 'Installing'), and 'The input file'. At the bottom of the sidebar, there is a 'Read the Docs' button and a version selector set to 'v: latest'.

E. Linscott, **NC**, et al. JCTC **19**, 7097 (2023)

Outlook: AiIDA integration

koopmans

- Simple by design
 - Local execution
 - Only serial step execution

AiIDA

- Powerful by design
 - Remote execution
 - parallel step execution

koopmans

UI practically unchanged:

```
$ koopmans tio2.json → $ koopmans --engine=aiida tio2.json
```

but executed remotely and in parallel:



Edward Linscott



Miki Bonacci

Outlook: Black-box accurate band-structures

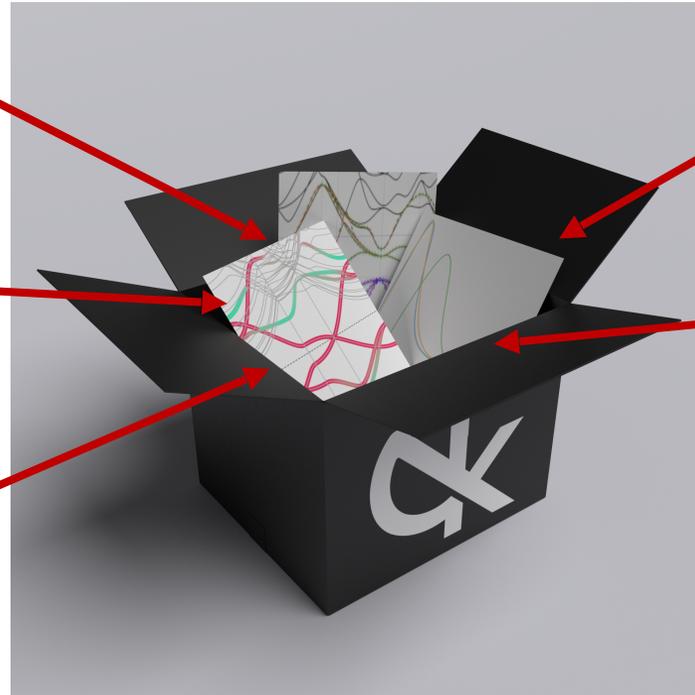
automated Wannierisation

a new AiiDA engine

Non-collinear
extension

screening parameters from
machine-learning

symmetries for faster
calculations of screening
parameters



Edward Linscott



<https://koopmans-functionals.org/>

E. Linscott, **NC**, *et al.* JCTC **19**, 7097 (2023)

Conclusions

- **AiiDAlab** as a platform to make advanced simulations methods accessible
- **Quantum ESPRESSO app** providing several plugins, including for neutron and muon experiments
- AiiDAlab platform being extended to support **secure data access and data processing for LSF experiments**
- **Koopmans functionals**: streamline excited-state properties calculations (ARPES, ABS, ultrafast)