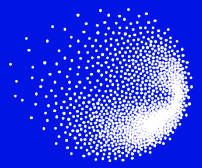


PSI Center for Scientific Computing, Theory and Data

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

PSI

- 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
  - […]

QUANTUMESPRESSO®

www.quantum-espresso.org

WANNIER90

www.wannier.org

AiiDA

www.aiida.net

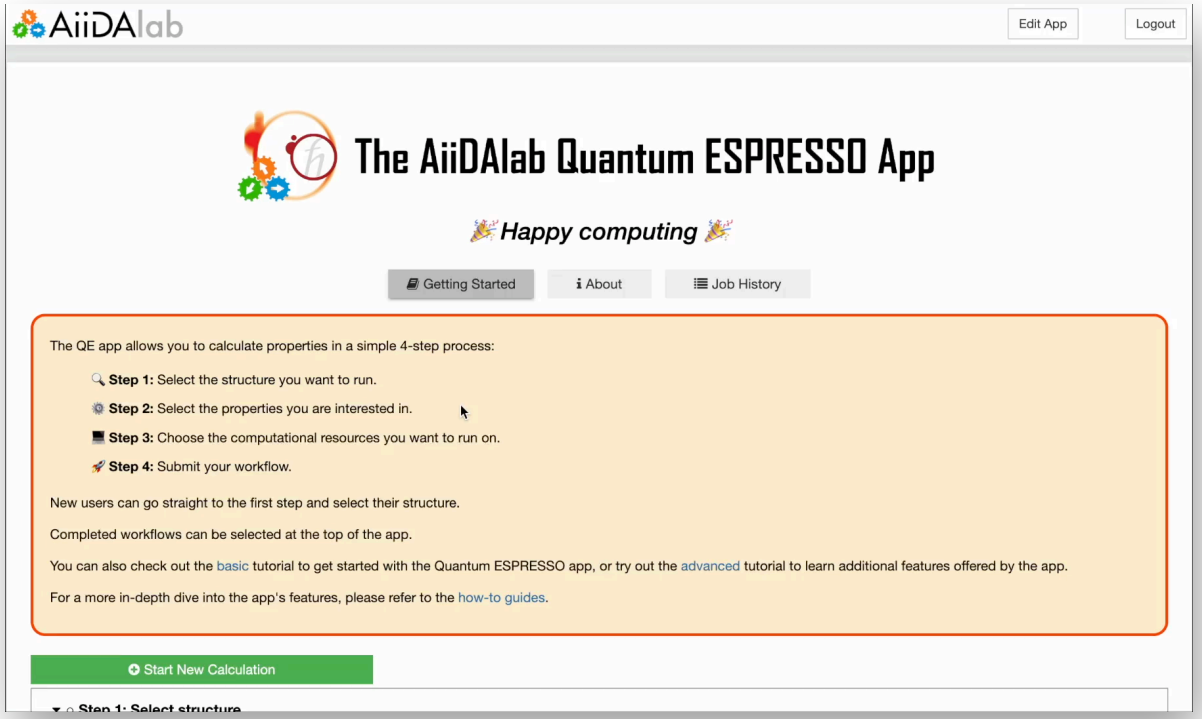
AiiDAlab

www.aiidalab.net

Making advanced simulation capabilities accessible

PSI

AiiDAlab Quantum ESPRESSO app

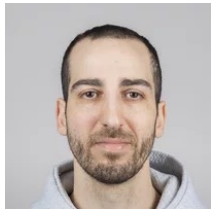


https://aiidalab-qe.readthedocs.io/

- 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

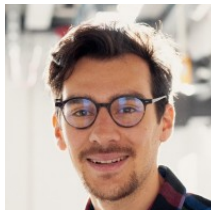

Miki Bonacci

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)

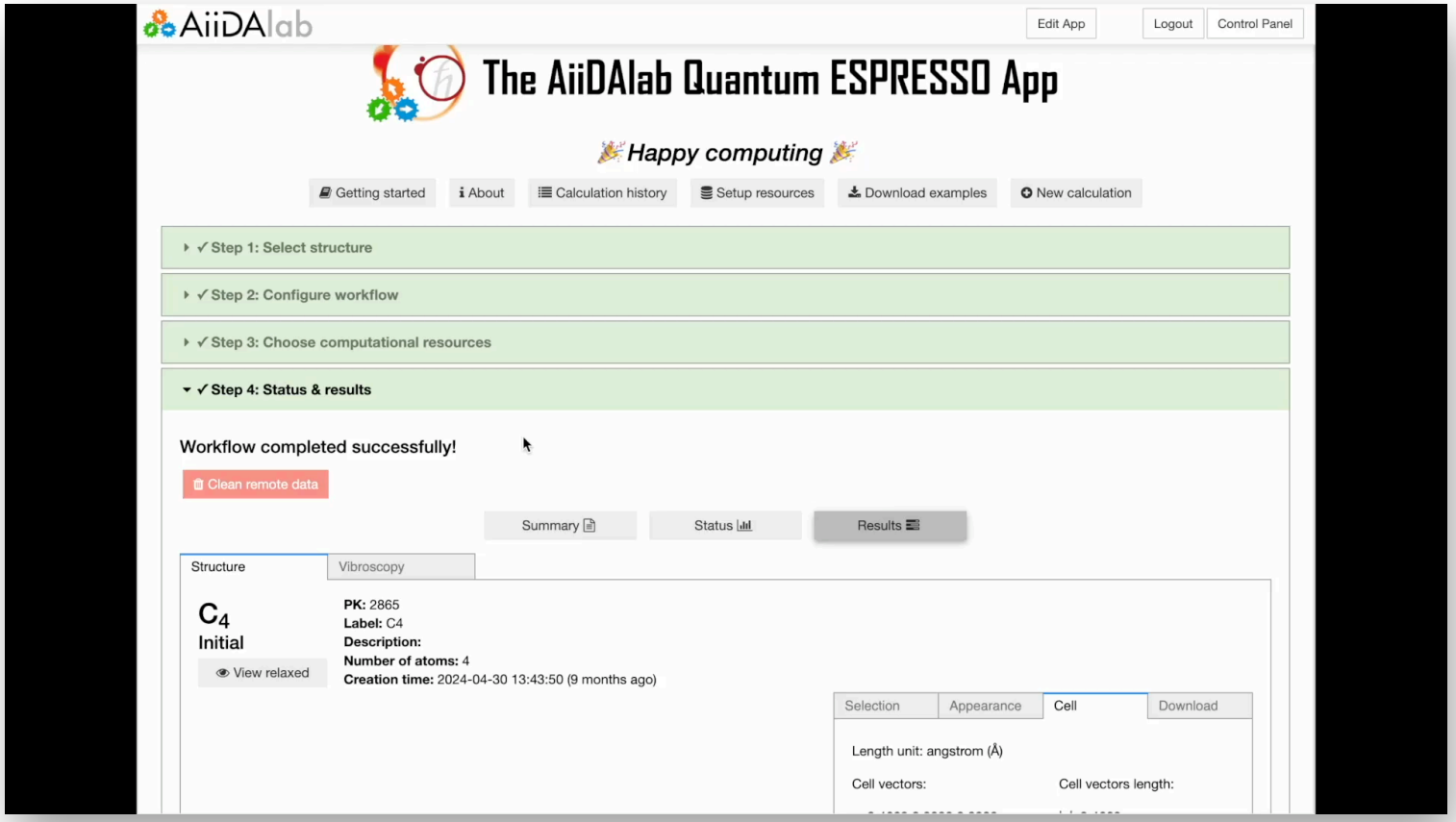
PSI

- 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)



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)

https://aiidalab-qe.readthedocs.io/
https://github.com/aiidalab/aiidalab-qe-vibroscopy

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

PSI

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- Support phonon **bands** **IR/Raman** spectra with **thermal** properties, …
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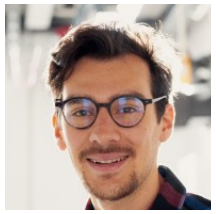
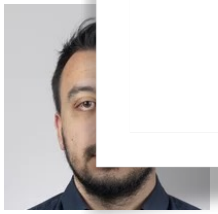
- Testing+feedback by **St** **and Tom Fennell (CNN**

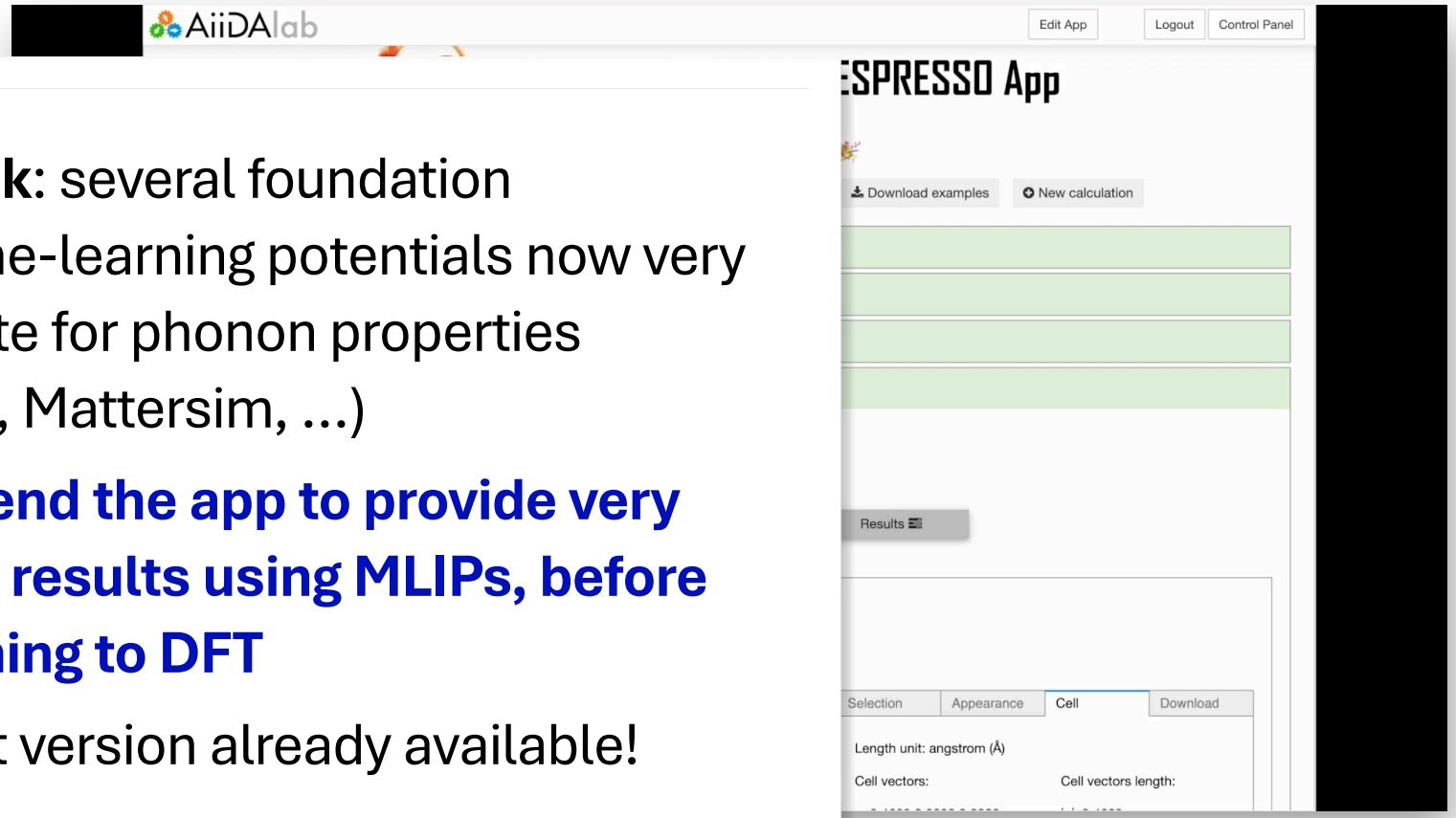


Lorenzo Bastonero
(Uni Bremen)



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!



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https://aiidalab-qe.readthedocs.io/
https://github.com/aiidalab/aiidalab-qe-vibroscopy

QE app plugin for muon spectroscopy with DFT+μ

PSI

- 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]

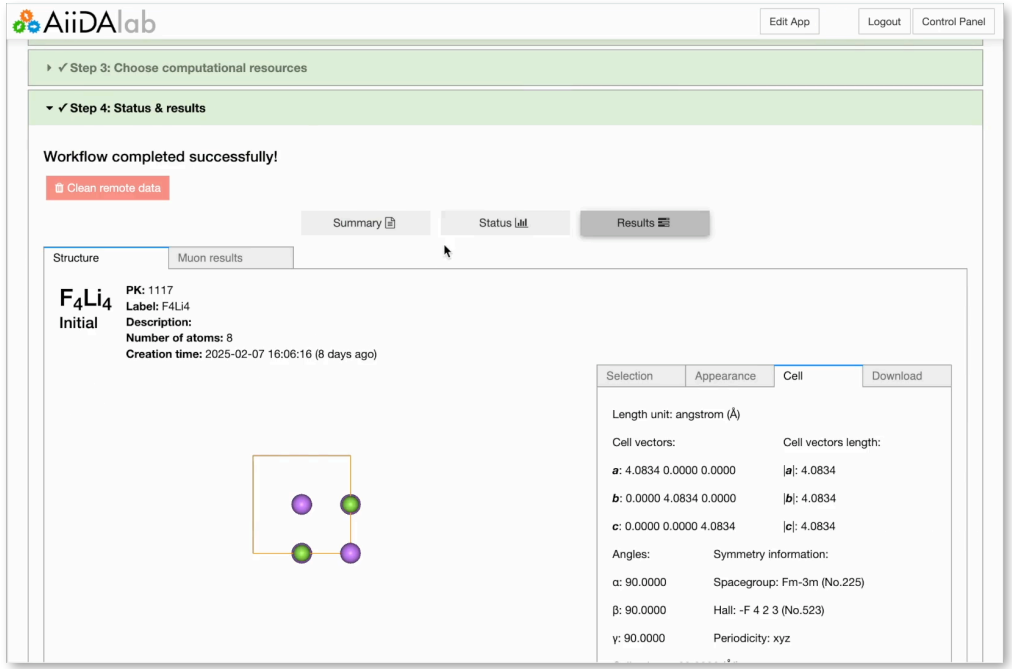
Ifeanyi J. Onuorah
(Uni Parma)

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]



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

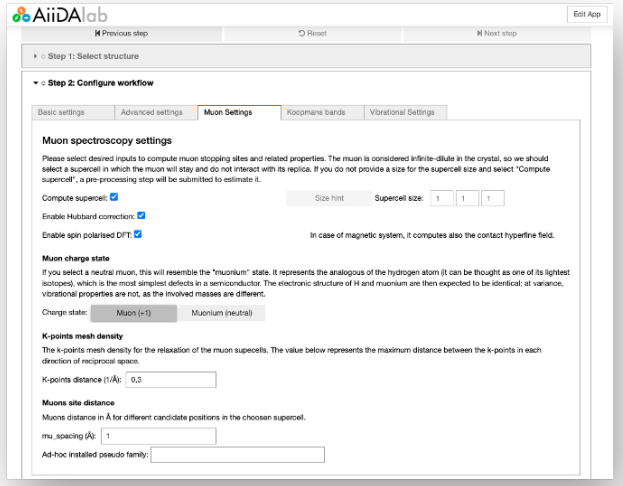
[2] J. S. Moller et al., Phys. Rev. B 87, 121108 (2013); F. Bernardini et al., Phys. Rev. B 87, 115148 (2013

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

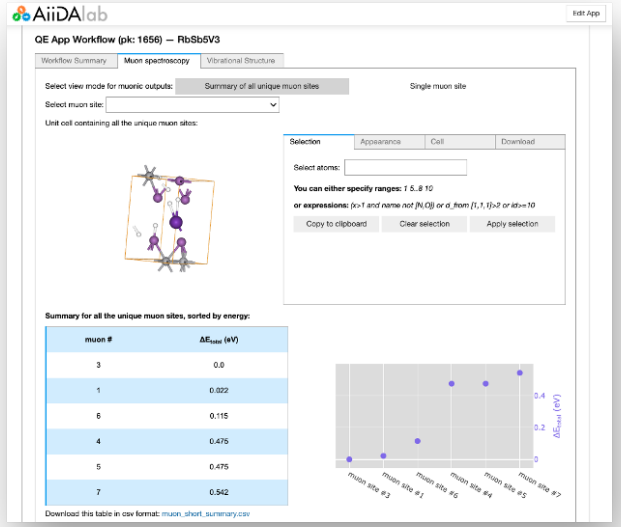
QE app plugin for muon spectroscopy with DFT+μ

PSI

- **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

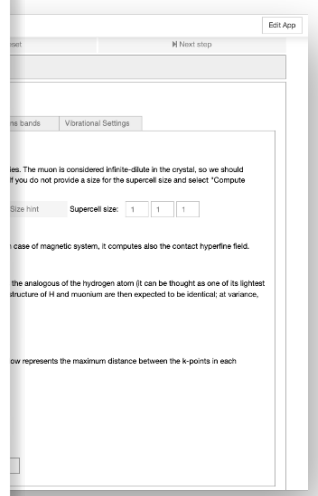
[1] I. J. Onourah, GP, et al., Digital Discovery, 4, 523 (2025)
[2] J. S. Moller et al., Phys. Rev. B 87, 121108 (2013); F. Bernardini et al., Phys. Rev. B 87, 115148 (2013
[3] https://aiidalab-qe.readthedocs.io/tutorials/muons.html

QE app

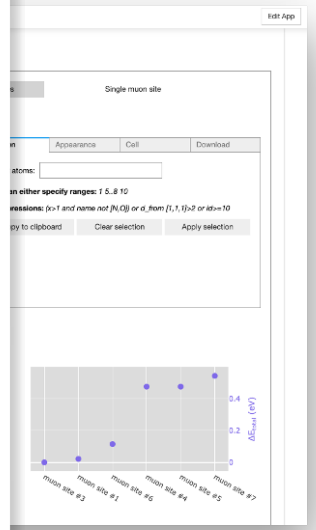
- **Available**
  - **muon** SOC,
  - **conta**
  - **class**
  - **Kubo** static
  - **time inter** (via U
- **Work-in-**
  - **quad** UNDI
  - **Effici** optim Bonfà

- **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)



s panel

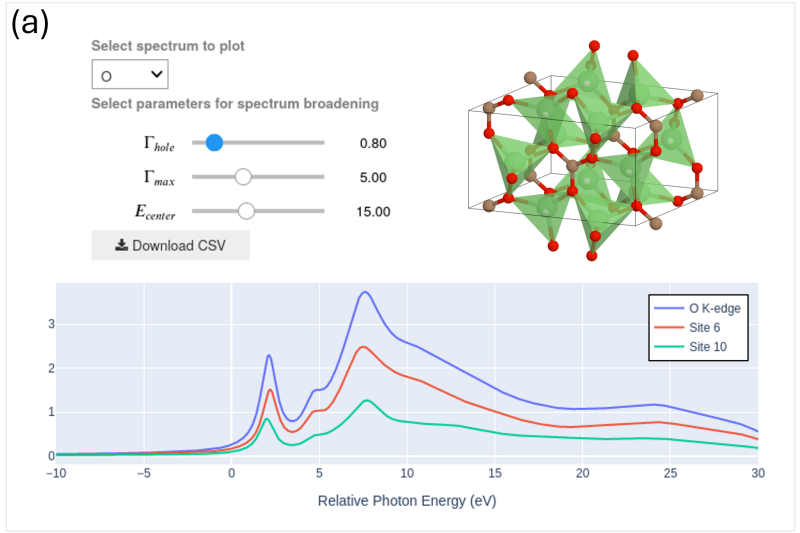


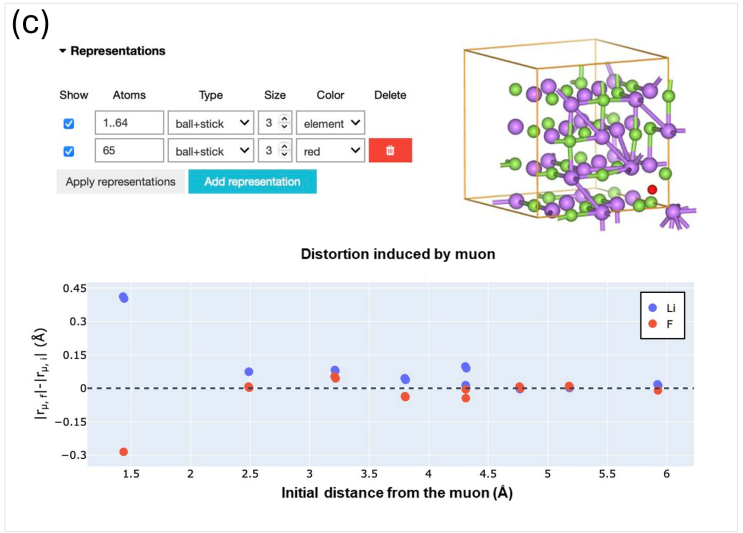
s panel

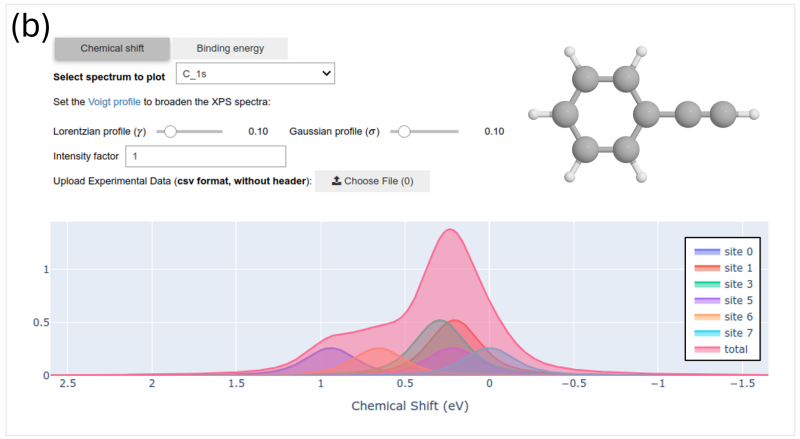
[1] I. J. Onourah, GP
[2] J. S. Moller et al
[3] https://aiidalab-qe.readthedocs.io/tutorials/muons.html

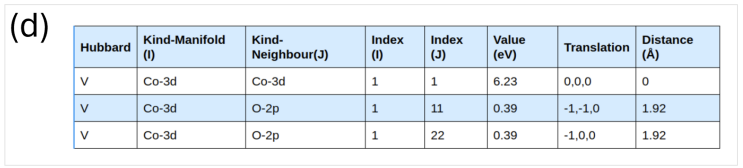
Many more robust workflows developed (and GUIs to drive them)

PSI



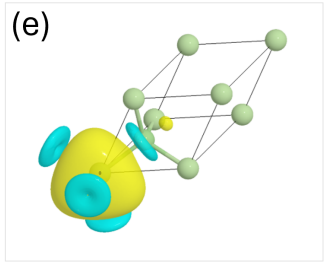


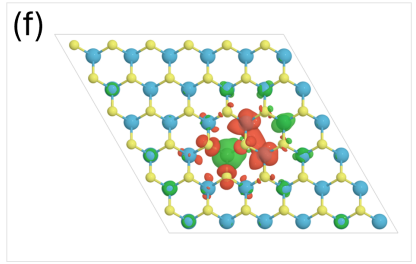




(d)

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





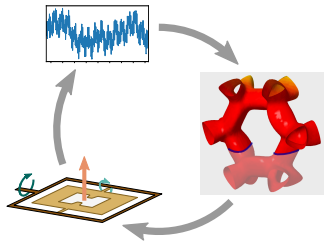
see X. Wang et al., npj Comput. Mater. 12, 72 (2026)

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, …

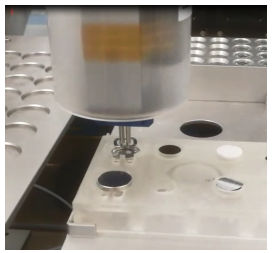
Agentic AI and autonomous labs

PSI

- Active investigation of using **AiiDA as part of Agentic AI workflows**
  - AI tool
  - Active learning workflows
  - …

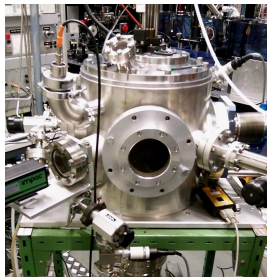


Accurate Fermi-surface mapping (Shubnikov-de Haas)



Battery assembly and testing

- 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



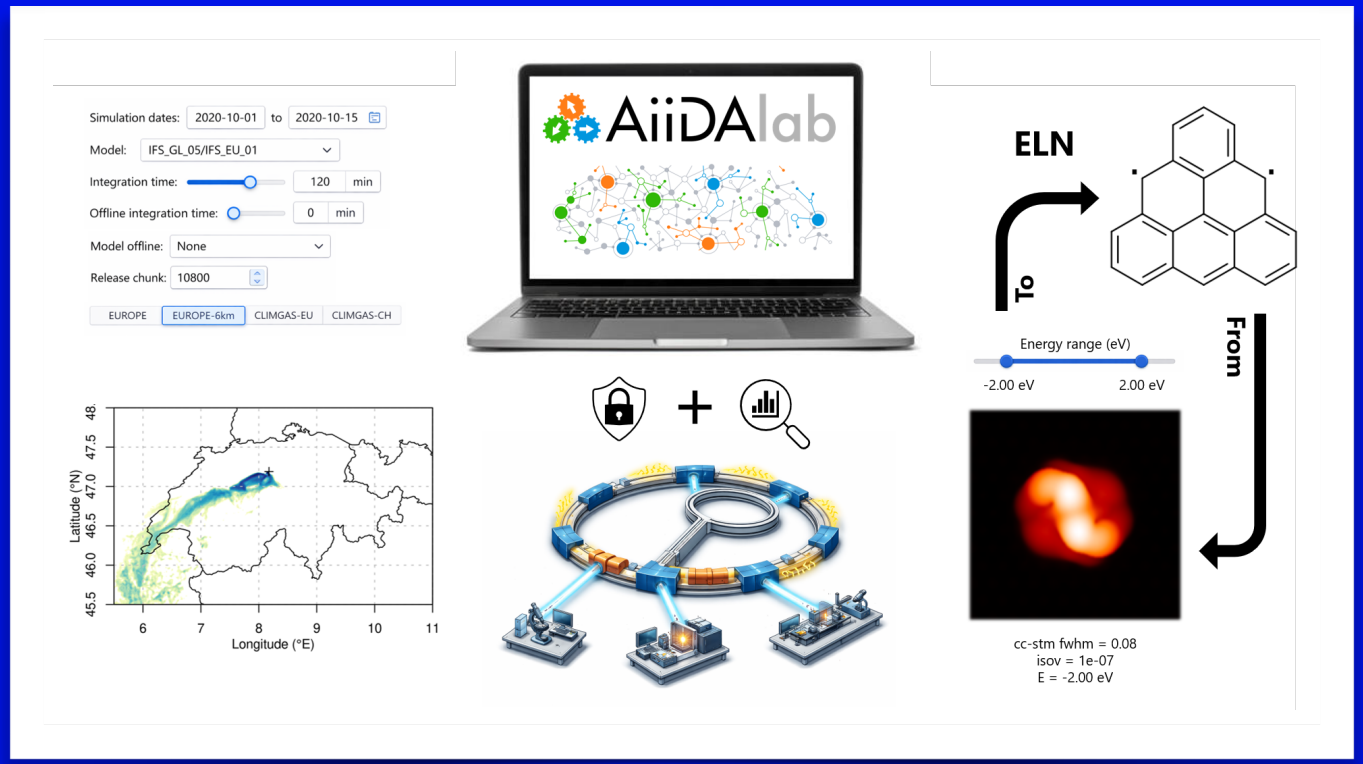
Pulsed laser deposition (autonomous crystal growth)

Nikita Shepelin

Pietro Mani

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

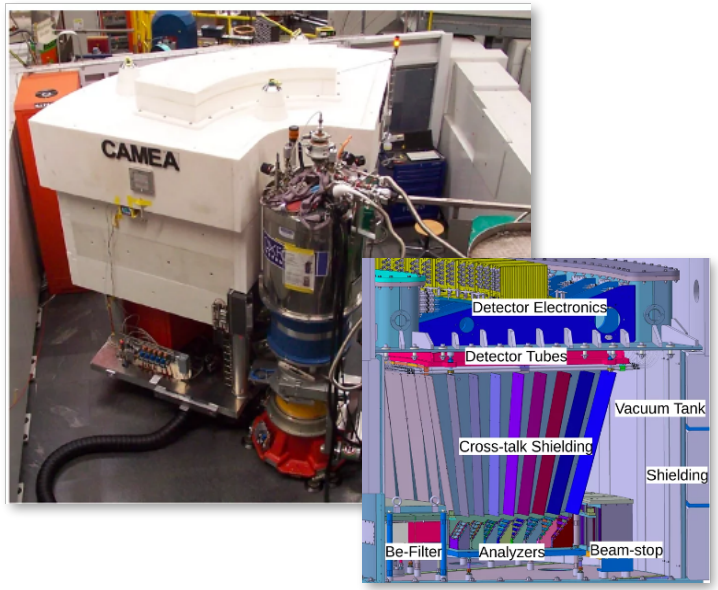
A. Yakutovich et al., arXiv:2512.22173 (2025)



AiiDAlab beyond DFT and AiiDA: the LNS apps

PSI

- 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/camea

(*q*,*E*) mapping of neutron excitations

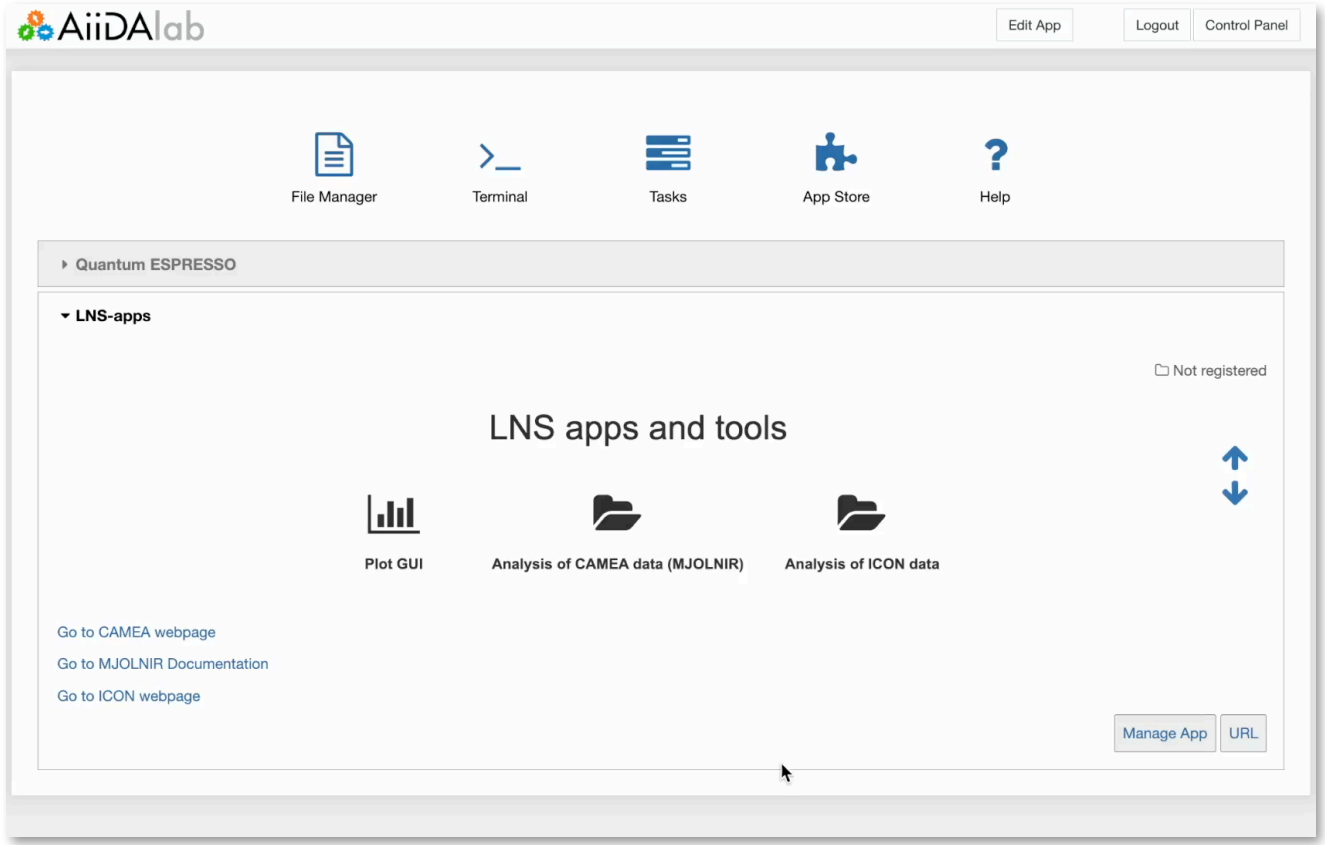
Daniel Mazzone

Jakob Lass

Our proposed solution: The AiiDAlab LNS app

PSI

- **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

PSI

Live data storage

CAMEA

NFS mount

PSI NFS mount for CAMEA da

HPC (Merlin, Ra, CSCS, …)
(Optional)

SSH via AiiDA

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

AiiDAlab
server (backend)

NFS mount

Login with PSI credentials
(authentication via Azure AD)

HTTPS

HTTPS

HTTPS

Web browser
AiiDAlab
frontend
/camea/20201923/
User 1

Web browser
AiiDAlab
frontend
/camea/20242013/
User 2

Web browser
AiiDAlab
frontend
/camea/20246188/
/camea/20242013/
User 3

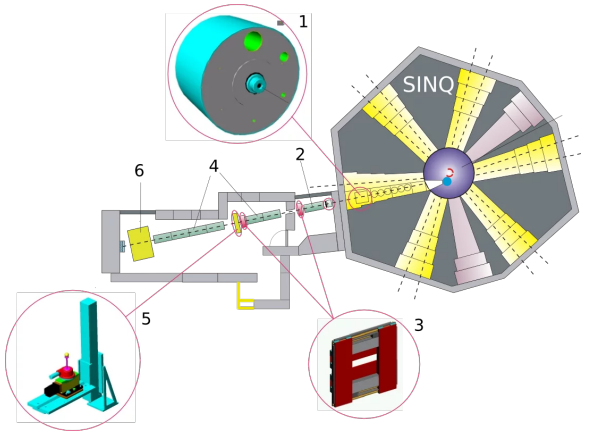
…

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

AiiDAlab beyond DFT and AiiDA: the LNS apps

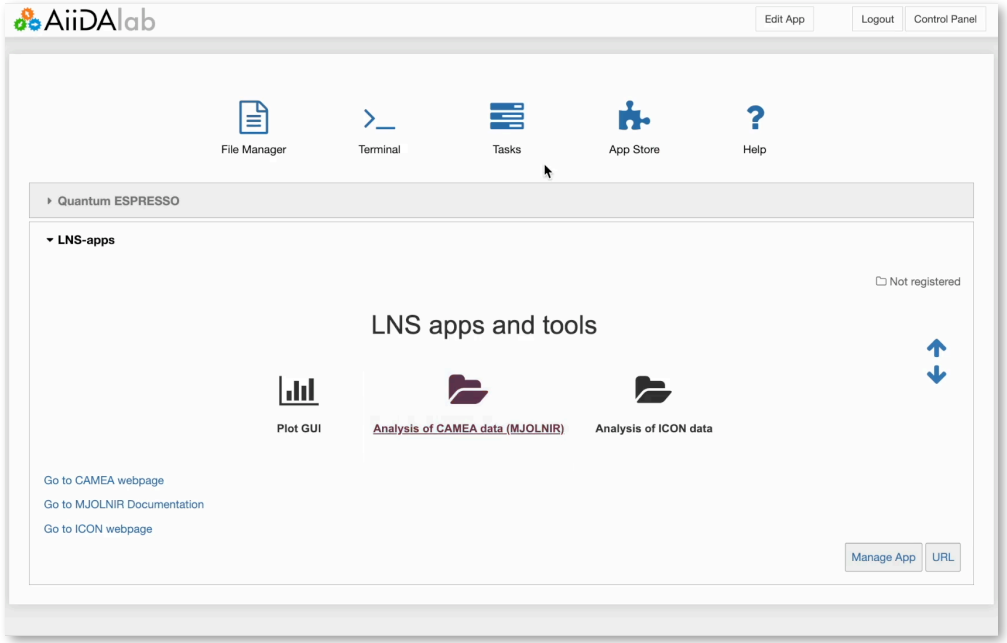
PSI

- **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

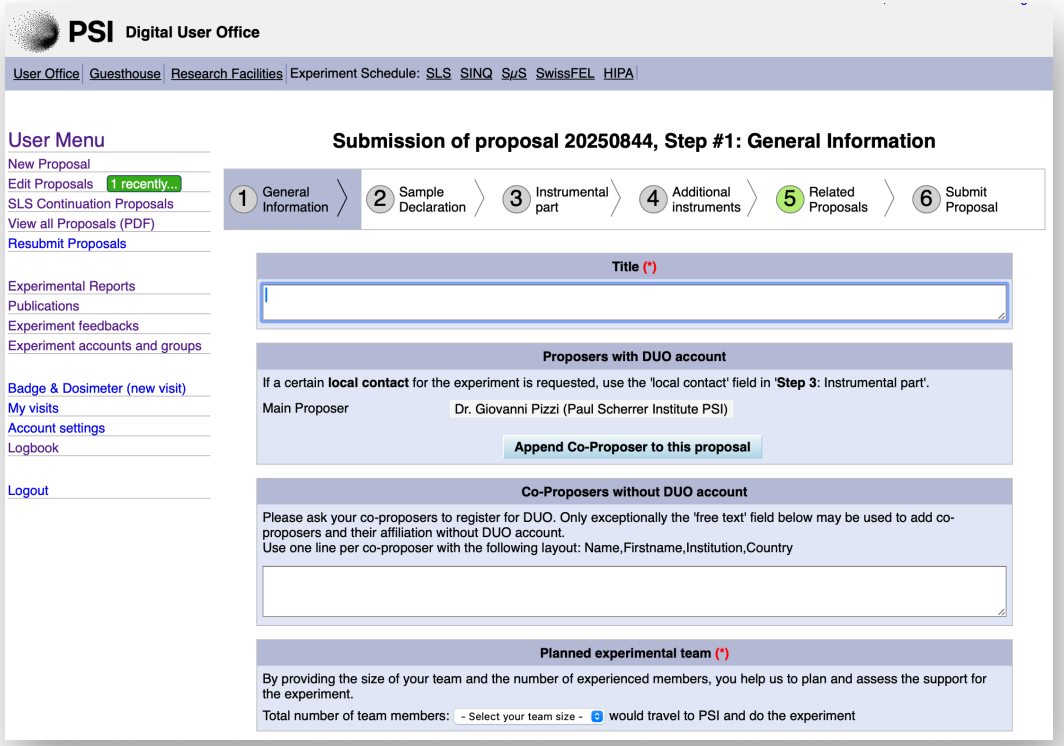


https://github.com/mikibonacci/LNS-app

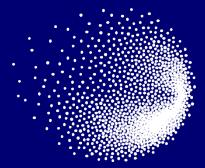
Vision for a computational facility

- **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 (AiiDAlab) interface to users**, both those interested in materials simulations, or only in data analysis and pre-/post-processing



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

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

- 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

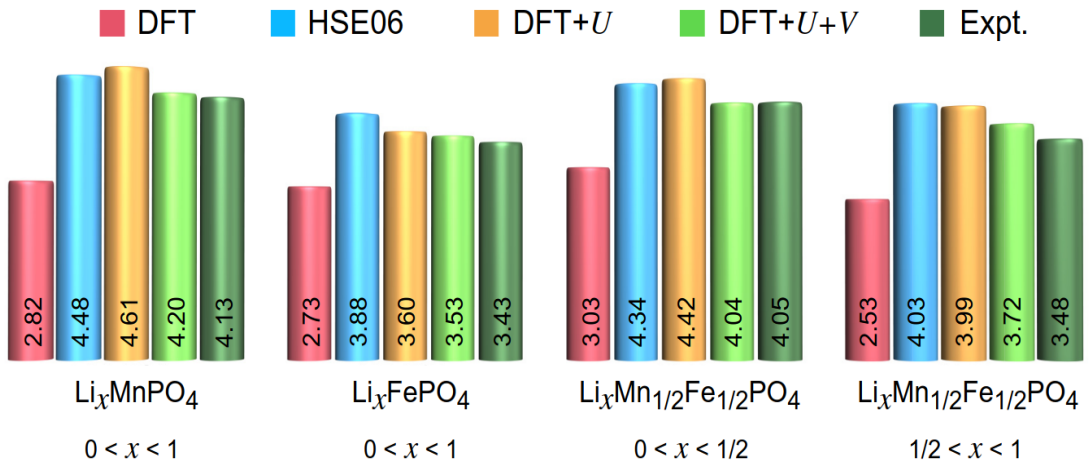
Advanced electronic structure: ground state

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

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

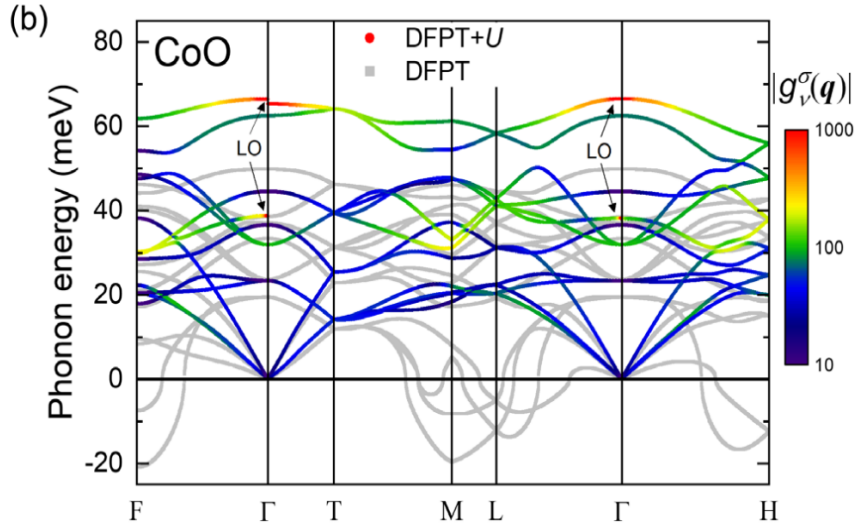
Iurii Timrov
PSI LMS

Li-ion batteries



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

Correlated oxides



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

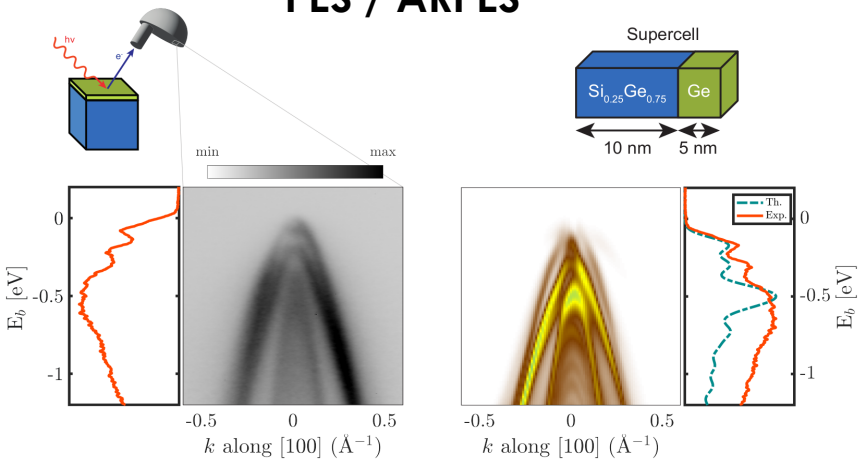
DFT+U+V calculations with QE and **automated Hubbard U(&V)** workflow already **available in the AiiDAlab QE app**

Advanced electronic structure: excited states

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

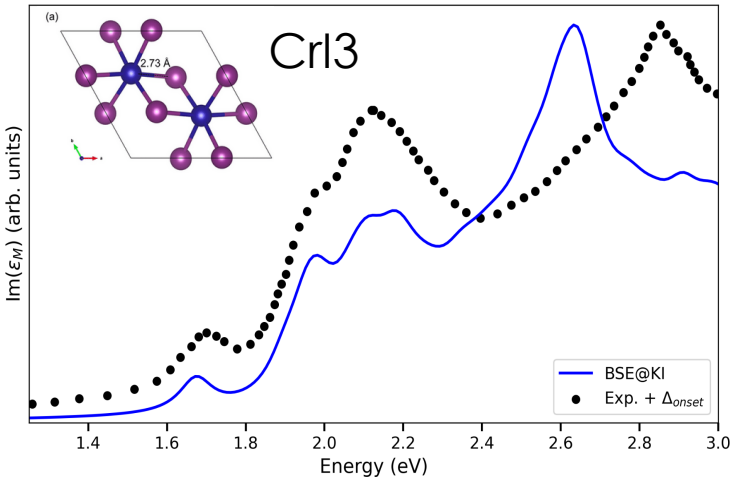
$$E^{\mathrm{KC}}[\rho,\{\rho_i\}] = E^{\mathrm{DFT}}[\rho] + \sum_i \alpha_i \Pi_i^{\mathrm{KC}}[\rho_i]$$

PES / ARPES



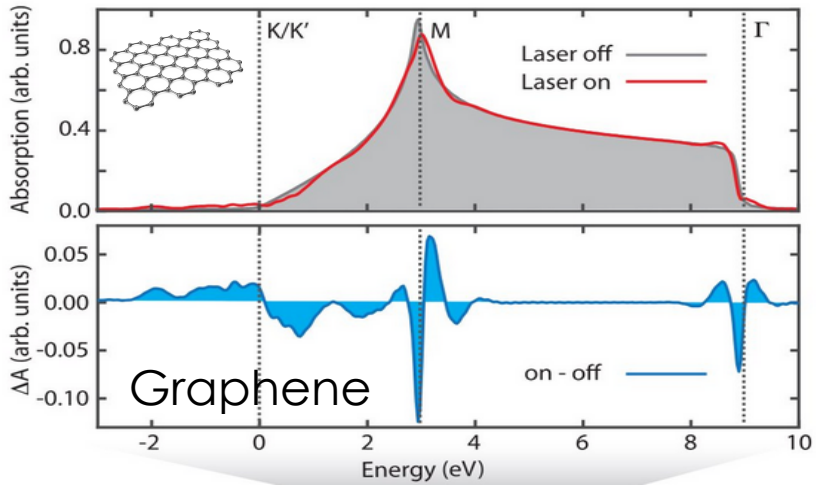
E. della Valle et al. submitted (2026)

Optical/Xray ABS, EELS, IXS, …

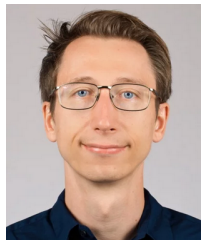


M. Bonacci et al. in preparation (2026)

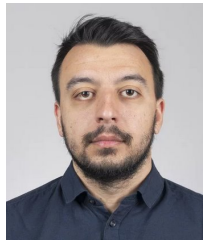
Time-resolved and **ultrafast**



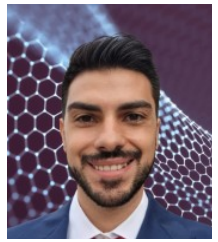
G. Cistaro et al. in preparation (2026)



Michael Schuler
PSI LMS



Miki Bonacci
PSI LMS



Giovanni Cistaro
CNR Milano

Open source

QUANTUMESPRESSO

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

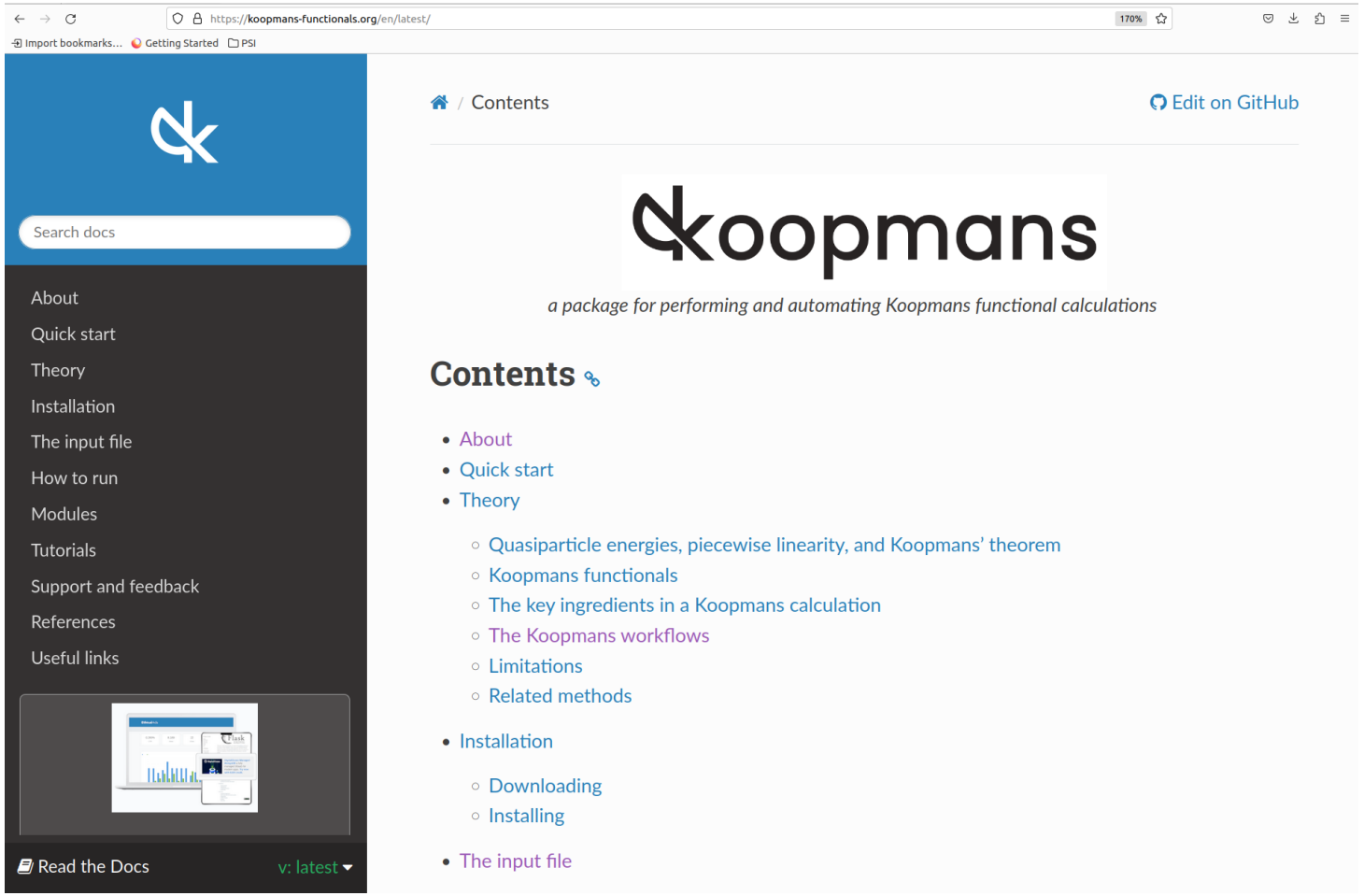
WANNIER90

https://wannier.org/

EDUS

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

koopmans-functionals.org



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

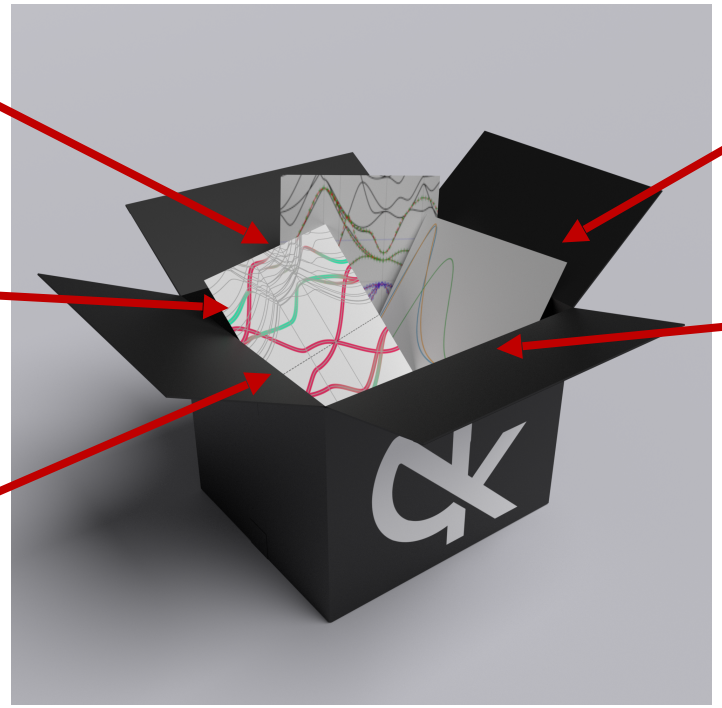
Miki Bonacci

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)