



Towards all-electron treatment in electronic structure machine learning

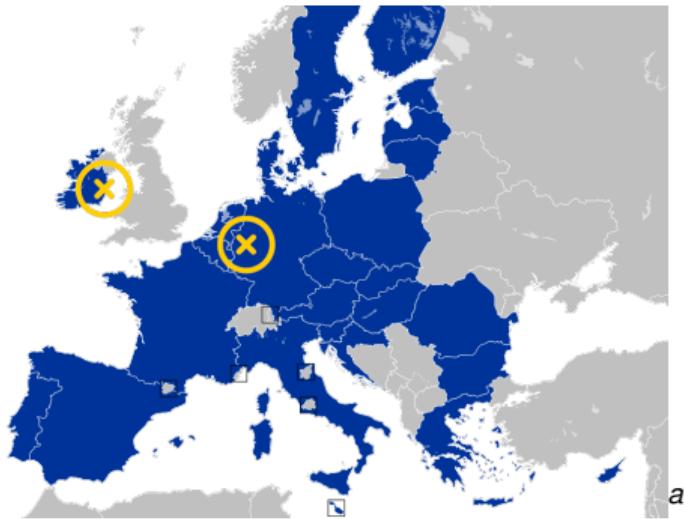
February 5, 2025 | Johannes Wasmer¹ Urvesh Patil² Philipp Rüßmann^{3,1} Stefano Sanvito² Stefan Blügel¹ | ¹Forschungszentrum Jülich ²Trinity College Dublin ³University of Würzburg

Talk held at DAEMON COST Action Meeting in Porto, February 2025 ([URL](#)).

Latest version of slides are [here](#).

My STSM

Short-term Scientific Mission, July 2024



^aKolja21 2020.

Members of /
Objectives:



Host



Trinity College Dublin
Coláiste na Trionóide, Baile Átha Cliath
The University of Dublin

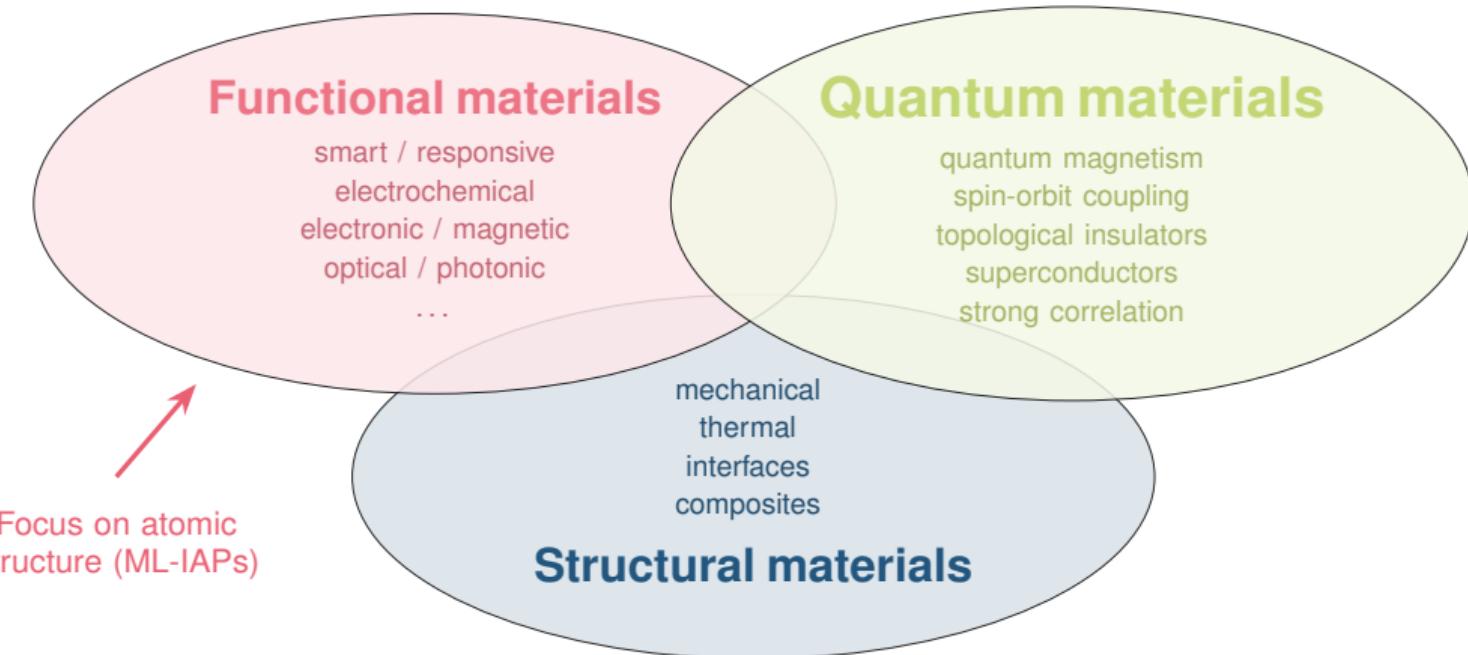
Prof. Dr. Stefano Sanvito
Computational Spintronics Group

Visitor

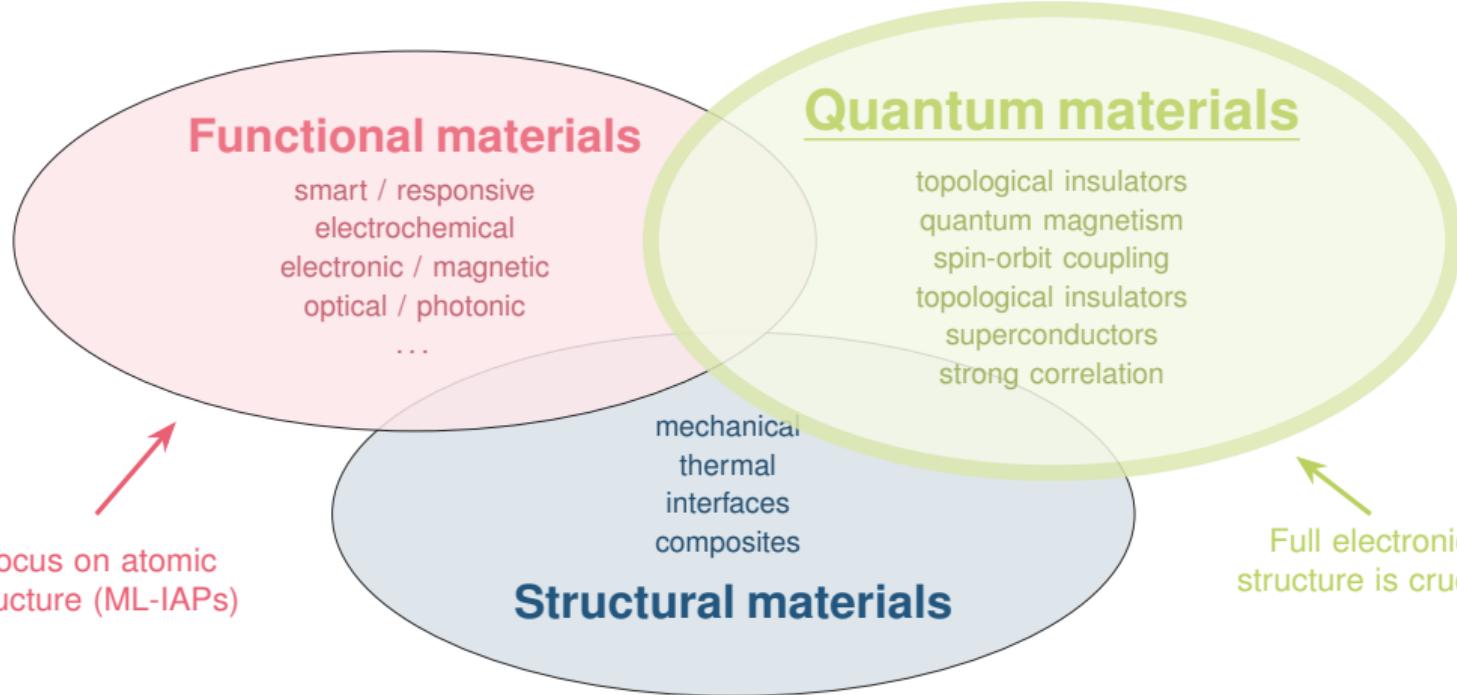


Johannes Wasmer
Quantum Theory of Materials Group

Materials realms



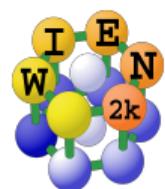
Materials realms



All-electron DFT for quantum materials

Only a handful of solid-state DFT codes are all-electron, full-potential, fully relativistic for data generation^a.

^aTalirz, Ghiringhelli, and Smit 2021.



juDFT



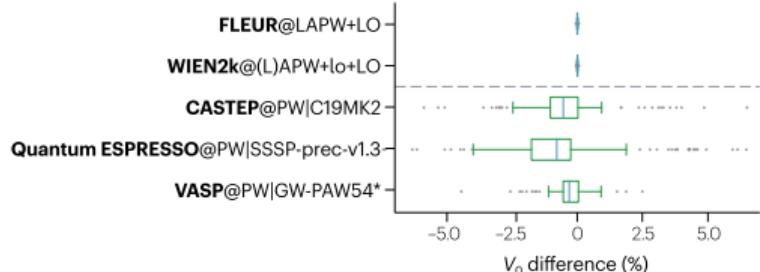
exciting

...

The **juDFT.de** codes are a “gold standard” for accuracy and HT-ready with AiiDA integration.



Materials set: $Z = 57\text{--}71$ (lanthanides: La to Lu)



Discrepancy of the equilibrium volume V_0 across popular DFT codes^a

^aBosoni et al. 2024.

High-throughput data generation

with perfectly labeled data



**Automated Interactive
Infrastructure and Database
for Computational Science**



Workflows

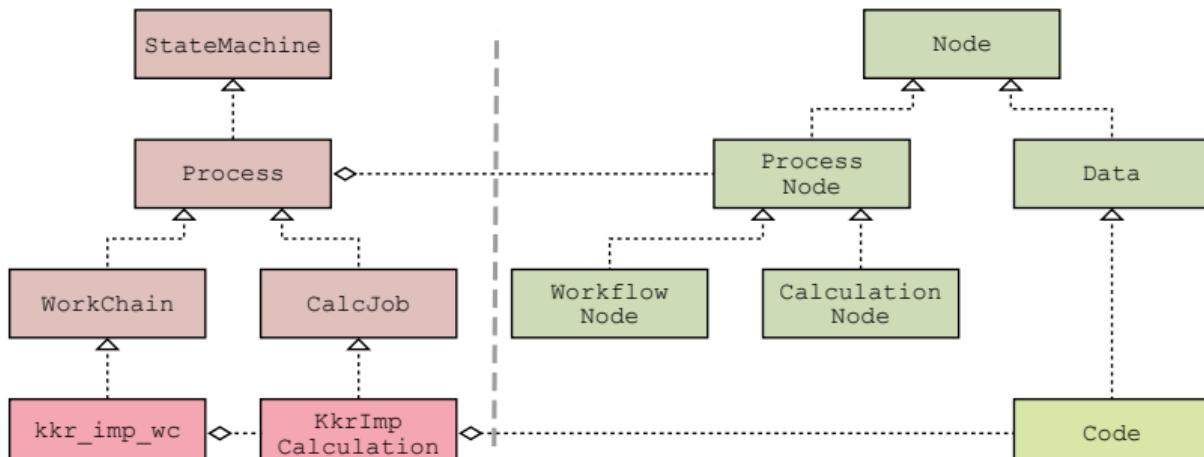
Provenance

Plugin Framework

HPC Interface

Open Science

Open source

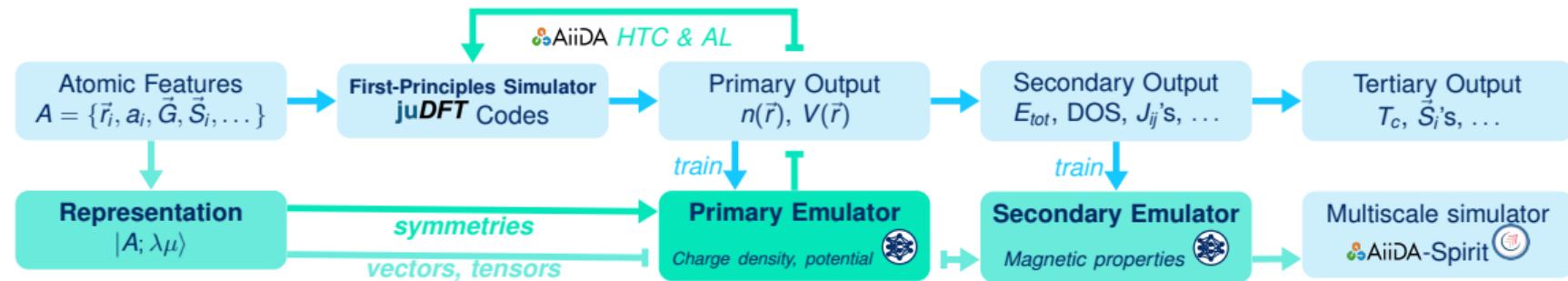


Engine

Database

Vision: Electronic structure learning

as integrated, high-level multiscale workflows



Smart “initial guess”
for fast SCF convergence

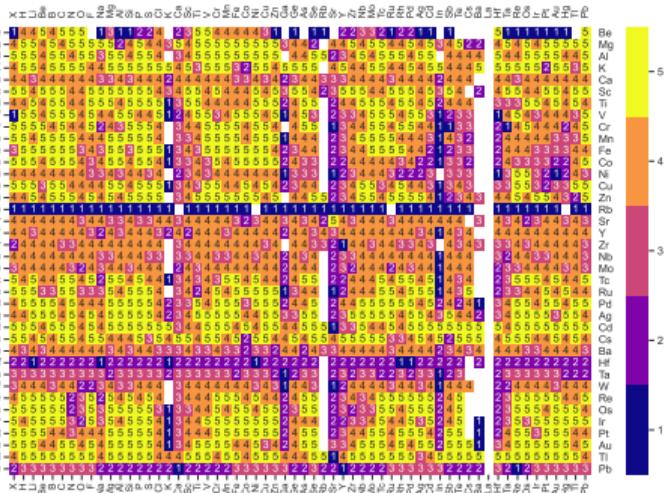
Magnetic property prediction
for spin dynamics simulation

Data generation

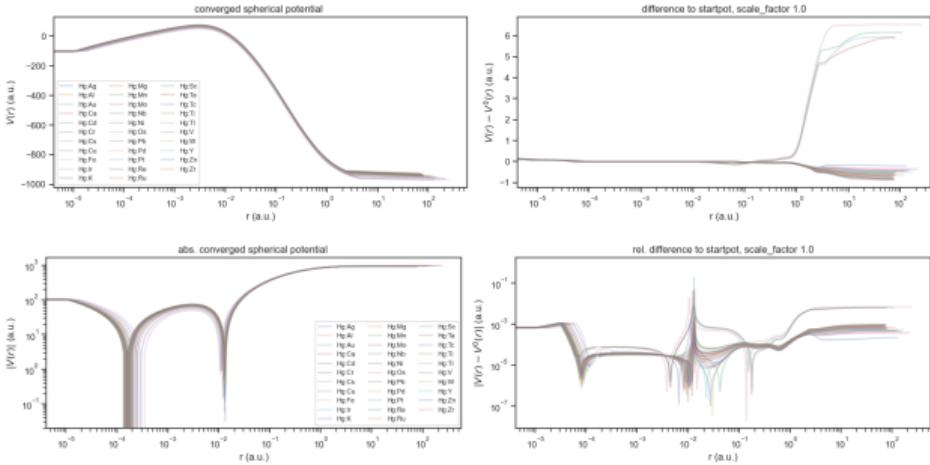
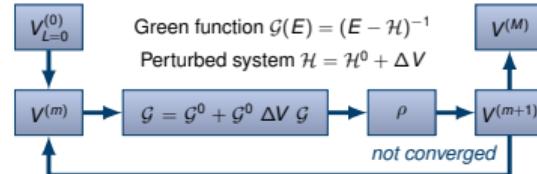
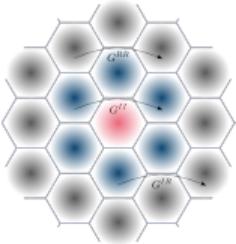
for this project, with  AiiDA-KKR

Data 10'000 impurity embeddings into elemental crystals

Target Electron potential difference $\Delta V_{imp}(\vec{r})$



Dataset map. Rows: Element of host crystal, columns: impurity atom, color: num. calculations.

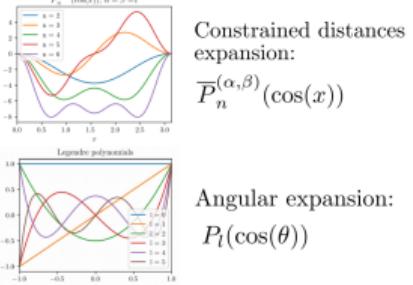
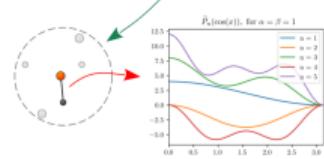
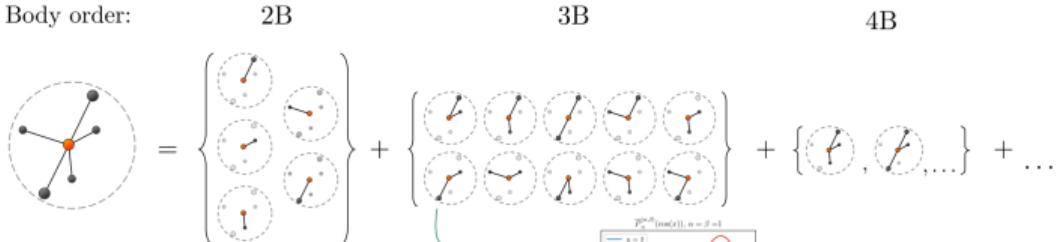


Spherical impurity potentials in first Voronoi cell of Hg:X embeddings,
 left upper to bottom right: V , $V - V^0$, $|V|$, $|V - V^0|$.

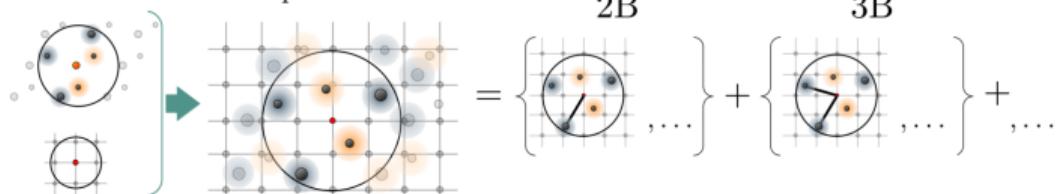
The Jacobi-Legendre framework¹

for electronic structure representation

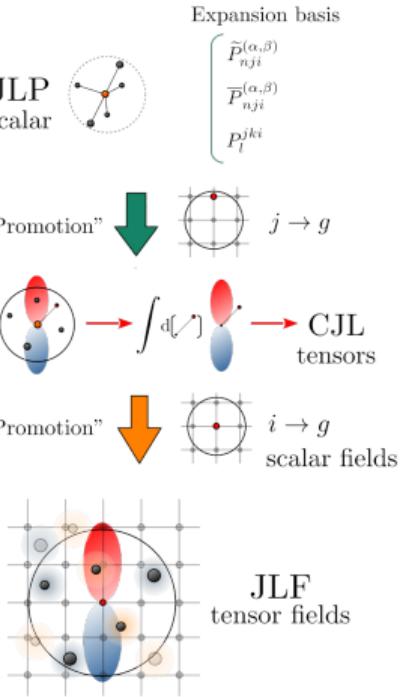
Body order:



Grid centered representation

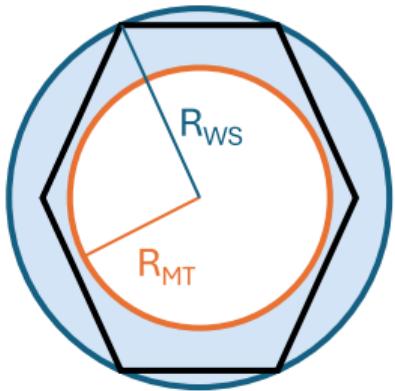


¹Domina 2024.

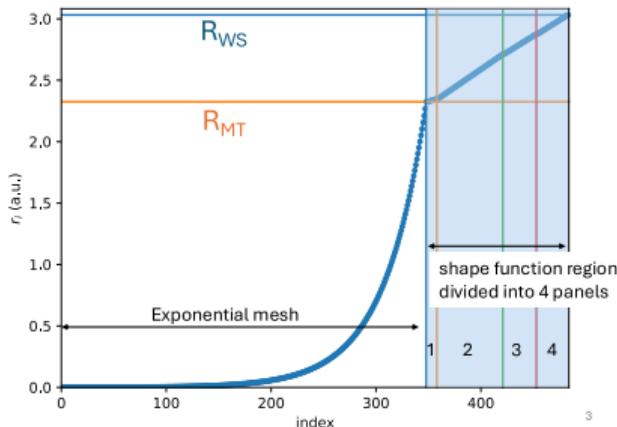


KKR potential conversion

from Voronoi decomposition to Cartesian grid



Space-filling Voronoi decomposition



Convolution with non-trivial shape functions $\Theta(\vec{r})$ outside MT sphere^a

^aStefanou, Akai, and Zeller 1990.

Conversion

Full potential convolution with shape functions

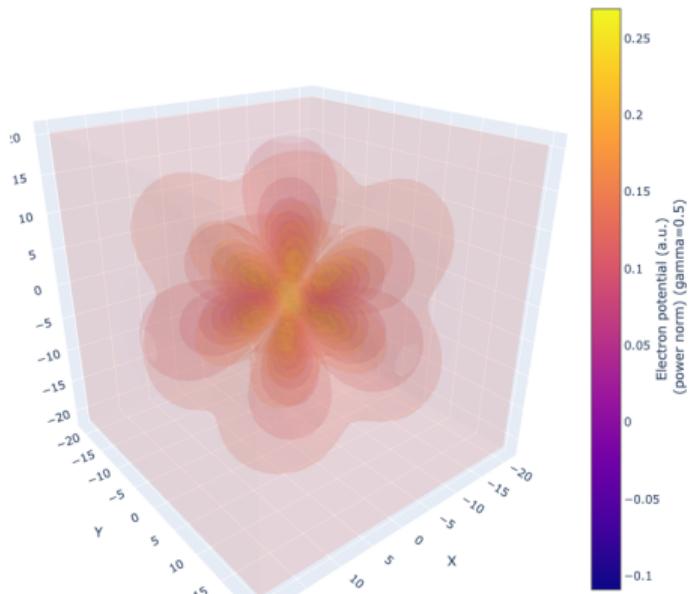
$$V_{LL'}(r) = \sum_{L''} C_{LL'L''} V_{L''}(r)$$

Conversion to real-space grid

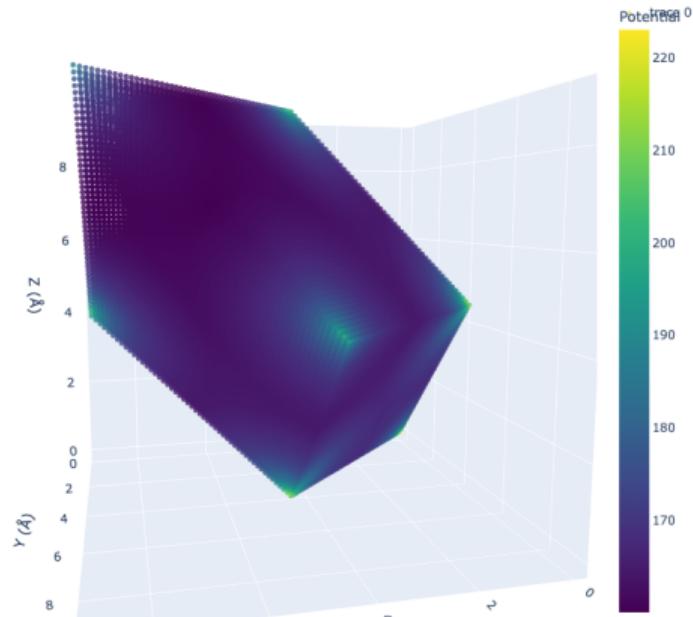
$$V(\vec{r}) = \sum_L V_L(r) Y_L(\theta, \phi)$$

Conversion example

Cu fcc host crystal



ΔV_{host} non-periodic



V_{host} mapped to unit cell

Community resources

Best of atomistic machine learning

JuDFTteam/best-of-atomistic-machine-learning

A ranked list of awesome atomistic machine learning projects 🏆.

5 Contributors | 83 Issues | 271 Stars | 19 Forks

GitHub - JuDFTteam/best-of-atomistic-machine-learning: 🏆 A ranked list of a...

Largest list of atomistic ML tools on the web (400+), auto-ranked, regular updates^a

go.fzj.de/baml

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^aWasmer et al. 2023.

Discussion slides

References I

-  Bosoni, Emanuele et al. (Jan. 2024). "How to Verify the Precision of Density-Functional-Theory Implementations via Reproducible and Universal Workflows". In: *Nature Reviews Physics* 6.1, pp. 45–58. ISSN: 2522-5820. DOI: [10.1038/s42254-023-00655-3](https://doi.org/10.1038/s42254-023-00655-3). URL: <https://www.nature.com/articles/s42254-023-00655-3>.
-  Domina, Michelangelo (Mar. 7, 2024). "The Jacobi-Legendre Framework for Machine Learning in Materials Investigation and Discovery". PhD thesis. Dublin: Trinity College Dublin. 184 pp. URL: <http://hdl.handle.net/2262/106636>.
-  Kolja21 (Feb. 1, 2020). File:European Union Main Map.Svg. URL: https://commons.wikimedia.org/wiki/File:European_Union_main_map.svg.
-  Stefanou, N., H. Akai, and R. Zeller (Sept. 1, 1990). "An Efficient Numerical Method to Calculate Shape Truncation Functions for Wigner-Seitz Atomic Polyhedra". In: *Computer Physics Communications* 60.2, pp. 231–238. ISSN: 0010-4655. DOI: [10.1016/0010-4655\(90\)90009-P](https://doi.org/10.1016/0010-4655(90)90009-P). URL: <https://www.sciencedirect.com/science/article/pii/001046559090009P>.

References II

- Talirz, Leopold, Luca M. Ghiringhelli, and Berend Smit (Oct. 25, 2021). "Trends in Atomistic Simulation Software Usage [Article v1.0]". In: Living Journal of Computational Molecular Science 3.1 (1), pp. 1483–1483. ISSN: 2575-6524. DOI: [10.33011/livecoms.3.1.1483](https://doi.org/10.33011/livecoms.3.1.1483). URL: <https://livecomsjournal.org/index.php/livecoms/article/view/v3i1e1483>.
- Wasmer, Johannes et al. (2023). Best of Atomistic Machine Learning. FZJ-2023-05862. Quanten-Theorie der Materialien. DOI: [10.5281/ZENODO.10430261](https://doi.org/10.5281/ZENODO.10430261). URL: <https://juser.fz-juelich.de/record/1020061>.