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AIDAS AI Data Analytics and Scalable Simulations

JÜLICH Forschungszentrum

Towards all-electron treatment in electronic structure machine learning

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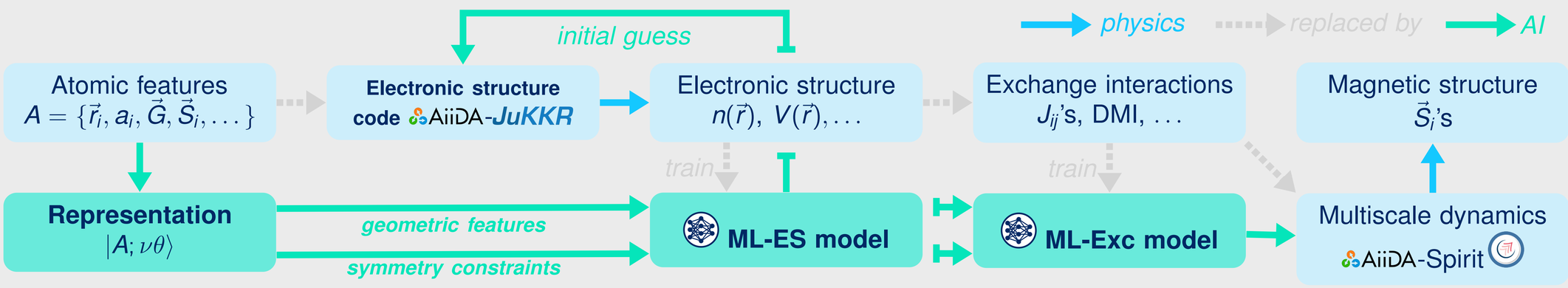
Hybrid physics-AI simulation workflows for quantum materials

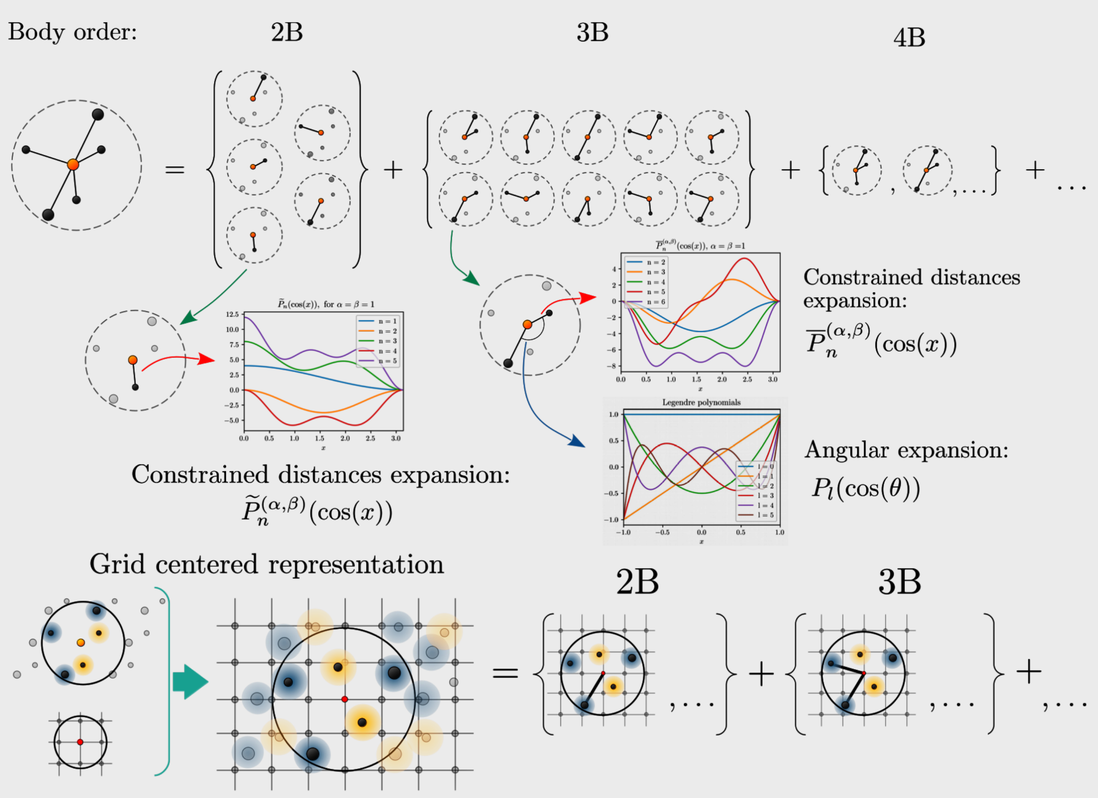
Quantum materials have enormous potential for low-energy, neuromorphic and quantum computing. The **all-electron** ***juDFT*** (judft.de) electronic structure codes uniquely provide the **high-end accuracy** needed to resolve and engineer their properties [1]. **Atomistic machine learning** techniques can accelerate these simulations from the nano- toward **device-relevant scales**. This PhD project integrates our codes with hybrid physics-AI workflows via the **high-throughput computing** engine and database AiiDA (aiida.net). This integrated system represents a significant step toward accurate datasets and **foundational models** of quantum materials.

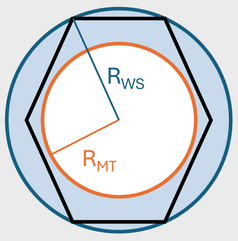


Electronic structure prediction — ML-ES

Grid-based, systematic cluster expansion of the full, converged ***JuKKR*** electron potential $\Delta V(\vec{r})$ with the Jacobi-Legendre (JL) framework [2].

Training database: 10k impurity embeddings, 60 chemical elements.





Space-filling Voronoi decomposition of $V^n(\vec{r})$

Potential convolution with shape functions $\Theta(\vec{r})$.

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

Conversion to Cartesian grid w. adaptive sampling.

$V(\vec{r}) = \sum_L V_L(r) Y_L(\hat{r})$; $P(\vec{r}) \propto \exp\left[-\frac{V(\vec{r})^{-2}}{2\sigma^2}\right]$

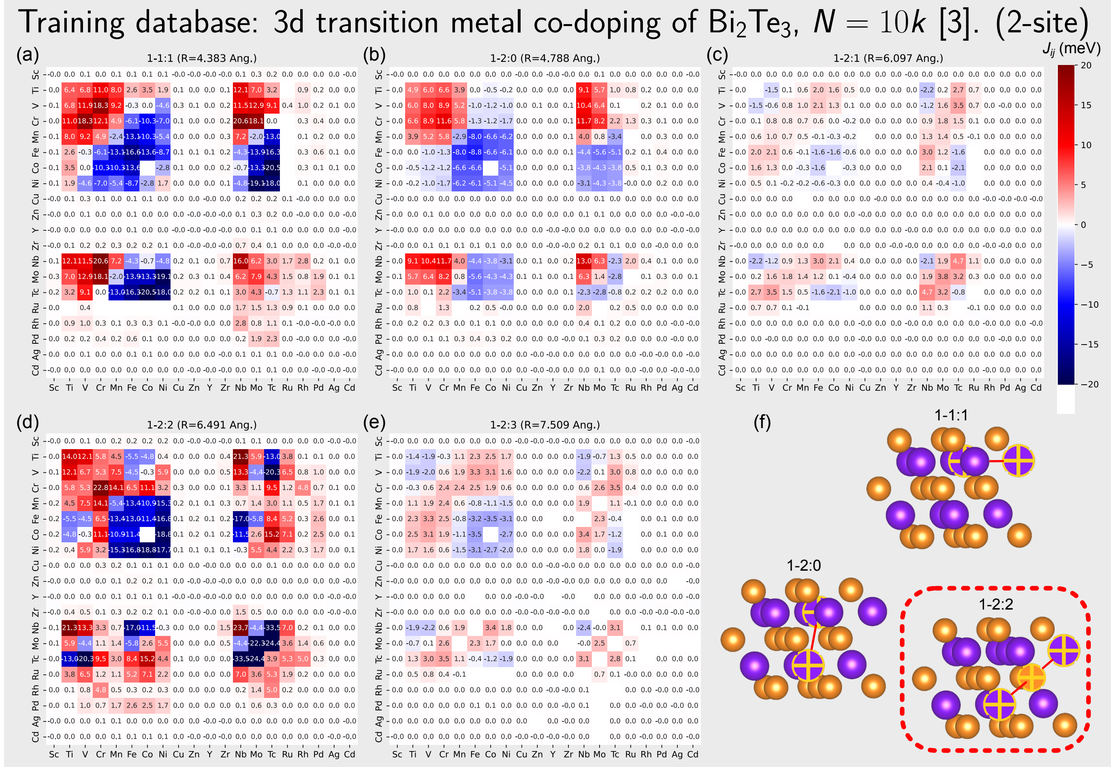
ML: JL cluster expansion ➞ **small linear models**.

$V(\vec{r}_g) = \sum_i \sum_n^{(2B)} a_n^i \tilde{P}_n^{gi} + \sum_{i,j} \sum_{n_1 n_2 L}^{(3B)} a_{n_1 n_2 l}^{ij} \bar{P}_{n_1}^{gi} \bar{P}_{n_2}^{ji} P_l^{gji} + \dots$

Exchange interaction prediction — ML-Exc

Equivariant neural networks explicitly predict exchange interaction tensors from first principles ***JuKKR*** to arbitrary order.

Training database: 3d transition metal co-doping of Bi_2Te_3, $N = 10k$ [3]. (2-site)



Systematic expansion of higher-order exchange interactions.

$\mathcal{H} = \frac{1}{2}\sum_{ij}{}' J_{ij} \vec{S}_i \cdot \vec{S}_j + \frac{1}{2}\sum_{ij}{}' B_{ij} (\vec{S}_i \cdot \vec{S}_j)^2 + \sum_{ij} \vec{D}_{ij} \cdot (\vec{S}_i \times \vec{S}_j) + \dots$ (2-site)

$+ \frac{1}{2}\sum_{ijk}{}' Y_{ijk} (\vec{S}_i \cdot \vec{S}_j)(\vec{S}_j \cdot \vec{S}_k) + \sum_{ijk} (\vec{F}_{ijk} \cdot \vec{S}_i)[\vec{S}_i \cdot (\vec{S}_j \times \vec{S}_k)] + \dots$ (3-site)

$+ \frac{1}{8}\sum_{i,j,k,l}{}' L_{ijkl} (\vec{S}_i \cdot \vec{S}_j)(\vec{S}_k \cdot \vec{S}_l) + \dots$ (4-site)

Extraction of exchange tensors from KKR Green function.

$\mathcal{J}_{ij} = -\frac{1}{\pi} \mathrm{Im} \int_{-\infty}^{E_F} \mathrm{d}E \, \mathrm{Tr}[\delta t_i G_{ij} \delta t_j G_{ji}]$; $J_{ij} = \frac{1}{3}\mathrm{Tr}(\mathcal{J}_{ij}), \dots$ (2-site)

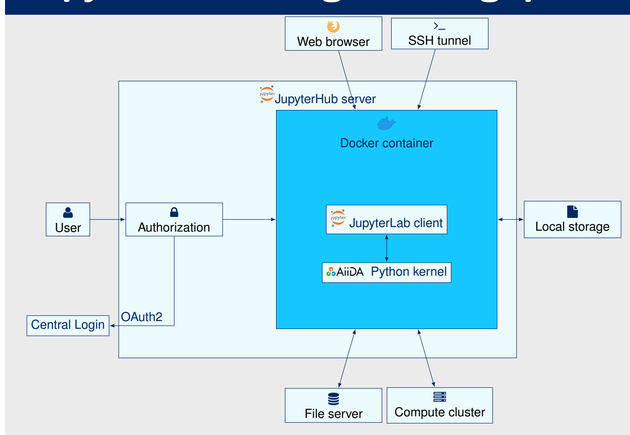
ML: Equivariant graph edge features ($Q \in \mathrm{O}(3)$, D Wigner matrix, $\mathbf{R}$ atom pos.).

$\mathcal{J}_{ij} \propto \sum_{k \in \mathcal{N}_{ij}} (\vec{e}_{ij})_k$; $e_{ij,\nu lm}(Q \cdot \mathbf{R}) = \sum_{m'} D^l_{mm'}(Q) e_{ij,\nu lm'}(\mathbf{R})$

AI4Science community building

Want to know more about atomistic machine learning? Have a look at our list go.fzj.de/baml **Best of Atomistic Machine Learning**. Over 500 tools, ranked, regular updates. The most comprehensive AML list available online.

Jupyter-based high-throughput cloud computing



The HTC workflow engine AiiDA provides plugins for 50+ atomistic simulation packages (LAMMPS, VASP, Quantum ESPRESSO, CP2K, GROMACS, FLEUR, etc.).

Our containerized, portable setup go.fzj.de/iffAiiDA gives users instant access with built-in high-quality, FAIR data management.

References, Acknowledgments

[1] Bosoni, E. et al. Nat Rev Phys 6, 45–58 (2024) | [2] Domina, M. The Jacobi-Legendre framework (Trinity College Dublin, Dublin, 2024) | [3] Mozumder, R. et al. Phys. Rev. Mater. 8, 104201 (2024).

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