Prediction of the magnetic exchange interaction in doped topological insulators

July 10, 2024 | **Johannes Wasmer**[1] Rubel Mozumder[1] David Antognini Silva[1] Philipp Rüßmann[2,1] Stefan Blügel[1] | [1]Forschungszentrum Jülich [2]University of Würzburg

Talk held at Psi-k Workshop 2024, “Machine Learning of First Principles Observables”, July 8-12 2024, in Berlin, Germany (URL).

Latest version of slides are here.

Outline

Introduction

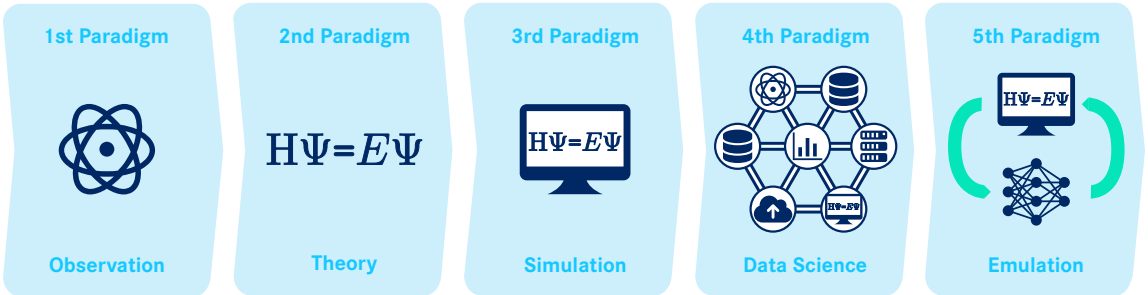
Magnetic co-doping of Bi_2Te_3

Machine learning exchange interactions

Odds and ends

A high-level perspective

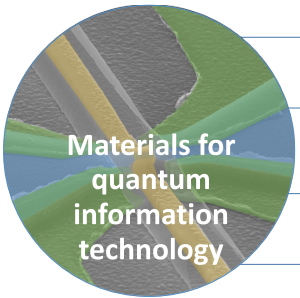
Learning simulation systems[1]



[1] Bishop, Welling, and Llorens 2022.

Affiliations

Research group



High-performance and high-throughput calculations

Superconductivity

Ab initio impurity embedding

First principles electronic structure calculations

juDFT

spirit

AiiDA

judft.de

Graduate school

HDS LEE

HELMHOLTZ School for Data Science in Life · Earth · Energy

European Joint Virtual Lab

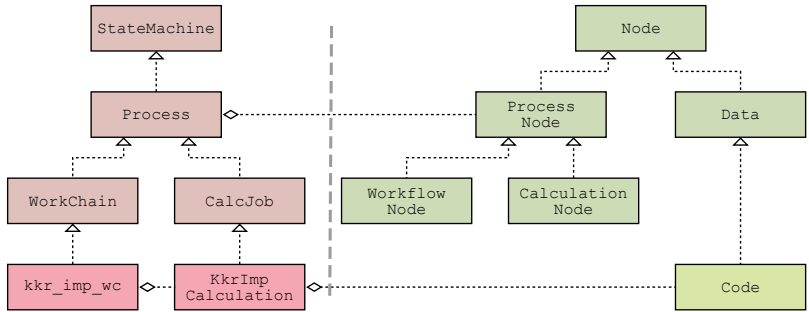
AIDAS

AI Data Analytics and Scalable Simulations

AiiDA

Automated Interactive Infrastructure and Database for Computational Science

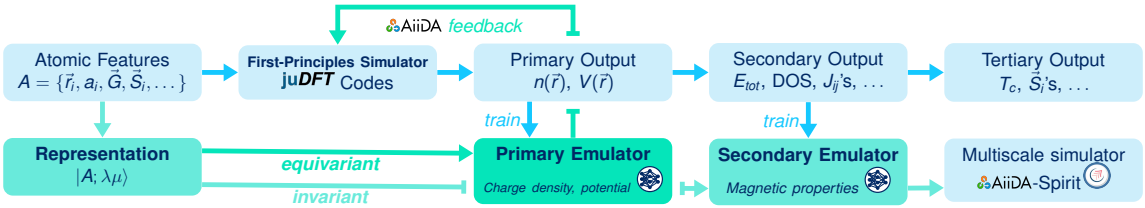
- Workflows
- Provenance
- Plugin Framework
- HPC Interface
- Open Science
- Open source



aiida.net

My PhD project

go.fzj.de/wasmer

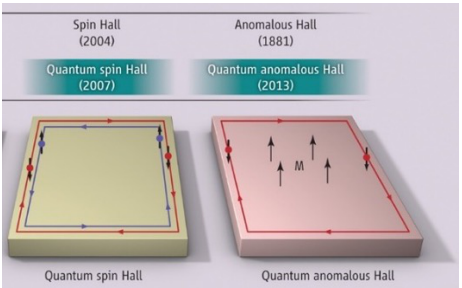


Electronic structure emulator
for fast SCF convergence

Magnetic property prediction
for spin dynamics simulation

Topological insulators and magnetic impurities

- Magnetic doping of topological insulators (**TIs**) can induce a topological phase transition
  - Ferromagnetic ordering
  - Out-of-plane anisotropy



S. Oh, Science **340**, 153 (2013)

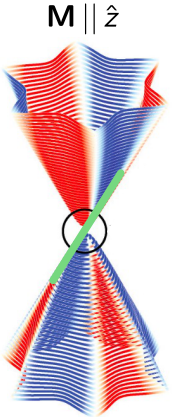
(QSHE)

→ Topological insulator

Two counter propagating edge states

(**QAHE**)

One single edge state

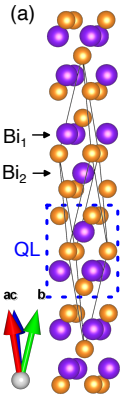


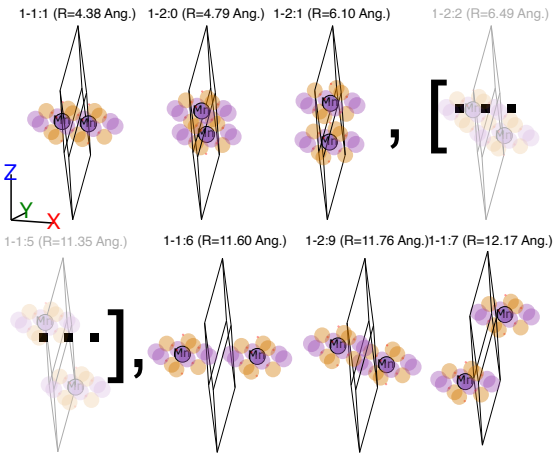
Henk *et al.*, PRL **109**, 076801 (2012)

Magnetic co-doping of topological insulators[1]

Bi_2Te_3

Dimer clusters of 3*d*, 4*d* transition metal defects





Single-impurity dabase, N=2'000.
go.fzj.de/judit

Dimer database (this), N=2'000.

Co-doping can help to control

- critical T_c of QAHE
- exchange splitting Δ_{xc}
- long-range magnetic ordering

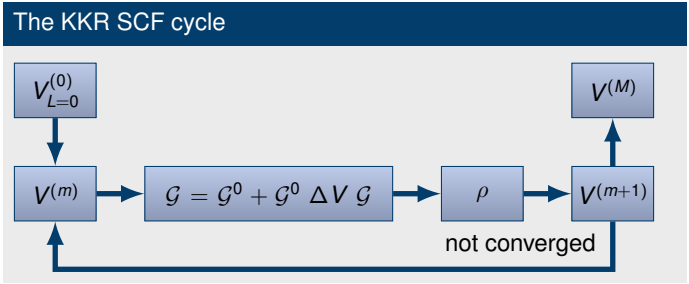
for applications in spintronics and fault-tolerant quantum computing.

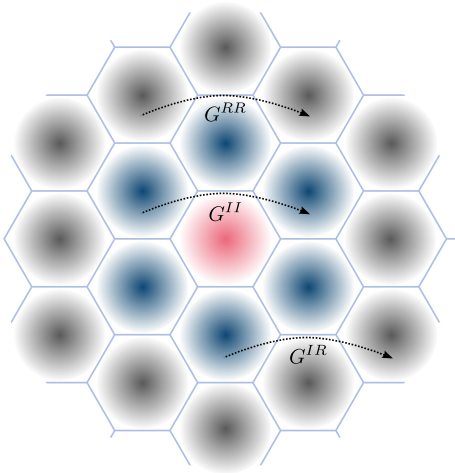
[1] Rubel Mozumder et al. (July 5, 2024). High-Throughput Magnetic Co-Doping and Design of Exchange Interactions in a Topological Insulator. arXiv: 2407.04413 [cond-mat]. URL: http://arxiv.org/abs/2407.04413 (visited on 07/08/2024). Pre-published.

Impurity embeddings with Korringa-Kohn-Rostoker

Green function
$\mathcal{G}(E) = (E - \mathcal{H})^{-1}$

Perturbed system
$\mathcal{H} = \mathcal{H}^0 + \Delta V$

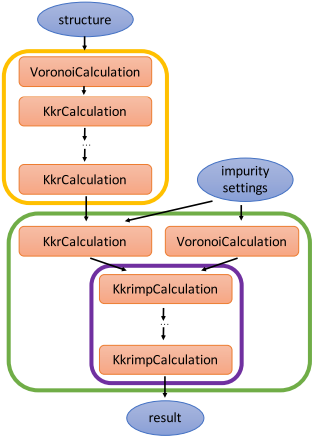


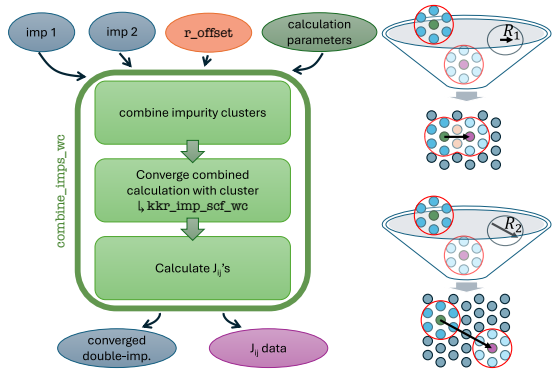


Observables $\langle \mathcal{O} \rangle = -\frac{1}{\pi} \mathrm{Im Tr} \int_{-\infty}^{E_F} dE\ \mathcal{O} G(E)$

Electron density $\langle \rho(\mathbf{r}) \rangle = -\frac{1}{\pi} \mathrm{Im} \int_{-\infty}^{E_F} dE\ G(\mathbf{r}, \mathbf{r}, E)$

AiiDA-KKR workflows[2]



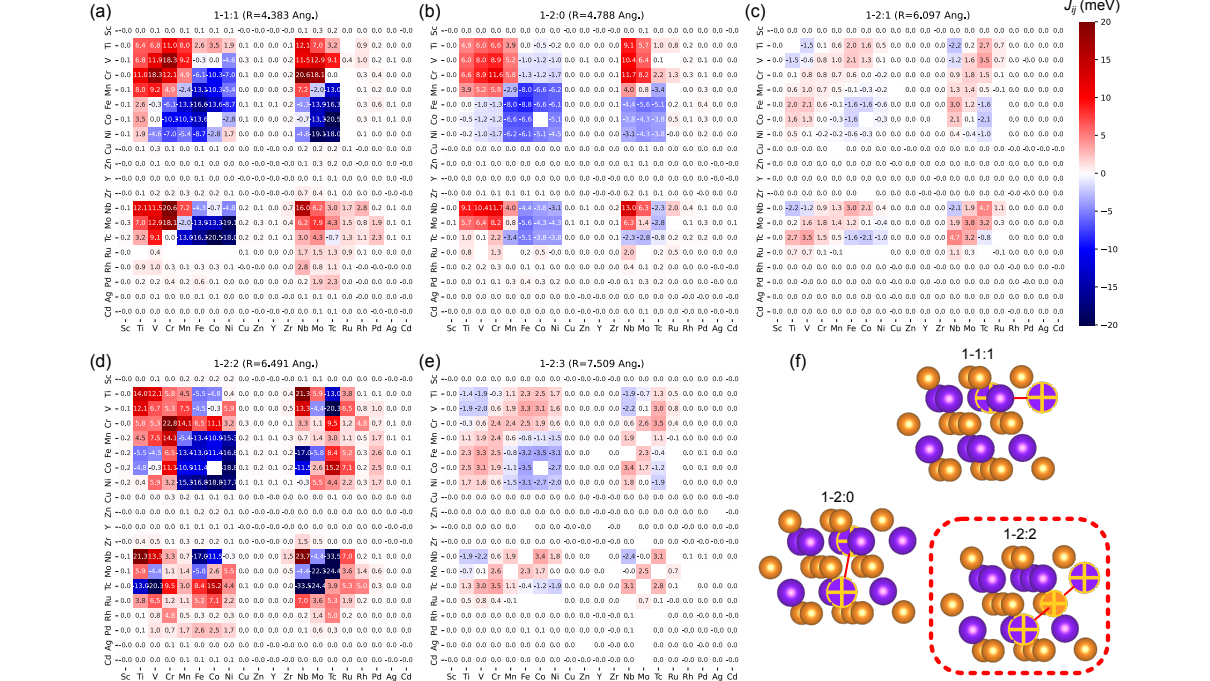


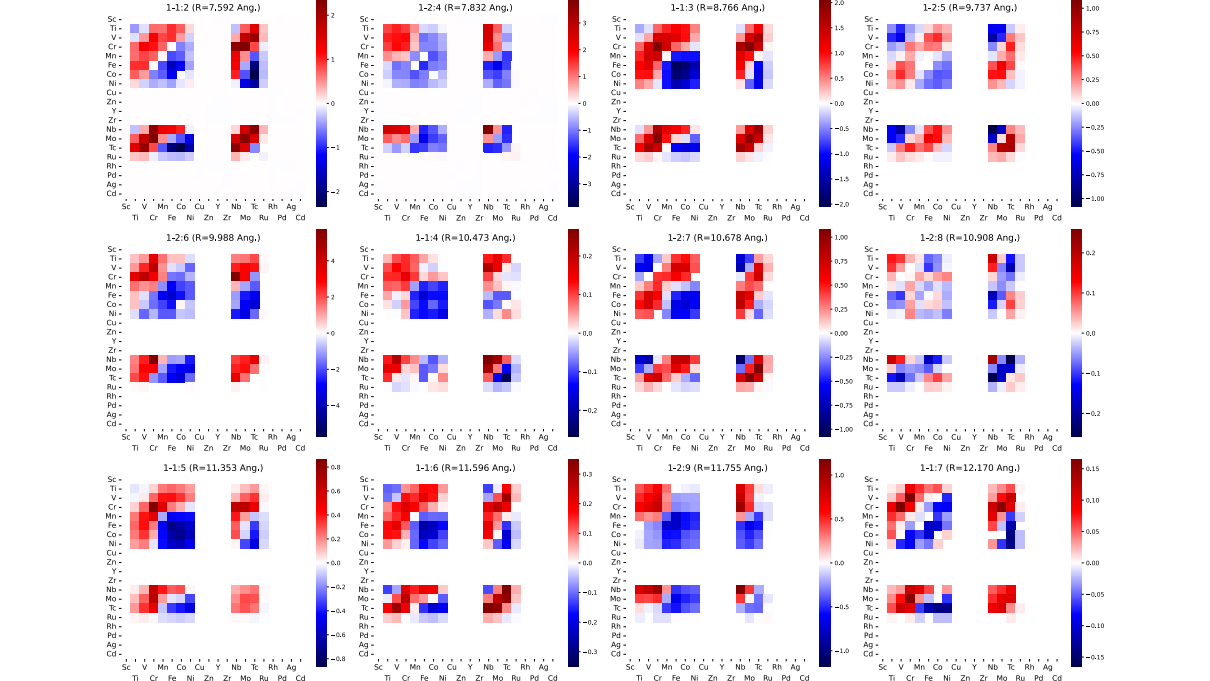
Extended Heisenberg Hamiltonian. $H = -\frac{1}{2}\sum_{i,j} J_{ij}\,\vec{S}_i \cdot \vec{S}_j - \frac{1}{2}\sum_{i,j} \vec{D}_{ij} \cdot \left(\vec{S}_i \times \vec{S}_j\right)$

Exchange constants from method of infinitesimal rotations[1]. $\mathcal{J}_{ij} = -\frac{1}{\pi}\,\mathrm{Im}\int_{-\infty}^{E_F} \mathrm{d}E\,\mathrm{Tr}[\delta t_i G_{ij} \delta t_j G_{ji}]$

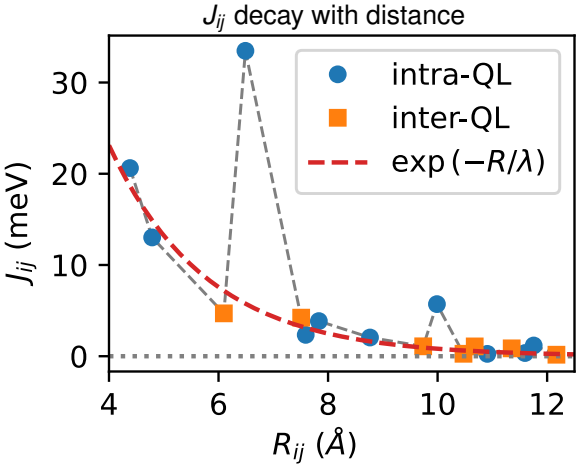
[1] Liechtenstein et al. 1987.

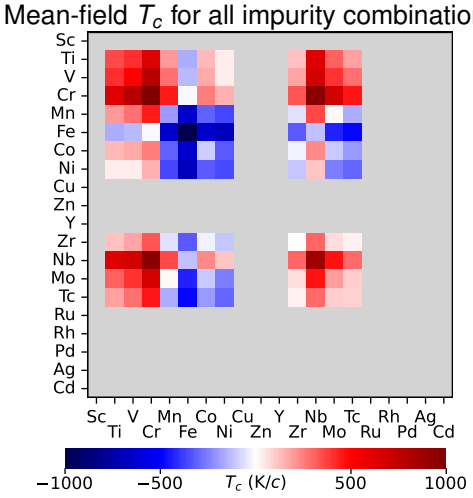
[2] Rüßmann, Bertoldo, and Blügel 2021.


(a)
1-1:1 (R=4.383 Ang.)
(b)
1-2:0 (R=4.788 Ang.)
(c)
1-2:1 (R=6.097 Ang.)
J_{ij} (meV)
20
15
10
5
0
−5
−10
−15
−20
(d)
1-2:2 (R=6.491 Ang.)
(e)
1-2:3 (R=7.509 Ang.)
(f)
1-1:1
1-2:0
1-2:2
Sc Ti V Cr Mn Fe Co Ni Cu Zn Y Zr Nb Mo Tc Ru Rh Pd Ag Cd


1-1:2 (R=7.592 Ang.)
1-2:4 (R=7.832 Ang.)
1-1:3 (R=8.766 Ang.)
1-2:5 (R=9.737 Ang.)
1-2:6 (R=9.988 Ang.)
1-1:4 (R=10.473 Ang.)
1-2:7 (R=10.678 Ang.)
1-2:8 (R=10.908 Ang.)
1-1:5 (R=11.353 Ang.)
1-1:6 (R=11.596 Ang.)
1-2:9 (R=11.755 Ang.)
1-1:7 (R=12.170 Ang.)
Sc V Mn Co Cu Y Nb Tc Rh Ag
Ti Cr Fe Ni Zn Zr Mo Ru Pd Cd

Long-range magnetic ordering





JÜLICH Forschungszentrum

Machine learning exchange interactions

Main idea

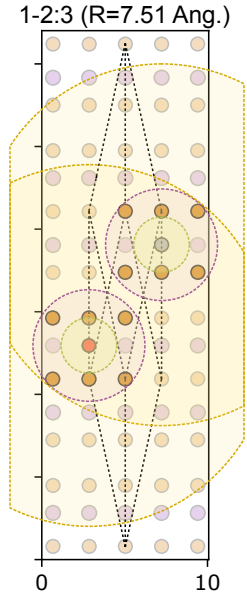
- Use ML potentials to fit the isotropic exchange interaction.

$$E_k = \sum_k E_k \longrightarrow J_{ij} = \sum_k \left(J_{ij}\right)_k$$

- Represent only the finite dimer clusters with $r_{\text{cut}}^{(\text{KKR})} \sim r_{\text{cut}}^{(\text{ML})}$

Challenges

- No MD, ground-state DFT only; enough variability?
- J_{ij} surface probably less smooth than a PES
- Tens of chemical elements, small dataset
- Small energy range (meV and below)
- Mix of non- / -periodic systems
- Transferability from dimer to n-mer clusters



Machine learning exchange interactions

Model selection

Model	Citation	Type	CSSP	NN	Defects	Spin	Symmetry
AutoML	Conrad et al. 2022	Composition	X			-	-
Coulomb matrix	Rupp et al. 2012	Descriptor				-	explicit
SOAP	Bartók, Kondor, and Csányi 2013	Descriptor				-	explicit
Alchemical SOAP	Lopanitsyna et al. 2023	Potential	X			-	explicit
Disordered SOAP	Sommer et al. 2023	Descriptor			X	-	explicit
GAP	Bartók, Payne, et al. 2010	Potential	X			?	explicit
ACE	Bochkarev et al. 2022	Potential				-	explicit
MEGNetSparse	Kazeev et al. 2023	Potential	X	X	X	-	explicit
MACE	Batatia, Kovács, et al. 2022	Potential	X	X		-	explicit
MACE-MP	Batatia, Benner, et al. 2023	UIP	X	X		-	explicit
Magnetic ACE	Rinaldi et al. 2024	Potential				noco	explicit
SpinGNN++	Yu et al. 2024	Potential	X	X		noco	explicit
CHGNet	Deng et al. 2023	UIP	X	X		coll	explicit
SNRep	Domina, Cobelli, and Sanvito 2022	Potential				coll	explicit
PET	Pozdnyakov and Ceriotti 2024	Potential	?	X		coll	approximate

Machine learning exchange interactions

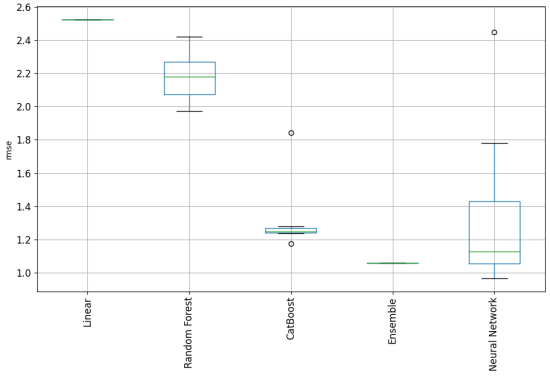
Results AutoML

"BaseLine" model with composition-based descriptor (`CBFV` package) with 318 tabulated features. `[r_distance, ..., dev_Atomic_Weight, ..., max_Boiling_Point_(K), ...]`.

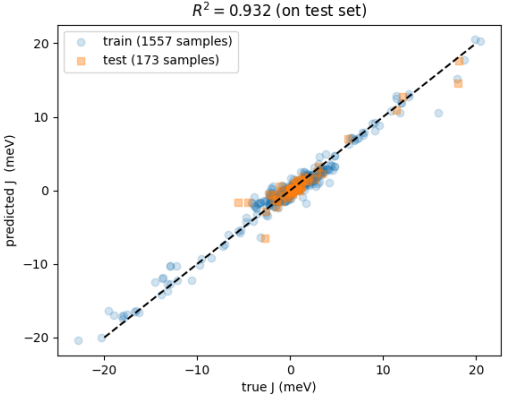
Model training with 

package's "Perform" mode. 90/10 train-test split, five models, 5-fold CV, Shuffle, Stratify.

Leaderboard performance.



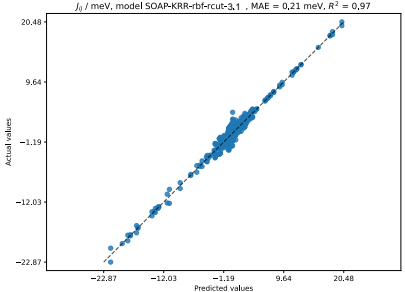
Best model on test set.



Machine learning exchange interactions

Results SOAP

Model SOAP+KRR
Training 80-20 train-test split, 5-fold CV
Best model $\mathrm{MAE} = 0.21$ meV, $\mathrm{R}^2 = 0.97$

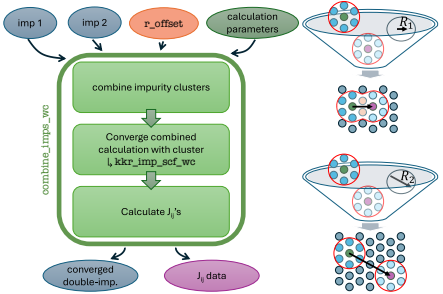


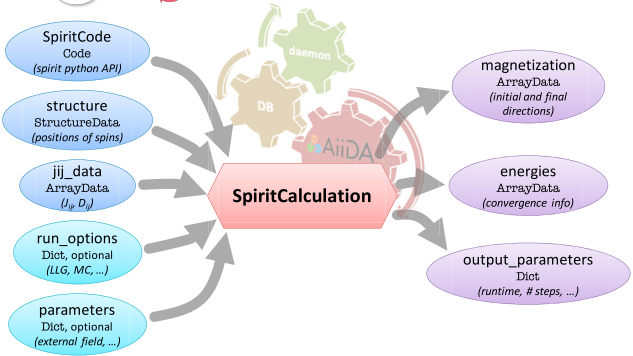
	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	
Sc	0	0.012	0.056	0.039	0.083	0.14	0.085	0.051	0	0	0	0	0.1	0.25	0.18	0	0	0	0	0	Sc
Ti	0.012	6.3	6.7	11	7.9	3	4.1	1.9	0.064	0	0	0.1	12	6.9	3.2	-1	0.83	0.2	0.025	0	Ti
V	0.055	6.6	12	18	9.1	0.65	1.3	-4.6	0.29	0.053	0.021	0.17	11	13	9.1	0.44	1	0.16	0.099	0.013	V
Cr	0.04	11	19	12	4.8	-6.6	-12	-7	0.061	0.048	0.021	0.15	20	18	0.079	-0.24	0.26	0.36	0.017	0.022	Cr
Mn	0.082	7.7	8.8	4.8	-2.4	-13	-12	-5.4	0.036	0.036	0.034	0.25	7.2	-2	-13	-3.6	0.092	0.17	0.013	0.023	Mn
Fe	0.11	2.6	-0.58	-5.5	-13	-20	-17	-8.5	0.1	0.051	0.06	0.16	-4.2	-14	-16	-1.9	0.25	0.55	0.063	0.042	Fe
Co	0.063	3.4	-0.34	-9.7	-11	-17	-14	-3.2	0.12	0.013	0.028	0.18	-0.61	-13	-20	-3.7	0.27	0.085	0.054	0.012	Co
Ni	0.05	1.4	-5.6	-7.2	-5.6	-9.6	-2.7	1.7	0.015	0	0.019	0.13	-4.7	-19	-18	-2.8	0.082	0.042	0	0	Ni
Cu	0	0.062	0.28	0.055	0.035	0.1	0.11	0.012	0	0	0	0	0.15	0.24	0.2	0.08	0	0	0	0	Cu
Zn	0	0	0.056	0.048	0.036	0.077	0.021	0	0	0	0	0	0.07	0.27	0.2	0	0	0	0	0	Zn
Y	0	0	0.021	0.021	0.034	0.074	0.038	0.019	0	0	0	0	0.029	0.12	0.11	0	0	0	0	0	Y
Zr	0	0.11	0.18	0.14	0.26	0.2	0.22	0.14	0	0	0	0	0.63	0.37	0.13	0	0	0	0	0	Zr
Nb	0.1	12	11	20	7.4	-3.9	0.024	-3.9	0.16	0.066	0.028	0.61	16	6.2	3	1.7	2.8	0.15	0.049	0.013	Nb
Mo	0.25	6.8	13	18	-1.8	-15	-14	-18	0.26	0.26	0.12	0.37	6.4	7.8	4.3	1.5	0.76	1.9	0.068	0.12	Mo
Tc	0.18	3.8	9.6	1.1	-13	-18	-23	-18	0.2	0.2	0.11	0.13	4.3	4.5	-0.72	1.2	1.1	2.3	0.12	0.14	Tc
Ru	0	-0.8	0.58	-1.1	-4.8	-1.3	-3.6	-2.8	0.076	0.01	0	0	1.6	1.7	1.5	0.87	0.048	0.017	0.038	0.011	Ru
Rh	0	1	1.1	0.24	0.099	0.23	0.23	0.065	0	0	0	0	3.2	0.75	1.4	0.051	0	0	0	0	Rh
Pd	0	0.16	0.24	0.44	0.22	0.89	0.14	0.049	0	0	0	0	0.18	2.4	2.3	0.015	0	0	0	0	Pd
Ag	0	0.024	0.093	0.015	0.013	0.063	0.052	0	0	0	0	0	0.046	0.064	0.12	0.039	0	0	0	0	Ag
Cd	0	0	0.014	0.022	0.023	0.041	0.019	0	0	0	0	0	0.014	0.13	0.14	0.011	0	0	0	0	Cd
	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	

10 5 0 −5 −10 −15

J_{ij} / meV

Spin dynamics with AiiDA-spirit [1]





Liechtenstein formula (ML target)

$$\mathcal{J}_{ij} = -\frac{1}{\pi}\,\mathrm{Im}\int_{-\infty}^{E_F} \mathrm{d}E\,\mathrm{Tr}[\delta t_i G_{ij} \delta t_j G_{ji}]$$

Landau-Lifshitz-Gilbert equation

$$\frac{\partial \vec{S}_i}{\partial t} = -\gamma' \vec{S}_i \times \vec{B}_i^{\mathrm{eff}} - \lambda \vec{S}_i \times \left(\vec{S}_i \times \vec{B}_i^{\mathrm{eff}}\right)$$

judft.de

[1] Rüßmann, Ribas Sobreviela, et al. 2022.

Machine learning exchange interactions

Tensorial interaction

Heisenberg Hamiltonian in tensor form.

$$\mathcal{H}_H = -\sum_{j>i} \vec{m}_i \cdot \mathcal{J}_{ij} \vec{m}_j$$

Tensor components: isotropic, anti-symmetric (DMI) and anisotropic or traceless symmetric part (neglected).

$$\mathcal{J}_{ij} = J_{ij}\mathbb{1} + \mathcal{J}_{ij}^A + \mathcal{J}_{ij}^S$$

with $J_{ij}^{xx} = J_{ij}^{yy} = J_{ij}^{zz} = \frac{1}{3} J_{ij}$ and

$$\mathcal{J}_{ij}^A = \begin{bmatrix} 0 & J_{ij}^{xy} & J_{ij}^{xz} \\ J_{ij}^{yx} & 0 & J_{ij}^{yz} \\ J_{ij}^{zx} & J_{ij}^{zy} & 0 \end{bmatrix} = \begin{bmatrix} 0 & J_{ij}^{xy} & -J_{ij}^{zx} \\ -J_{ij}^{xy} & 0 & J_{ij}^{yz} \\ J_{ij}^{zx} & -J_{ij}^{yz} & 0 \end{bmatrix} = \begin{bmatrix} 0 & -D_{ij}^{z} & D_{ij}^{y} \\ D_{ij}^{z} & 0 & -D_{ij}^{x} \\ -D_{ij}^{y} & D_{ij}^{x} & 0 \end{bmatrix}$$

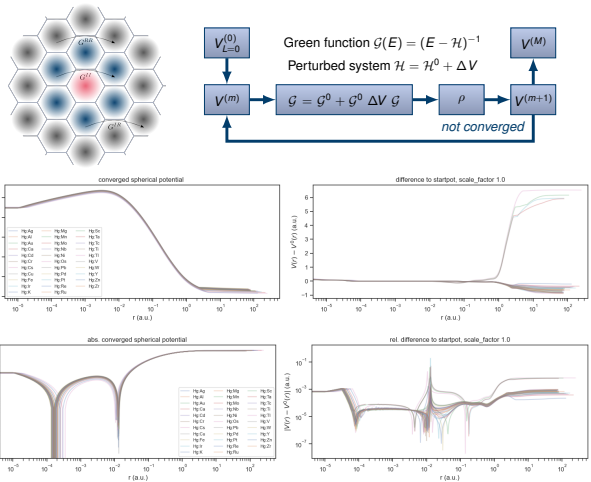
Electronic structure emulator

Task Predict electron potential difference $\Delta V_{imp}(\vec{r})$ & use as initial guess for AiiDA-KKR

Data 10'000 single impurity in elemental crystal combinations (60 $\times$ 40 elements) from DFT

Challenges

- **Collaboration** Adapt the linear Jacobi-Legendre Charge Density Model (JLCDM)[a] to all-electron DFT
  - Large chemical feature space
  - From radial to full equivariant potential
  - Intermediate SCF results
  - Should be code-agnostic
  - From collinear to noco magnetism

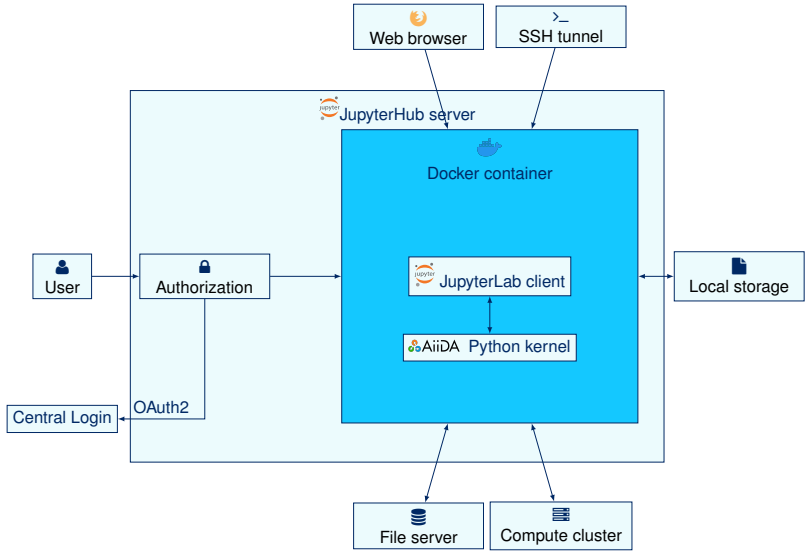


Spherical impurity potentials in first Voronoi cell of Hg:X embeddings, left upper to bottom right: V, $V - V^0$, $|V|$, $|V - V^0|$.

[a] Focassio et al. 2023.

Reproducible software environments

Problem with AiiDA: High setup cost ☹ Solution: Portable, self-hosted cloud computing ☺



Community resources

Best of atomistic machine learning

Largest list of atomistic ML tools on the web (350+), auto-ranked, regular updates

go.fzj.de/baml

Contents

Community resources

The DAEMON Network

Join via

cost-daemon.eu

European network for data-driven materials science

WG1: Community standards: data, workflows and codes for materials design.

WG2: Representations and algorithms for materials design for “single-modality” use.

WG3: Multi-modal machine learning methods for advanced materials design.

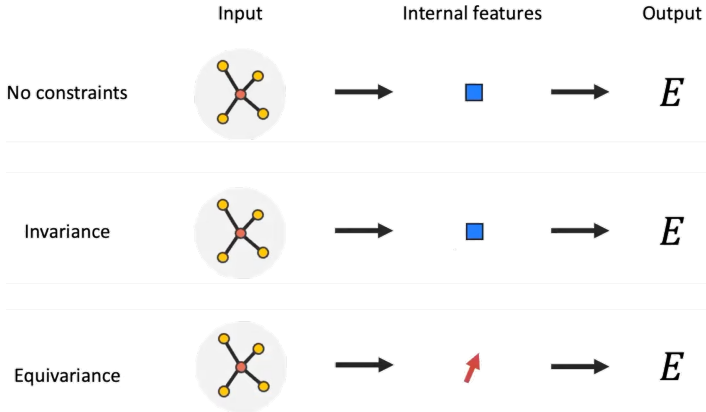
WG4: Process-structure-property relationships in materials. Novel insights and applications.

WG5: Training, Dissemination, Exploitation, Outreach

Discussion slides

Inductive bias

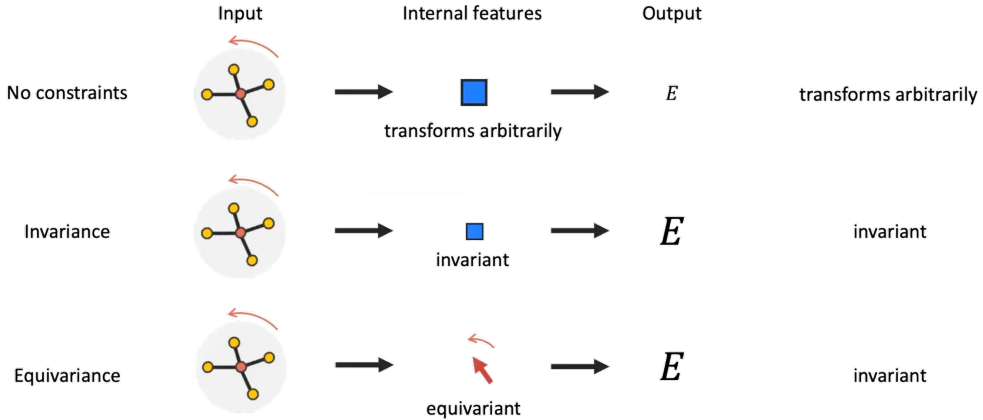
Example: O(3) symmetry



[1] Adapted from (Musaelian 2023)

Inductive bias

Example: O(3) symmetry



[1] Adapted from (Musaelian 2023)

Feature engineering

Example: O(3)-invariant SOAP

Descriptor: 3-body

Smooth overlap of atomic positions (SOAP)[a]

Feature vector $\phi(A) = \mathbf{p} \in \mathbb{R}^n$

Model: Kernel regression

Kernel $\kappa(A, A') = \langle \phi(A), \phi(A') \rangle_{\mathcal{F}} = \langle \mathbf{p}, \mathbf{p}' \rangle_{\mathcal{F}} \in \mathbb{R}$

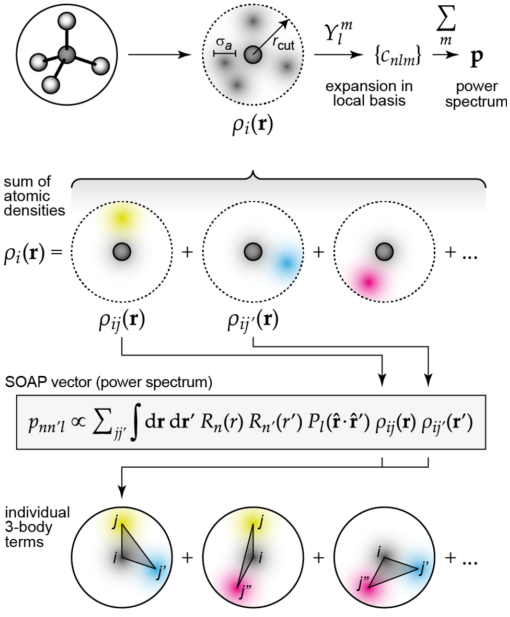
Gram matrix $\mathbf{K} = \left(\kappa(A^{(i)}, A^{(j)}) \right)_{i,j} \in \mathbb{R}^{m \times m}$

Cost function $\mathcal{C}(\mathbf{y}, \hat{\mathbf{y}}) = ||\mathbf{y} - \hat{\mathbf{y}}||^2 + \alpha\, \mathbf{c}^\intercal\, \mathbf{K}\, \mathbf{c}$

Training $\mathbf{c} = (\mathbf{K} + \alpha\, \mathbf{I}_m)^{-1} \mathbf{y}$

Inference $\hat{y}(A) = \sum_i^m c_i\, \kappa(A, A^{(i)})$

[a] Adapted from (Deringer et al. 2021)



Feature learning

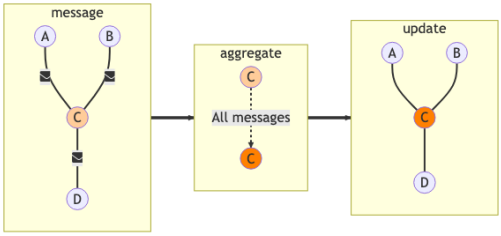
Example: O(3)-equivariant MPNN

Model: Graph neural network

Message-passing formalism (MPNN)

1. Message $\mathbf{m}_{ij}^{(t)} = \mathcal{M}\left(\mathbf{h}_i^{(t)}, \mathbf{h}_j^{(t)}, \mathbf{e}_{ij}\right)$
2. Aggregation $\hat{\mathbf{m}}_i = \bigoplus_{j \in \mathcal{N}_i} \mathbf{m}_{ij}$
3. Update $\mathbf{h}_i^{(t+1)} = \phi\left(\mathbf{h}_i^{(t)}, \hat{\mathbf{m}}_i^{(t)}\right)$

Where $\mathbf{h}_i^{(t)}$ node features at step t, $\mathbf{e}_{ij}$ edge features, $\mathcal{N}_i$ neighborhood of node i, ϕ update function.



Equivariance

Internal features $\mathbf{h}_i$ transform under rotations $Q \in \mathrm{O}(3)$.

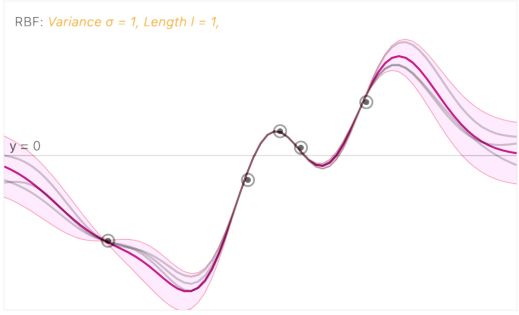
$$h^{(t)}_{i,klm}(Q \cdot \mathbf{R}) = \sum_{m'} D^{l}_{mm'}(Q) h^{(t)}_{i,klm'}(\mathbf{R})$$

Where k feature index, $\mathbf{R}$ atom positions, D^l Wigner D-matrix, $l = 0$ invariant scalars.

Active learning

Materials space too large for true generalizability → Couple data generation & model training

- AL improves data efficiency drastically[a]
- Offline AL: Test on simulations, manual. Online AL: Model has built-in uncertainty prediction → automatable retraining.
- Uncertainty methods: Ensemble learning (indirect), Bayesian (direct, e.g. Gaussian process)
- Sampling criteria: uncertainty (min. error), dissimilarity measure (max. diversity), ...



[a] Jinnouchi et al. 2019.

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