



# From physics to physics-AI hybrids in quantum materials simulation

September 10, 2024 | **Johannes Wasmer**<sup>1</sup>   Philipp Rüßmann<sup>2,1</sup>   Ira Asent<sup>3</sup>   Stefan Blügel<sup>1</sup> | <sup>1</sup>Forschungszentrum Jülich   <sup>2</sup>University of Würzburg   <sup>3</sup>Aarhus University

Talk held at HDS-LEE Retreat 2024 ([URL](#)).

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

What is the most important problem,  
right now?\*

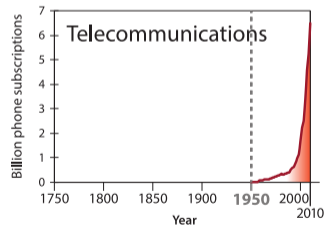
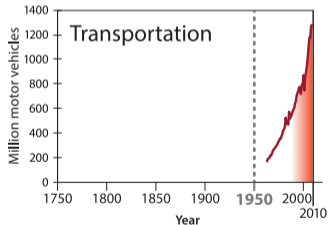
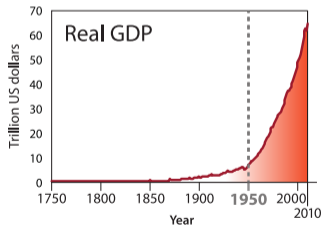
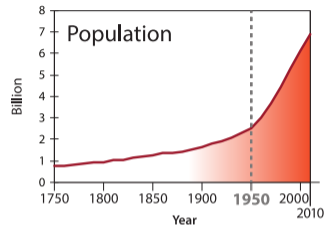
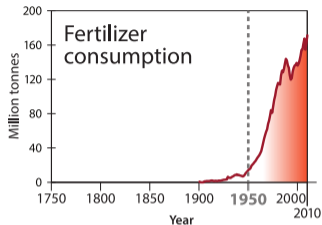
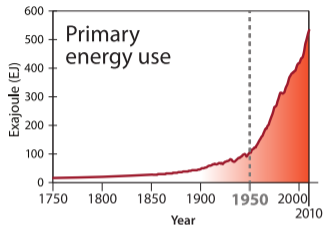
What is the most important problem,  
right now?\*

\*imho

# The most important problem

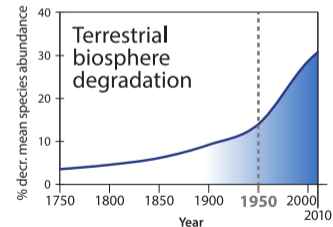
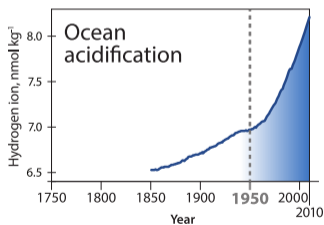
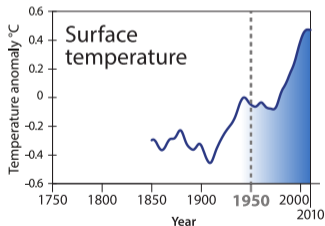
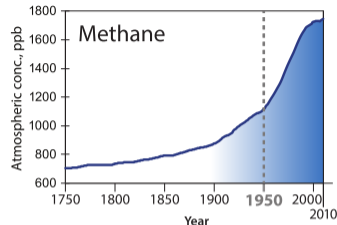
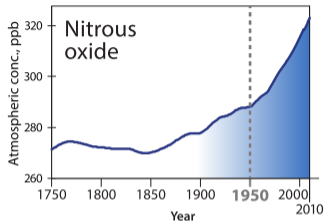
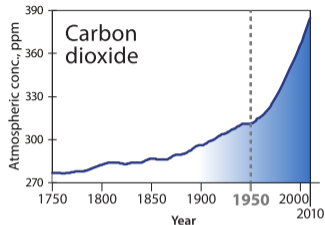
The  
Great Acceleration

# Socio-economic trends<sup>1</sup>



<sup>1</sup>Steffen et al. 2015.

# Earth system trends<sup>1</sup>



<sup>1</sup>Steffen et al. 2015.

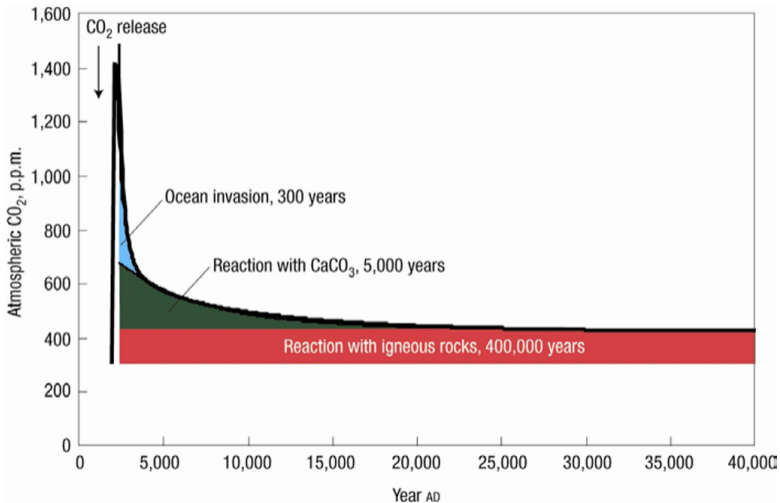
# The most important problem

The  
Great Acceleration



Changes Earth's  
atmosphere

# How long will the change last?



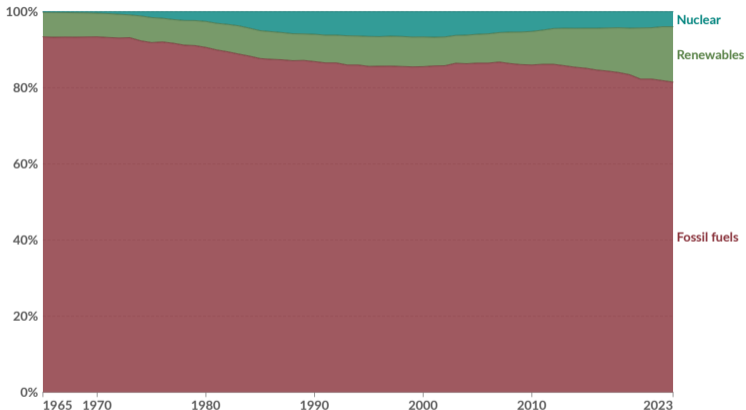
Model simulation of atmospheric CO<sub>2</sub> concentration from combustion of fossil fuels<sup>a</sup>.

<sup>a</sup>Inman 2008.

# The most important problem



# We are 20 percent done



Data source: Energy Institute - Statistical Review of World Energy (2024)

OurWorldInData.org/energy | CC BY

Primary energy consumption from fossil fuels, nuclear and renewables, World<sup>a</sup>.

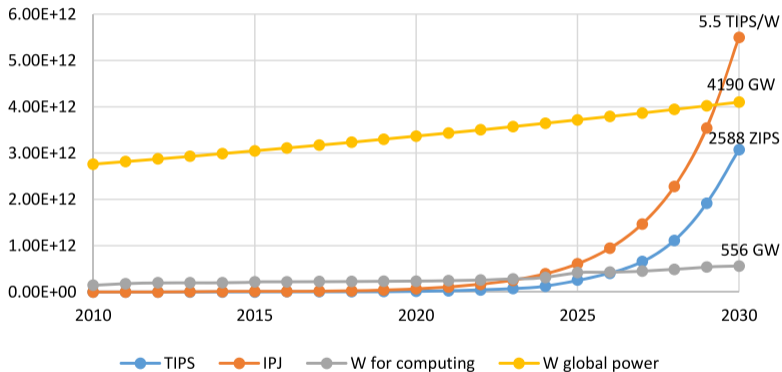
<sup>a</sup>Ritchie, Rosado, and Roser 2024.

# The most important problem



## Example: The Energy Challenge in Information Technology

### Overall power use



Computing power trends in relation to global power consumption 2010 to 2030. The share rises from 5 to 15 % from 2010 to 2030<sup>a</sup>.

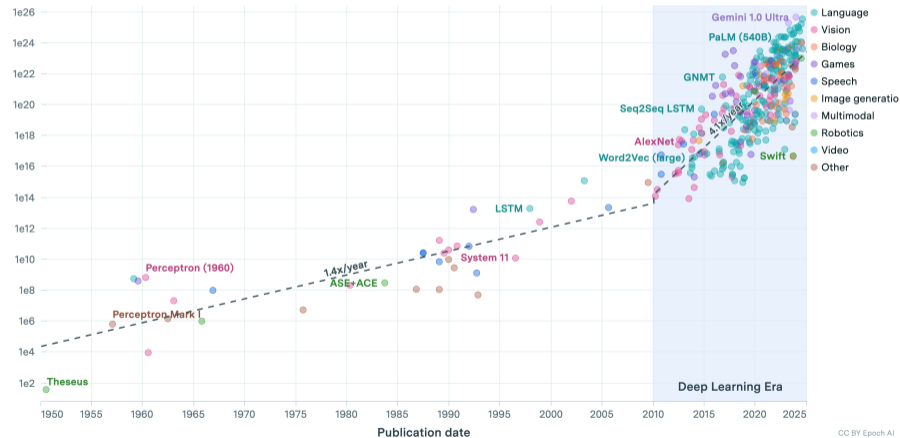
<sup>a</sup>Andrae 2020.

# Example: The Energy Challenge in Information Technology

## Notable AI Models



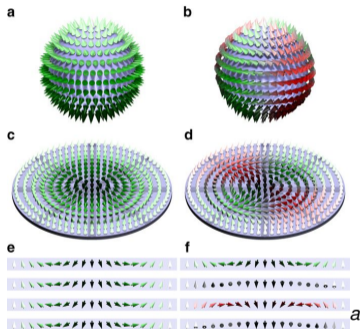
Training compute (FLOP)



<sup>1</sup> Sevilla et al. 2022.

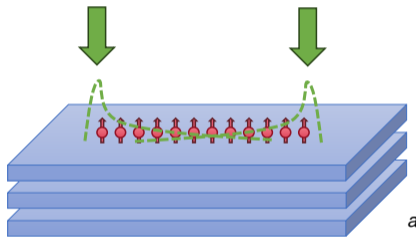
# A disruptive technology: Quantum Materials

Precise control of the electron spin will enable ultra-low power, neuromorphic and quantum computing



Magnetic skyrmion

<sup>a</sup>Hoffmann et al. 2017.



Majorana zero modes

<sup>a</sup>Rüßmann, Silva, et al. 2023.

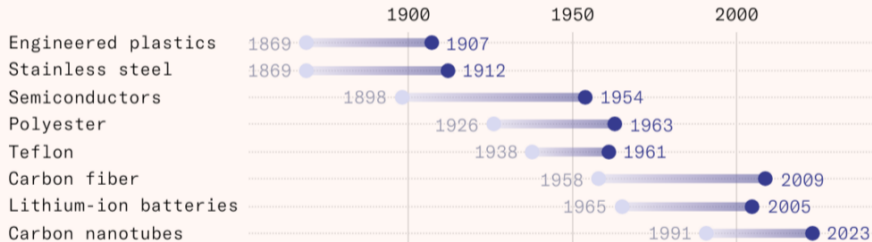
# The most important problem



# Materials discovery is too slow

Materials take decades to make it out of the lab

Time between invention and charismatic application



The year of charismatic application refers to when the material became a key component of a mainstream product. This definition is inherently nebulous.

Source: Reinhardt (2024)

# The most important problem



# Accelerate materials discovery

With emerging scientific paradigms

1st Paradigm



Observation

2nd Paradigm

$$H\Psi = E\Psi$$

Theory

3rd Paradigm



Simulation

4th Paradigm



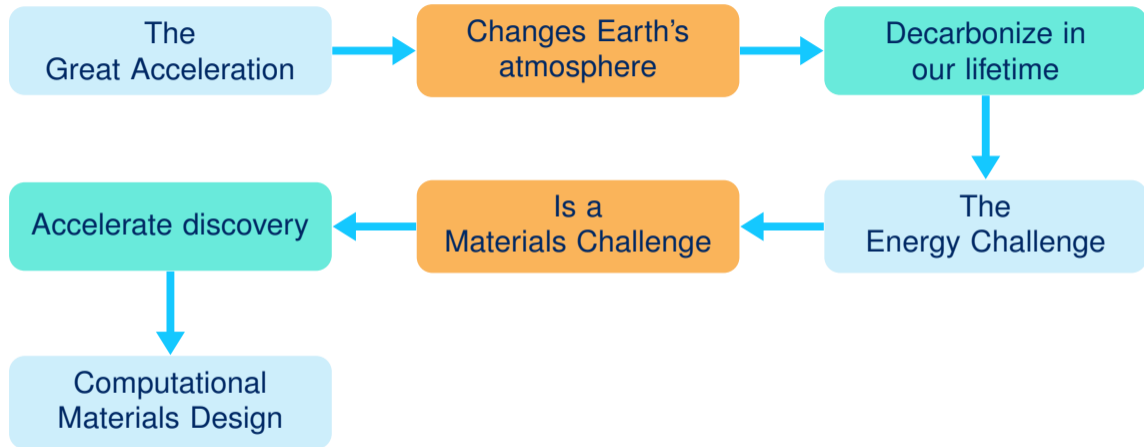
Data Science

5th Paradigm



Emulation

# The most important problem



# First-principles electronic structure methods

*“The underlying laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that exact applications of these laws lead to equations which are too complicated to be soluble.”*

*P.M.A. Dirac, Proceedings of the Royal Society A123, 714 (1929)*



**Schrödinger equation**

$$\mathcal{H} |\Psi\rangle = E |\Psi\rangle, \quad \Psi(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N)$$

$$\mathcal{O}(3^N)$$

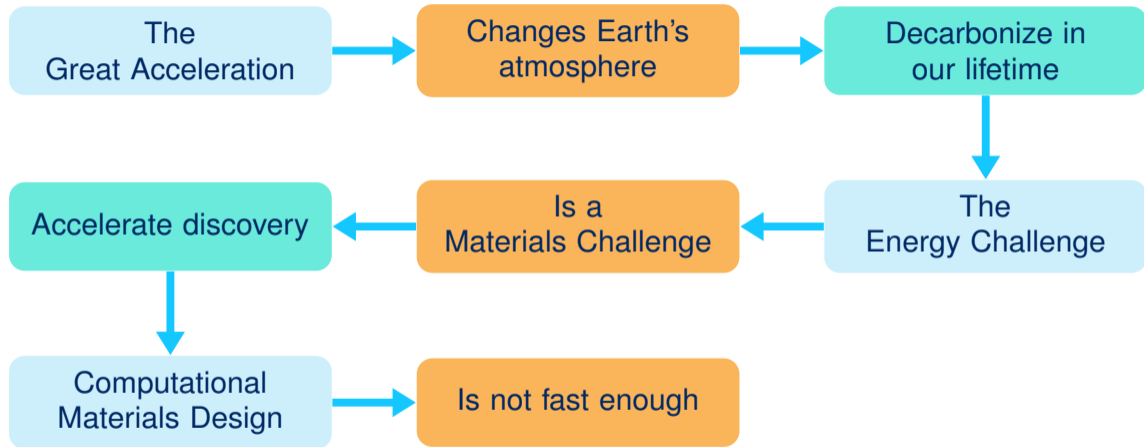


**Density functional theory**

$$(-\nabla_i^2 + v_{\text{eff}}(\mathbf{r})) \varphi_i(\mathbf{r}) = \varepsilon_i \varphi_i(\mathbf{r})$$

$$\mathcal{O}(N_{\text{el}}^3)$$

# The most important problem



# “Big AI” has joined the game

Google DeepMind

RESEARCH

Millions of new materials  
discovered with deep learning

Research

< Return to Blog Home

Microsoft Research Blog

## MatterSim: A deep-learning model for materials under real-world conditions

Published May 13, 2024

By [Han Yang](#), Senior Researcher; [Jielan Li](#), Researcher 2; [Hongxia Hao](#), Senior Researcher;  
[Ziheng Lu](#), Principal Researcher

Meta

Discover  
climate  
change  
solutions  
with AI

## Open Catalyst

AI at Meta and Carnegie Mellon University join forces to find more  
efficient and scalable ways to store and use renewable energy.

Orbital Materials

Introducing ‘Orb’ - the world’s  
fastest and most accurate AI model  
for simulating advanced materials

September 3, 2024  
Jonathan Godwin

MATLANTIS

Matlantis™ supports  
companies exploring innovative materials  
for a sustainable  
future.

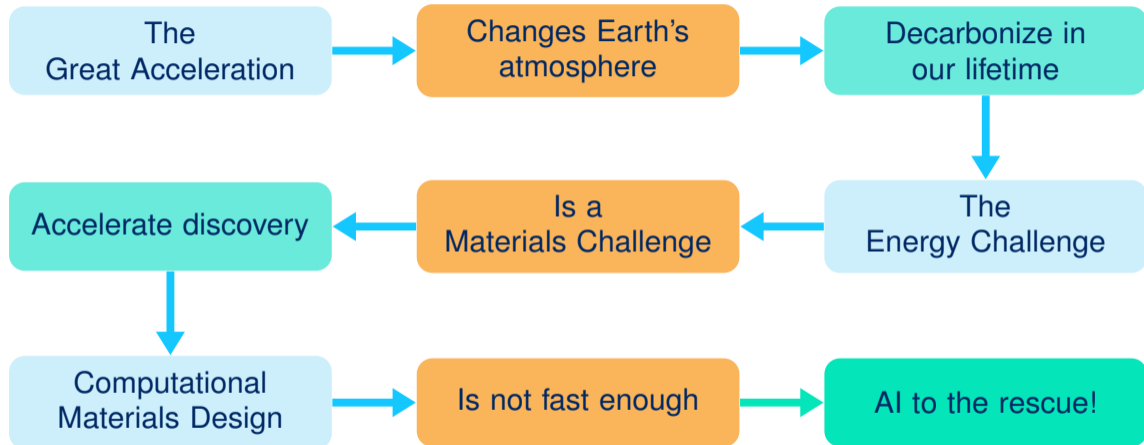
Out of  $10^{60}$  functional molecules that are theoretically possible,  
mankind has discovered only a handful of useful materials.  
Powered by an AI technique known as deep learning, Matlantis sheds  
light on promising candidates in the vast ocean of unknown  
molecules with its high-speed, versatile atomistic simulation.

DP Technology

Advancing AI for

DP Technology is a pioneer  
leverages AI to learn and ap  
in scientific research and ind

# The most important problem



# All-electron DFT is the gold standard

A frontier for electronic structure machine learning, developed in Jülich

*Fleur*

*JuKKR*

 spirit

 AiiDA

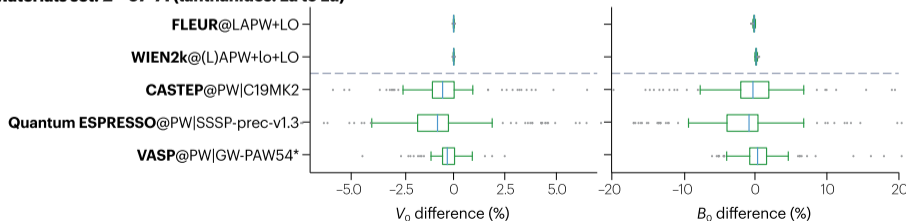
judft.de

//



JuDFTteam

Materials set: **Z = 57–71 (lanthanides: La to Lu)**

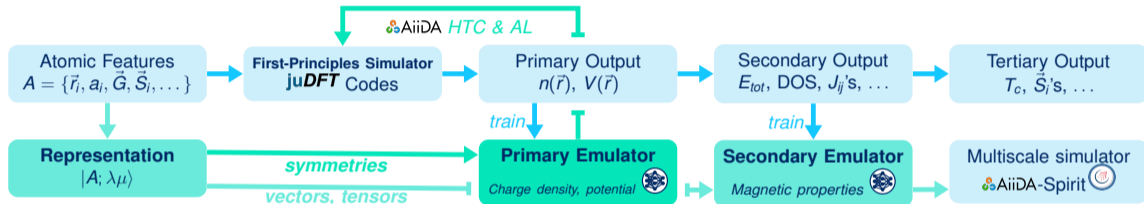


Discrepancy of the equilibrium volume  $V_0$ , the bulk modulus  $B_0$  across popular DFT codes<sup>a</sup>

<sup>a</sup>Bosoni et al. 2024.

# The full proposed hybrid physics/AI pipeline

For all-electron DFT codes



Electronic structure learning  
for fast SCF convergence

Magnetic property prediction  
for spin dynamics simulation

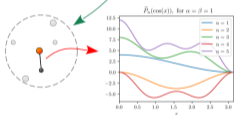
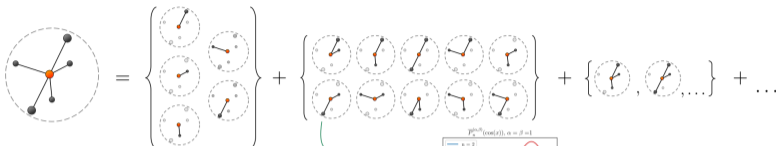
# Electronic structure learning

Body order:

2B

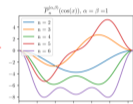
3B

4B



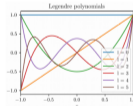
Constrained distances expansion:

$$\tilde{P}_n^{(\alpha,\beta)}(\cos(x))$$



Constrained distances expansion:

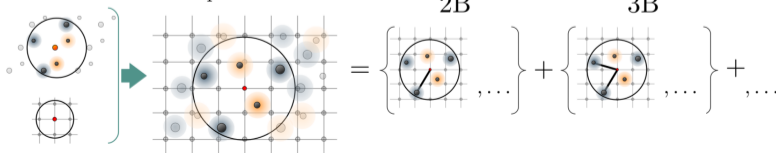
$$\tilde{P}_n^{(\alpha,\beta)}(\cos(x))$$



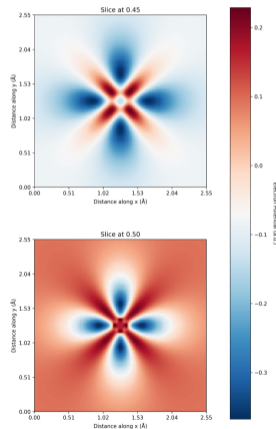
Angular expansion:

$$P_l(\cos(\theta))$$

Grid centered representation

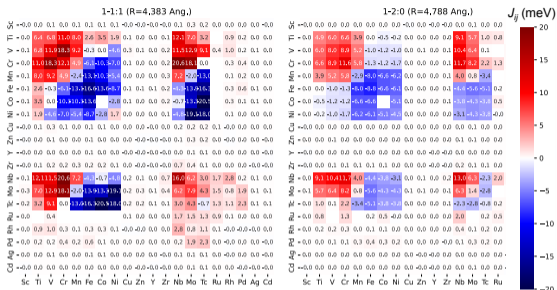


Extension of the Jacobi-Legendre framework<sup>a</sup> to all-electron potentials



<sup>a</sup>Domina 2024.

# Magnetic property prediction

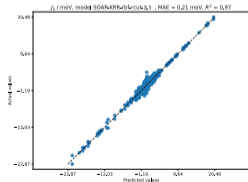
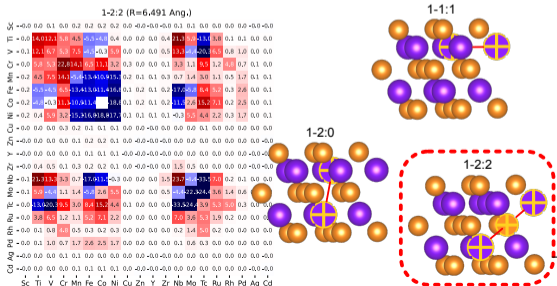


AiiDA-KKR database of transition metal defects embedded into a topological insulator, in review<sup>a</sup>

Benchmark study of ML interatomic potentials trained on the exchange interaction  $J_{ij}$  for spin dynamics, ongoing

$$\mathcal{J}_{ij} = -\frac{1}{\pi} \text{Im} \int_{-E_F}^{E_F} dE \text{Tr}[\delta t_i G_{ij} \delta t_j G_{ji}] \longrightarrow$$

$$H = -\frac{1}{2} \sum_{i,j} J_{ij} \vec{S}_i \cdot \vec{S}_j \longrightarrow J_{ij} = \sum_k (J_{ij})_k$$



Data size 2'000 calculations  
Model SOAP+KRR  
Best model MAE = 0.21,  
 $R^2 = 0.97$

<sup>a</sup>Mozumder et al. 2024.

# Acknowledgment

## Collaborations

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## Support

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# Community resources

## Best of atomistic machine learning



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

[go.fzj.de/baml](https://go.fzj.de/baml)

<sup>a</sup>Wasmer et al. 2023.

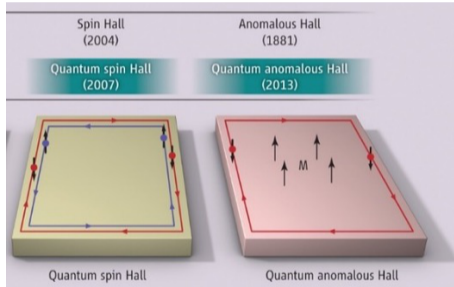
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Discussion slides

# Topological insulators and magnetic impurities

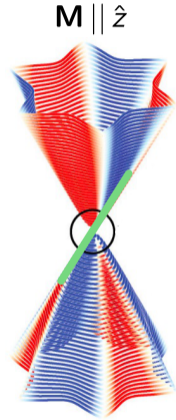
- Magnetic doping of topological insulators (**TIs**) can induce a topological phase transition
  - Ferromagnetic ordering
  - Out-of-plane anisotropy



(QSHE)  
→ Topological insulator  
*Two counter propagating  
edge states*

(QAHE)  
*One single edge state*

S. Oh, Science 340, 153 (2013)

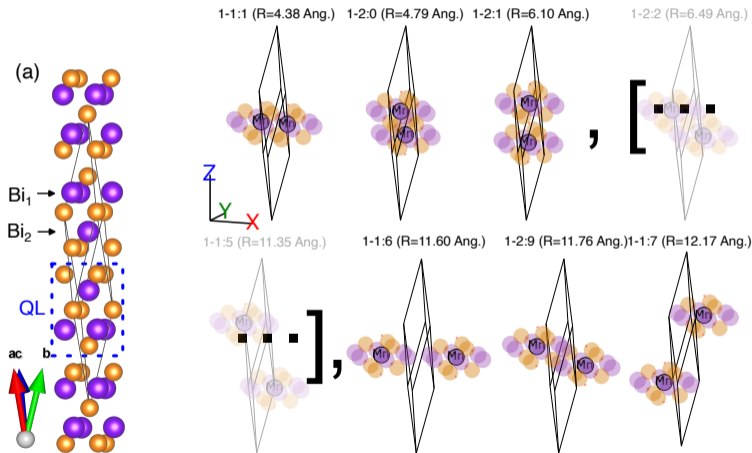


Henk et al., PRL 109, 076801 (2012)

# Magnetic co-doping of topological insulators<sup>1</sup>

$\text{Bi}_2\text{Te}_3$

Dimer clusters of 3d, 4d transition metal defects



Single-impurity database, N=2'000.

[go.fzj.de/judit](http://go.fzj.de/judit)

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

Co-doping can help to control

- critical  $T_c$  of QAHE
- exchange splitting  $\Delta_{xc}$
- long-range magnetic ordering

for applications in spintronics and fault-tolerant quantum computing.

<sup>1</sup>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

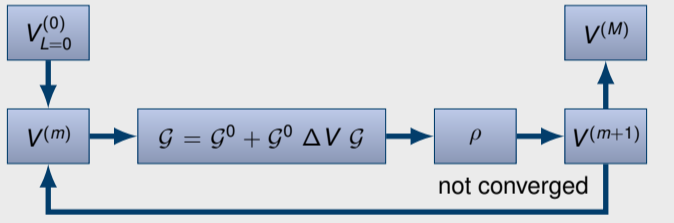
Green function

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

Perturbed system

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

## The KKR SCF cycle

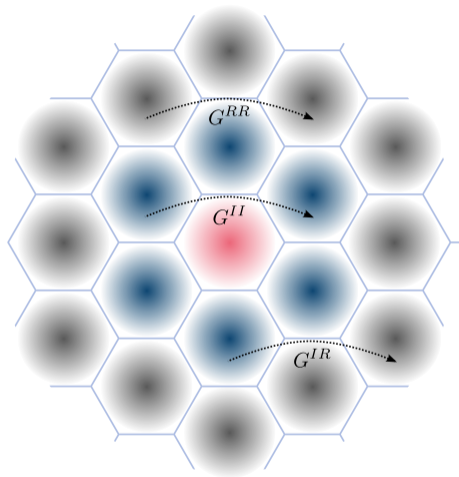


Observables  $\langle \mathcal{O} \rangle =$   

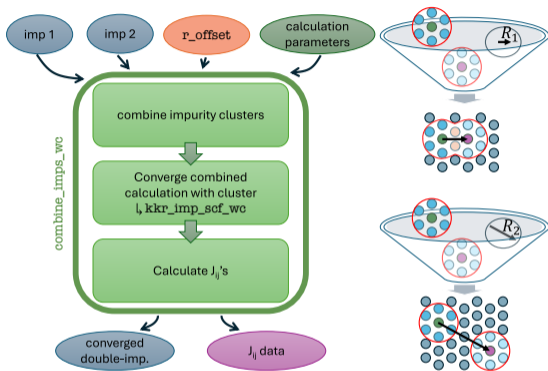
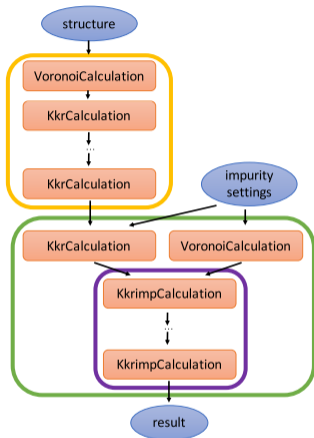
$$-\frac{1}{\pi} \text{Im} \text{Tr} \int_{-\infty}^{E_F} dE \mathcal{O} G(E)$$

Electron density  $\langle \rho(\mathbf{r}) \rangle =$   

$$-\frac{1}{\pi} \text{Im} \int_{-\infty}^{E_F} dE G(\mathbf{r}, \mathbf{r}, E)$$



# AiiDA-KKR workflows<sup>2</sup>

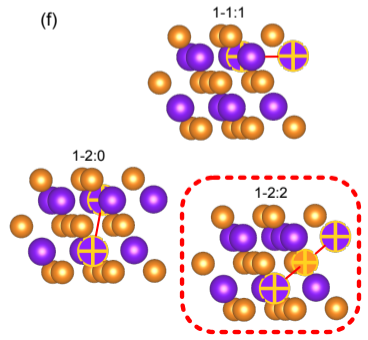
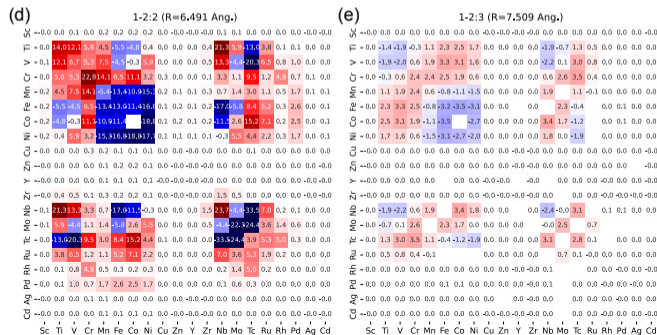
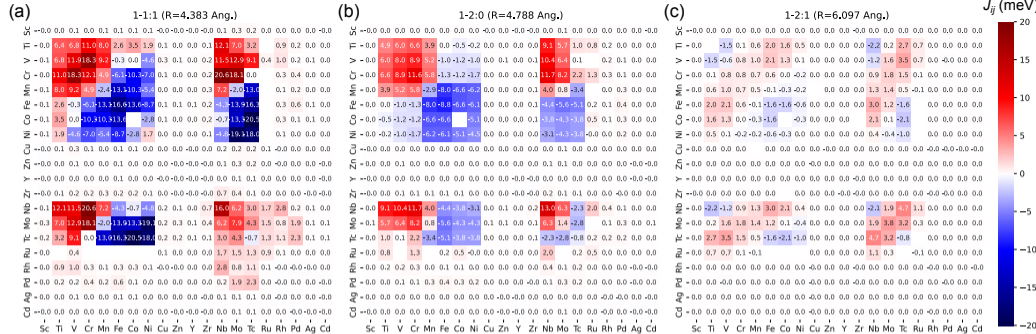


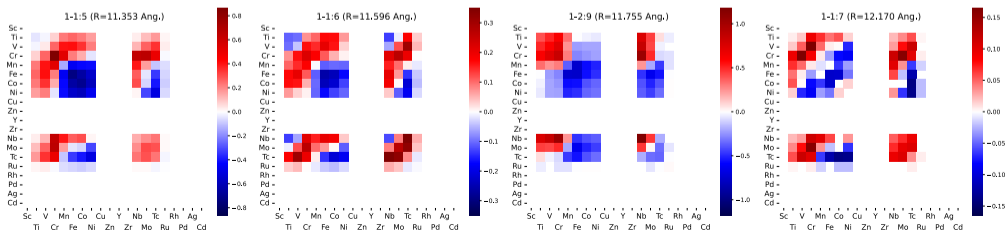
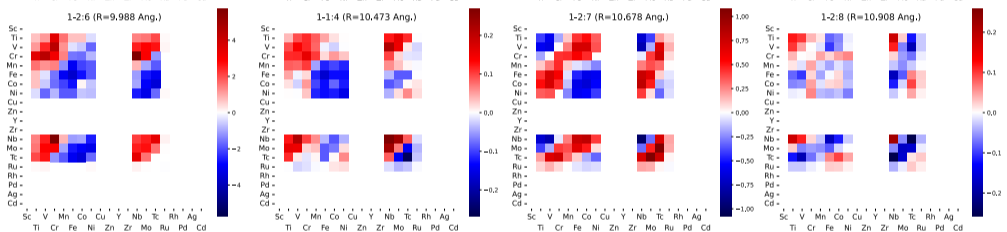
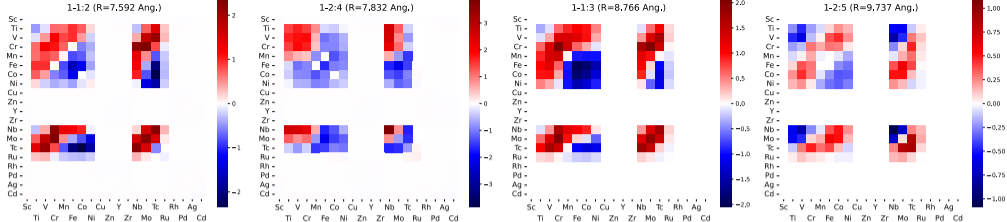
Extended Heisenberg Hamiltonian.  $H = -\frac{1}{2} \sum_{i,j} J_{ij} \vec{S}_i \cdot \vec{S}_j - \frac{1}{2} \sum_{i,j} \vec{D}_{ij} \cdot (\vec{S}_i \times \vec{S}_j)$

Exchange constants from method of infinitesimal rotations<sup>1</sup>.  $\mathcal{J}_{ij} = -\frac{1}{\pi} \text{Im} \int_{-\infty}^{E_F} dE \text{Tr}[\delta t_i G_{ij} \delta t_j G_{ji}]$

<sup>1</sup> Liechtenstein et al. 1987.

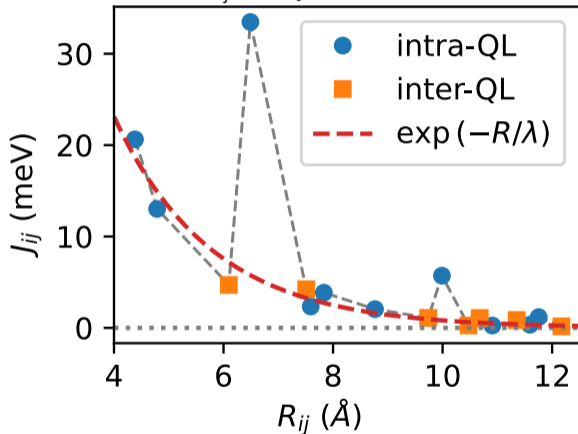
<sup>2</sup> Rüßmann, Bertoldo, and Blügel 2021.



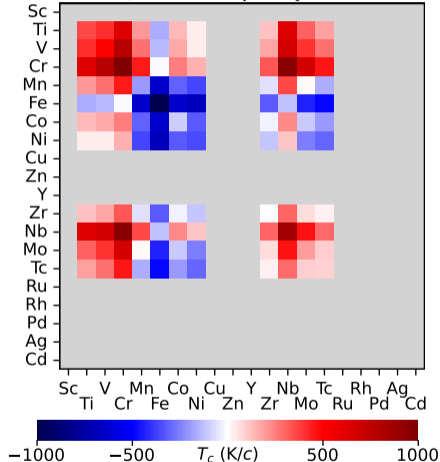


# Long-range magnetic ordering




$J_{ij}$  decay with distance






Mean-field  $T_c$  for all impurity combinations







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-  Liechtenstein, A. I. et al. (May 1, 1987). “Local Spin Density Functional Approach to the Theory of Exchange Interactions in Ferromagnetic Metals and Alloys”. In: *Journal of Magnetism and Magnetic Materials* 67.1, pp. 65–74. ISSN: 0304-8853. DOI: [10.1016/0304-8853\(87\)90721-9](https://doi.org/10.1016/0304-8853(87)90721-9). URL: <https://www.sciencedirect.com/science/article/pii/0304885387907219> (visited on 09/20/2023).

# References III

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