Machine Learning Emulators

for First-Principles Simulations of Quantum Materials

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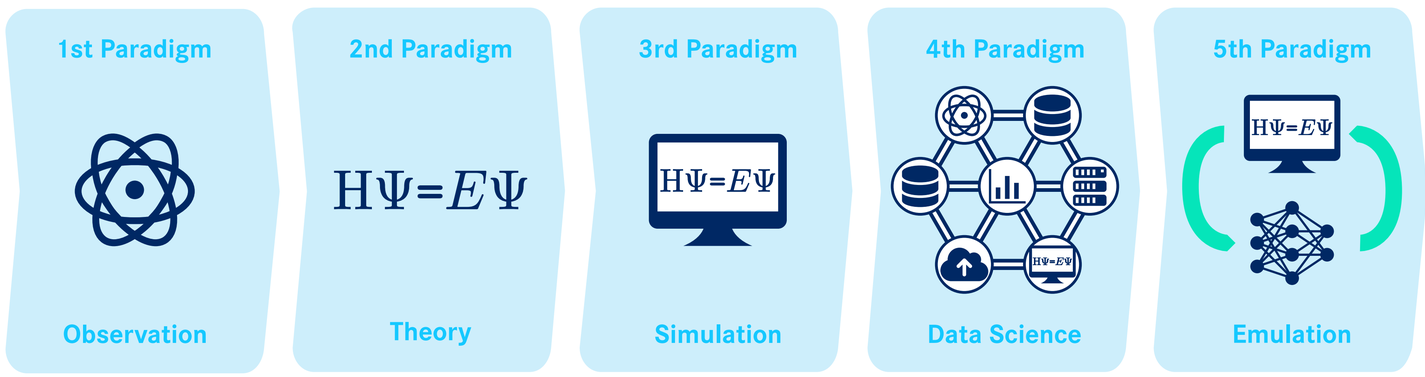
EMULATORS — A NEW PARADIGM OF SCIENTIFIC DISCOVERY[1]



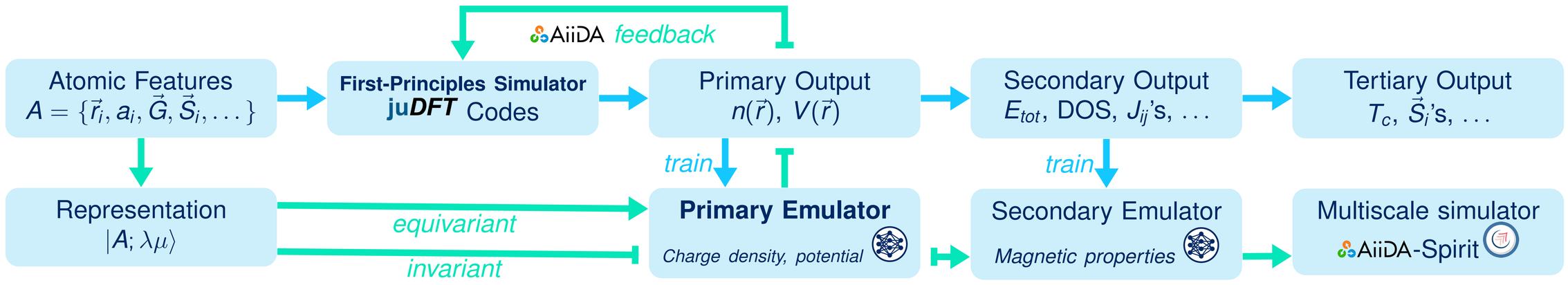
PROJECT GOALS

- **Extension** of state-of-the-art atomistic machine learning approaches to magnetic materials for energy-efficient future computing devices
- **Integration** of first-principles simulation and ML emulation into a single software package
- **Self-improving** feedback loop via high-throughput data generation
- **Harnessing the full data provenance** for ML via FAIR scientific workflows[2]

EMULATORS FOR QUANTUM MATERIALS

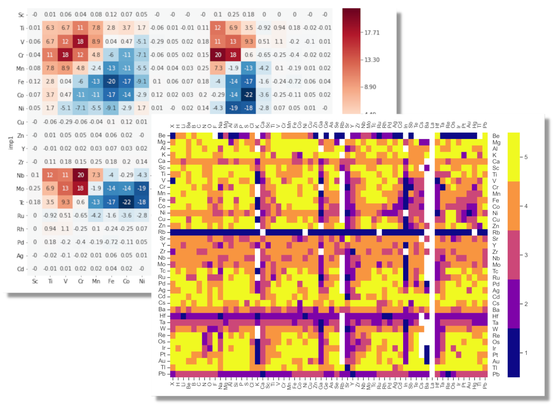
- Surrogate ML models have improved molecular dynamics simulations by orders of magnitude[3].
- We extend this success to electronic structure simulations.

1. Feeding back better initial guesses into the simulation to improve convergence
2. Direct property prediction for multiscale simulations.[4]



PROJECT COMPONENTS

DATA GENERATION



Training datasets of 10'000 impurity calculations.

- Integrate high-throughput data generation
- First-principles calcuation with the **juDFT** code ***JuKKR***
- Embedding of magnetic impurities in a topological insulator
- Candidate materials for future quantum technologies like quantum computers

MODEL CREATION

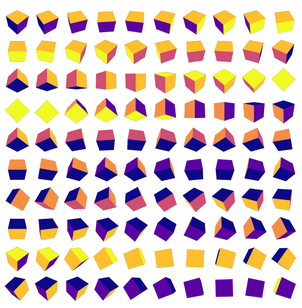
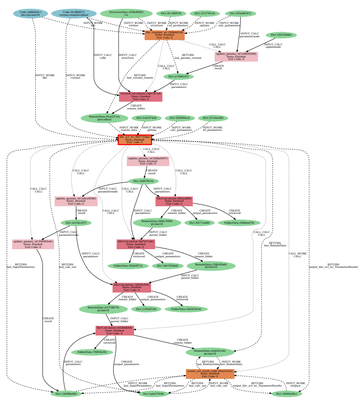


Image courtesy of Prof. Dr. Tess Smidt.

- Data efficiency with Euclidean symmetry-aware models
- Evaluation of state-of-the-art models
- Extension to quantum materials systems

	Invariant	Equivariant
Feature Engineering	SOAP	λ-SOAP, ACE
Representation Learning	SchNet	e3nn, MACE

SCIENTIFIC WORKFLOWS

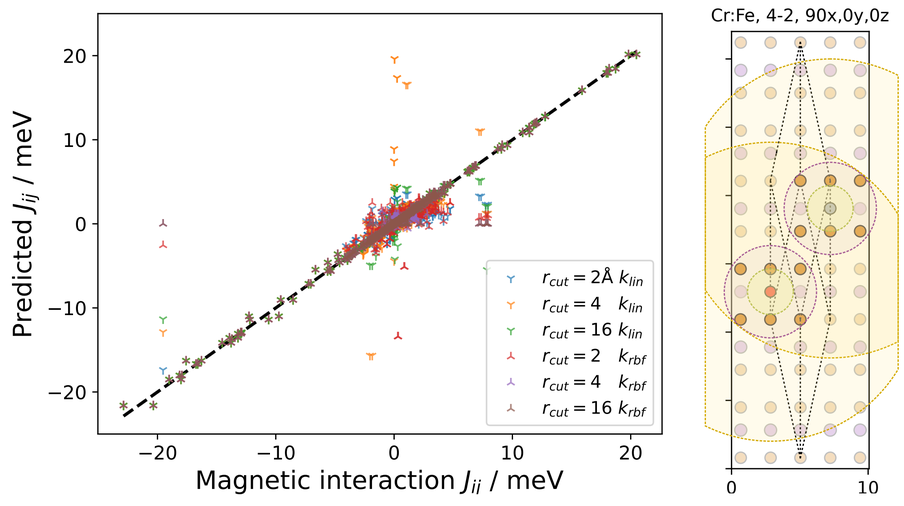


Subgraph of a single calculation.

- Full data provenance tracked with workflow engine AiiDA
- Intermediate calculation stages reused for learning

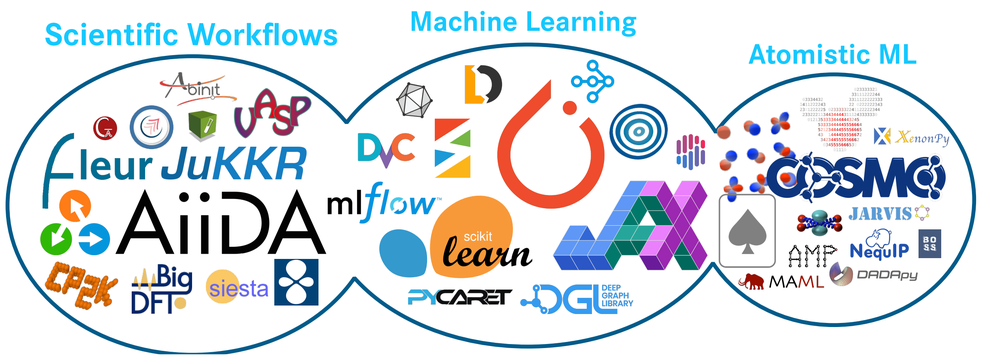
MODEL PERFORMANCE

Prediction of magnetic interaction strength J_{ij} of 2000 dimer impurities embedded into the topological insulator Bi_2Te_3 (secondary emulator). Model: SOAP + Kernel regression. MAE = 0.08 meV, R^2 = 0.94.



AI CLOUD INFRASTRUCTURE

- Deployment of full-stack (atomistic) machine learning platform
- iffAiiDA.fz-juelich.de available to all Jülich researchers



REFERENCES

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2. M. Uhrin, et int., G. Pizzi. Workflows in AiiDA: Engineering a High-Throughput, Event-Based Engine for Robust and Modular Computational Workflows. *Computational Materials Science* **187**, 110086 (Feb. 1, 2021).
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4. P. Rüßmann, et int., S. Blügel. The AiiDA-Spirit Plugin for Automated Spin-Dynamics Simulations and Multi-Scale Modeling Based on First-Principles Calculations. *Frontiers in Materials* 9 (2022).