JÜLICH Forschungszentrum

HDSLEE HELMHOLTZ School for Data Science in Life · Earth · Energy

# Curie Temperature Prediction of Magnetic Heusler Alloys Using Ab-initio Data

## Classifying Heusler compounds for potential industrial application


r.hilgers@fz-juelich.de

Robin Hilgers*†, Stefan Blügel*†, Ira Assent‡, Daniel Wortmann†, Dirk Witthaut§

* Department of Physics, RWTH Aachen University, Aachen, Germany
† Institute of Advanced Simulation (IAS-1), Forschungszentrum Jülich, Jülich, Germany
‡ Department of Computer Science, Aarhus University, Aarhus, Denmark
§ Institute for Theoretical Physics, University of Cologne, Köln, Germany


## INTRODUCTION

- Computational Materials Science: Predict macroscopic properties from molecular structure.
- Example: Predicting the material specific Curie temperature $T_c$ for different Heusler alloys based on simulation data.[1]
  ⇒Application in magnetic storage devices requires high $T_c$.
  ⇒Aim for a regression as well as a classification approach.
- Challenge: Training data is sparse and expensive to get.
- Complementary work at IAS-1/HDS-LEE to establish reference data base.

## METHODS

Established - but computationally costly - way to predict $T_c$:

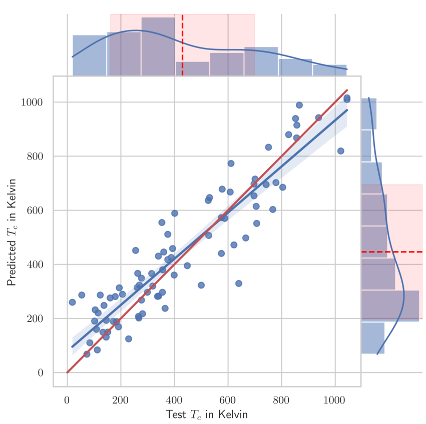
Structure Data → DFT Calculation => Charge Density at $T = 0$ K → Monte-Carlo Simulation => Behavior at $T > 0$ K → $T_c$

Step 1: DFT — Step 2: MC

Our goal is to either replace both simulation steps or at least the MC step by ML algorithms.

| Input Features | ML-Models | Outputs |
|---|---|---|
| Structural<br>Atomistic<br>opt: Magnetic | Extra Trees<br>Logistic Reg.<br>LASSO ... | $T_c$ (reg.)<br>"High" or<br>"Low" $T_c$ (class.) |

## Results

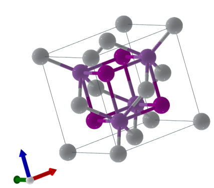



- Classification works well even without DFT data.
- Regression requires DFT generated magnetic structure data.
- Using Shapley Additive exPlanation (SHAP) we could validate the magnetic compound properties are crucial for the $T_c$.[2]
- We published the developed code and the data we processed from the Heusler data base JuHemd.[3,4]

| Model | Test F1 Score | Test Accuracy |
|---|---|---|
| Extra Trees | 0.90625 | 0.92683 |
| Logistic Reg. | 0.83871 | 0.87805 |

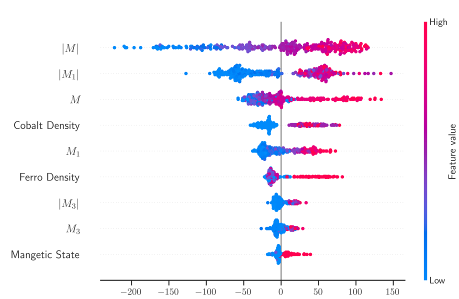
**Upcoming Paper:**

1. In preparation: Hilgers, R. et al. Curie temperature prediction models of magnetic Heusler alloys using machine learning methods based on first-principles data from ab-initio KKR-GF calculations, to be submitted to Physical Review Materials



## Conclusion

- False negative classification rate $< 3\%$ without DFT data
  ⇒Meets industry requirements for high-throughput screening.
- Physical insights can be derived from explainable models (XAI) which have no information about the underlying physics.




## Future work

- Extending the materials space to general 2-D materials instead of picking a subclass.
- Extending the presented approach to other magnetic material classes.
- Predicting further magnetic material quantities using ML models.

## REFERENCES


1. Kováčik, R., Mavropoulos, P. & Blügel, S. *The JuHemd (Jülich-Heusler-magnetic-database) of the Monte Carlo simulated critical temperatures of the magnetic phase transition for experimentally reported Heusler and Heusler-like materials.* 2022.
2. Lundberg, S. M. *et al.* From local explanations to global understanding with explainable AI for trees. *Nature Machine Intelligence* 2, 56–67 (Jan. 2020).
3. Hilgers, R., Wortmann, D. & Blügel, S. *ML-ready Curie temperatures and descriptors extracted from the JuHemd database.* 2022.
4. Hilgers, R., Wortmann, D. & Blügel, S. *Data processing for the JuHemd database and ML-training and evaluation scripts.* 2022.