Application of Machine-Learning Models and XAI in Materials Science Using Magnetic DFT Data

Classifying Heusler compounds for potential industrial application

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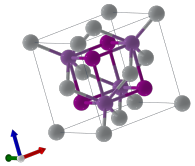

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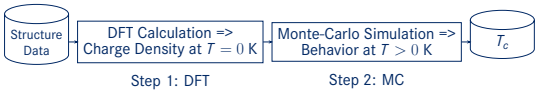
INTRODUCTION

- 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.

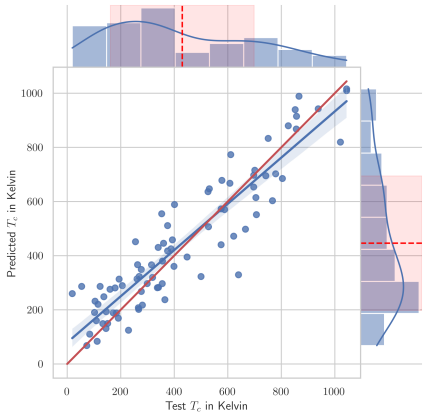
METHODS

Established - but computationally costly - way to predict T_c:



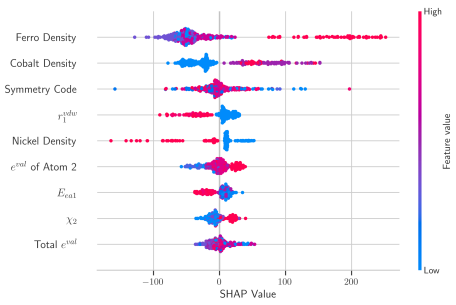
Our goal is to either replace both simulation steps or at least the MC step by ML algorithms.

Results



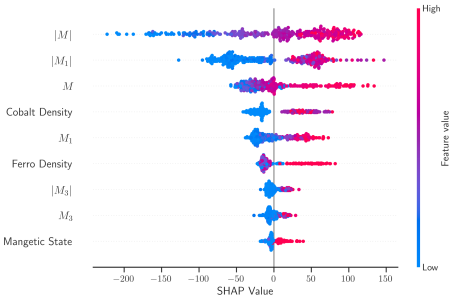
- Classification works well even without DFT/magnetic data.
- Regression requires DFT generated magnetic structure data.
- Using Shapley Additive exPlanation (SHAP) we could validate the magnetic compound properties are crucial for the T_c.[2]
- We published the developed code and the data we processed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



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. (In Progress)
- Predicting further magnetic material quantities using ML models e.g. screen for half-metallic properties (Paper in preparation)

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.
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3. Hilgers, R., Wortmann, D. & Blügel, S. *ML-ready Curie temperatures and descriptors extracted from the JuHemd database.* 2022.
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