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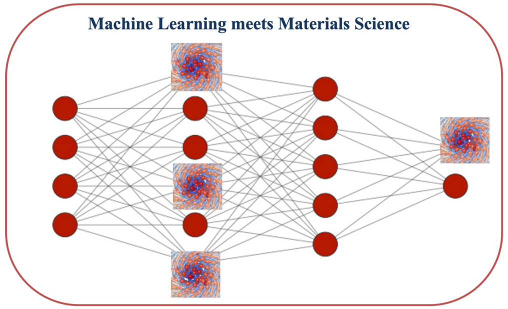

Predicting Magnetic Interactions from Time-Series Magnetization Data Using Explainable Machine Learning

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Knut and Alice Wallenberg Foundation

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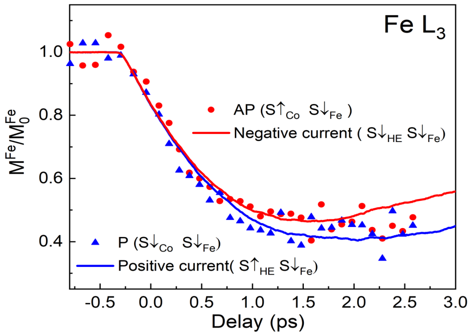
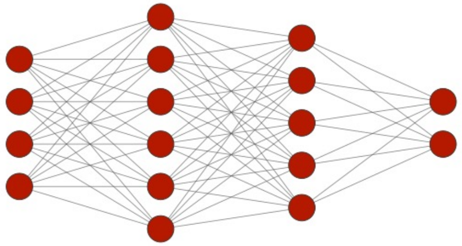
Explainable machine learning for magnetic interactions extraction

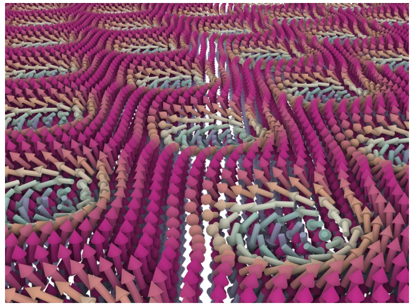
Magnetization dynamics



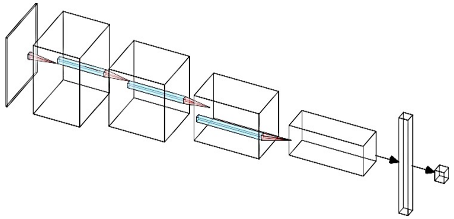
Machine learning



Magnetic images



Machine learning



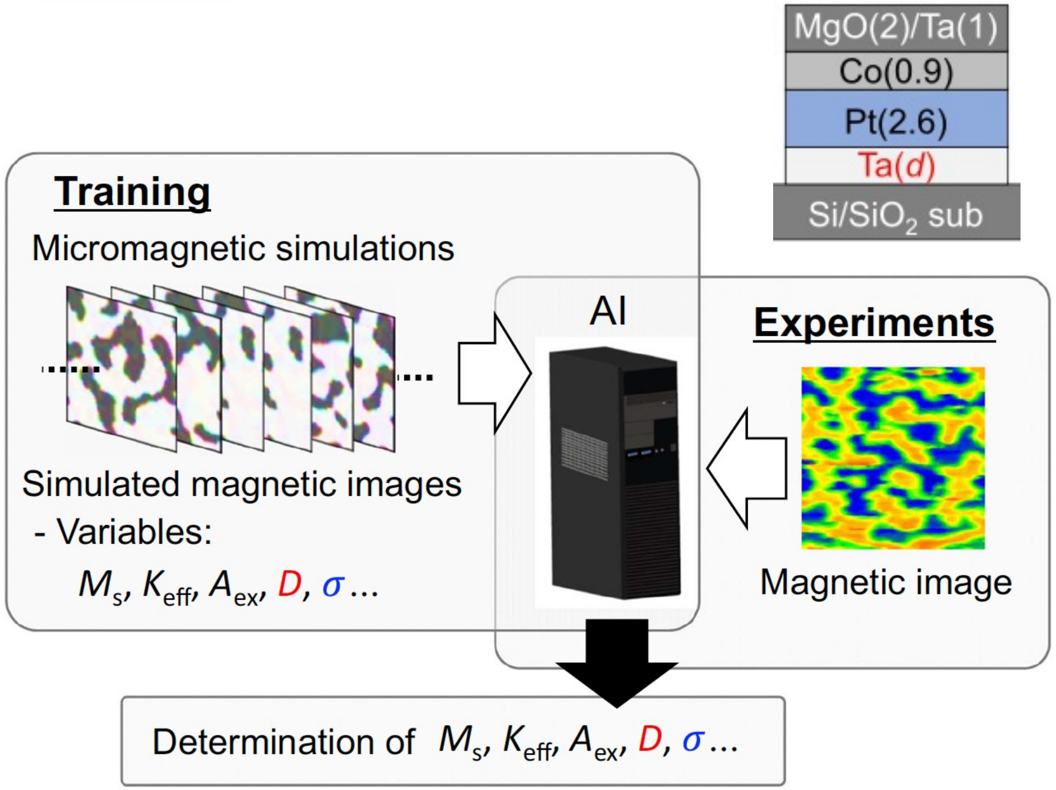
Extraction of exchange interaction, anisotropy, DMI

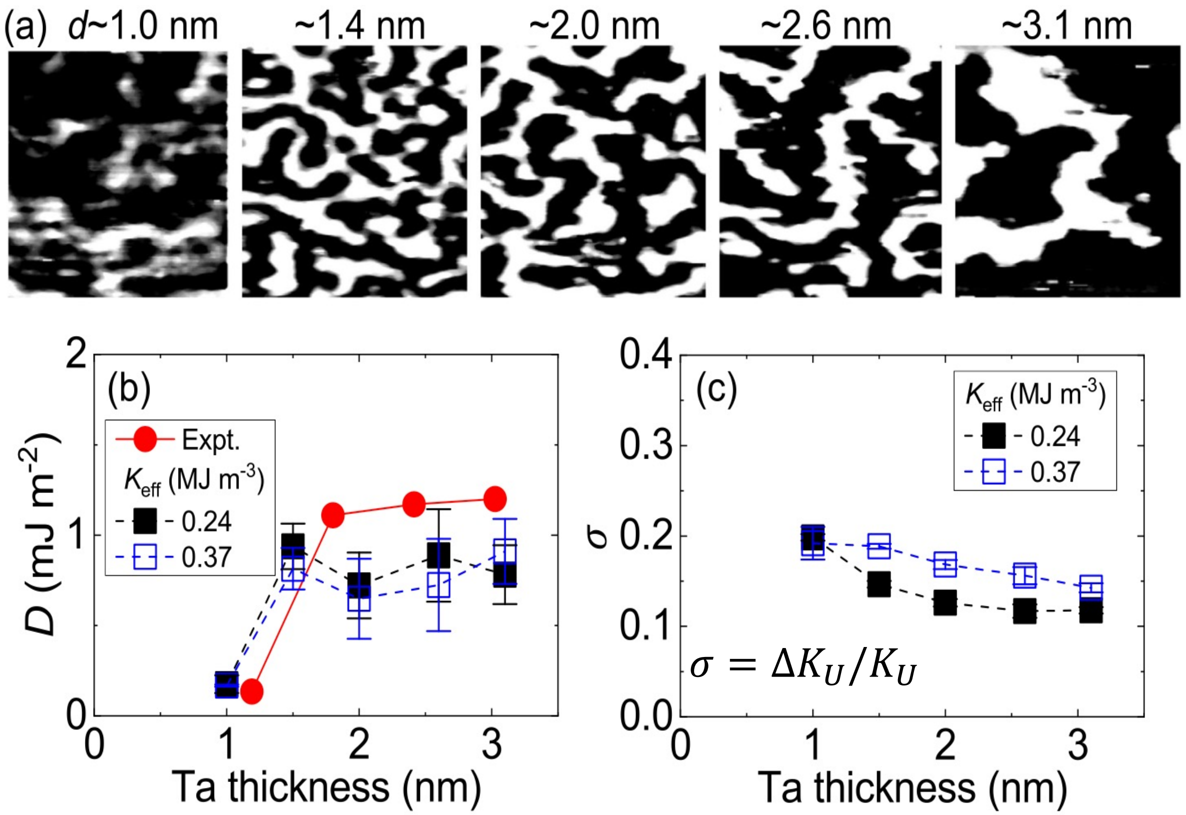
Here, we focus on **FeGd, bccFe, and FM-AFM bilayer**

Comparison of method accuracy and performance

Machine learning explainability

Introduction. Determination of the Dzyaloshinskii-Moriya interaction using pattern recognition and machine learning

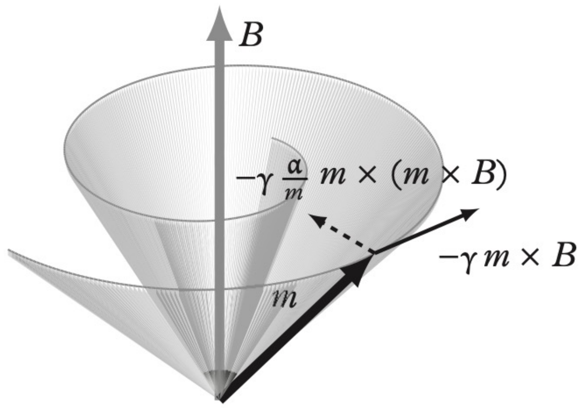




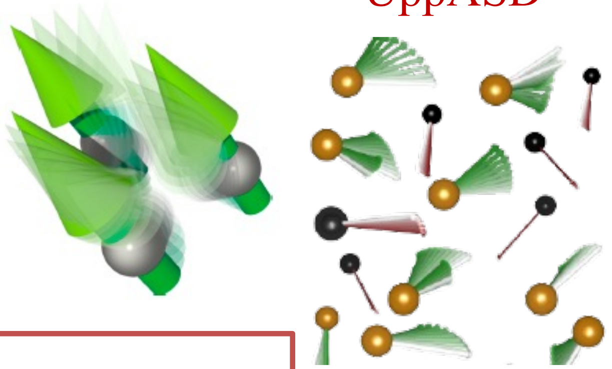
From: npj Computational Materials (2021)
https://doi.org/10.1038/s41524-020-00485-2

Introduction. Atomistic spin dynamics simulations.

Atomistic spin:
Localized magnetic moments
Classical description
Described by a spin Hamiltonian



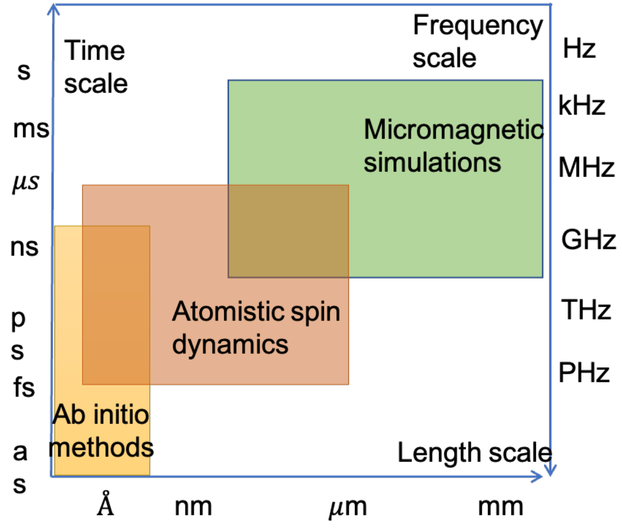
UppASD



Landau–Lifshitz–Gilbert equation Spin part

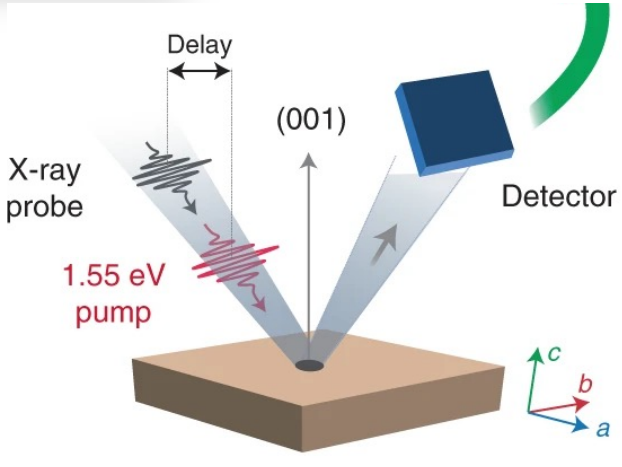
$$\frac{dm_i}{dt} = -\underbrace{\frac{\gamma}{(1+\alpha^2)} m_i \times \left(B_i + B_i^{fl}\right)}_{\text{Precession}} - \underbrace{\frac{\gamma}{(1+\alpha^2)} \frac{\alpha}{m_i} m_i \times \left(m_i \times [B_i + B_i^{fl}]\right)}_{\text{Damping}}$$

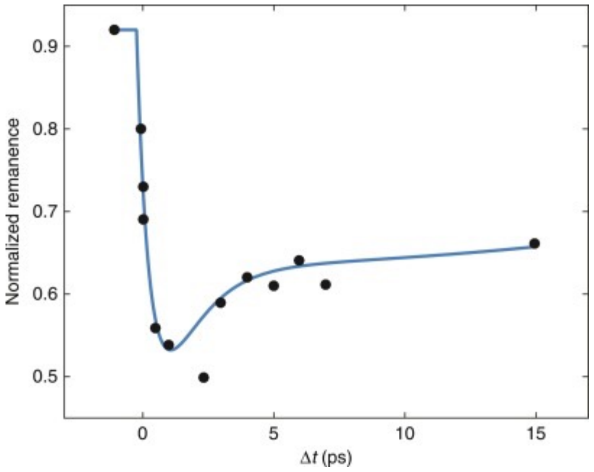
$$-\frac{1}{2} \sum_{ij} J_{ij}^{\alpha\beta}\, m_i^{\alpha} m_j^{\beta} \qquad \textbf{Spin}$$



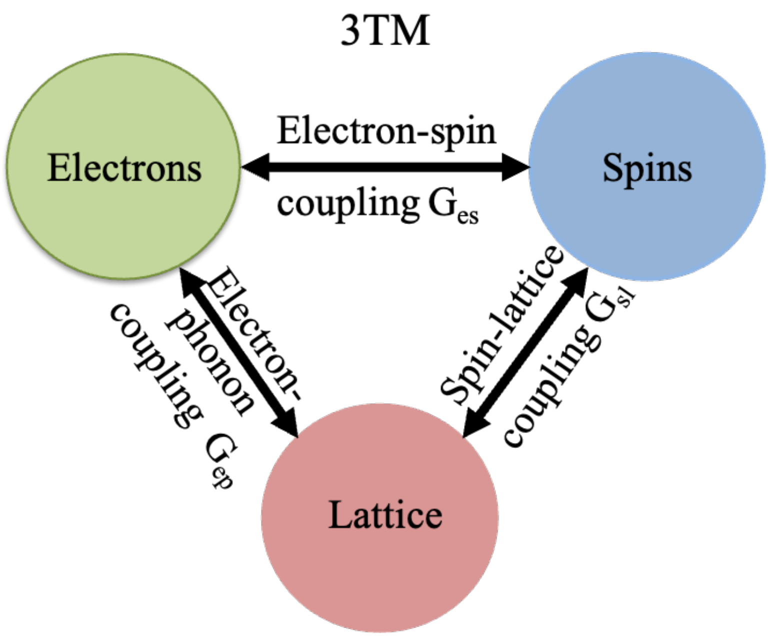
O. Eriksson et al, Atomistic Spin Dynamics Foundations and Applications, 2016

Introduction. Ultrafast demagnetisation





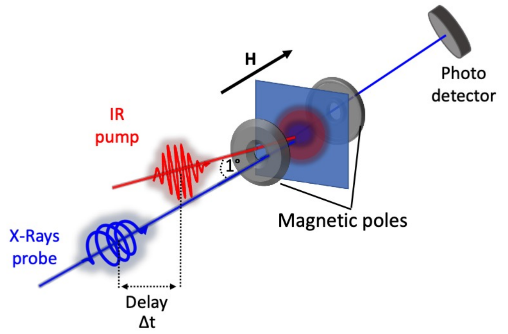
$$C_e(T_e)\frac{dT_e}{dt} = -G_{el}(T_e - T_l) - G_{es}(T_e - T_s) + P(t)$$
$$C_s(T_s)\frac{dT_s}{dt} = -G_{es}(T_s - T_e) - G_{sl}(T_s - T_l)$$
$$C_l(T_l)\frac{dT_l}{dt} = -G_{el}(T_l - T_e) - G_{sl}(T_l - T_s)$$



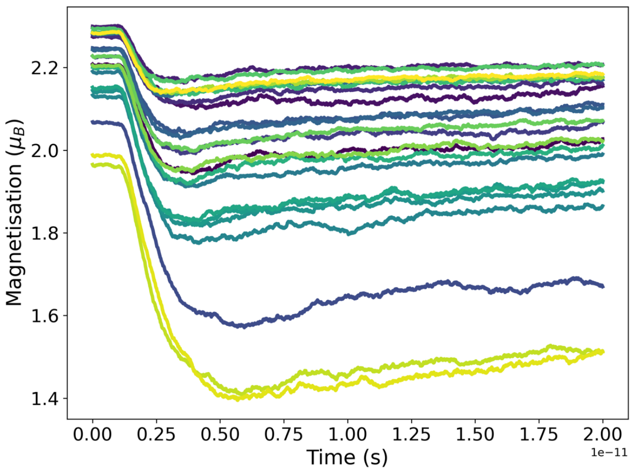
Nature Materials volume 21, pages 514–517 (2022)

E. Beaurepaire, et al, Phys Rev Lett. 76 (1996)

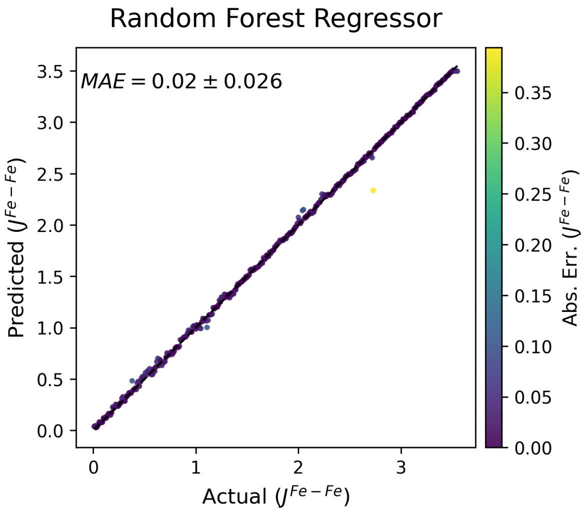
Extracting exchange interactions using explainable machine learning



Step I. Generate time series using atomistic simulations



Step II: Use ML to extract exchange interaction values



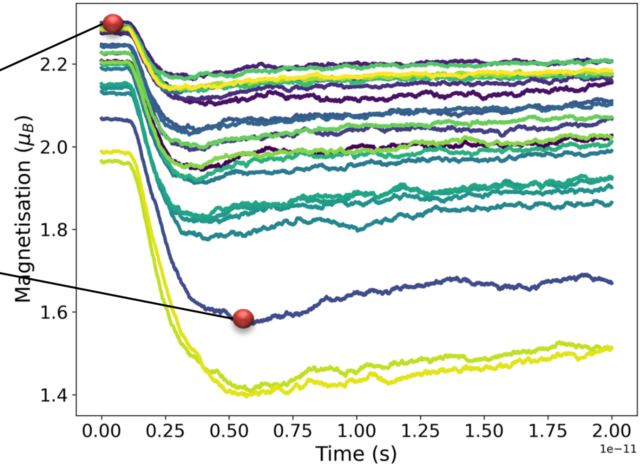
Step III. Apply the post-hoc explainability

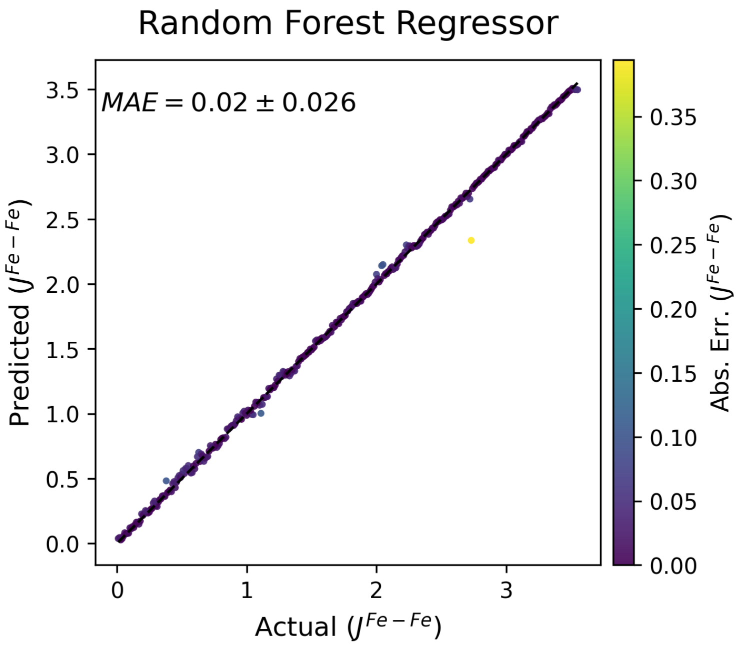
TreeSHAP algorithm
for tree-based ML

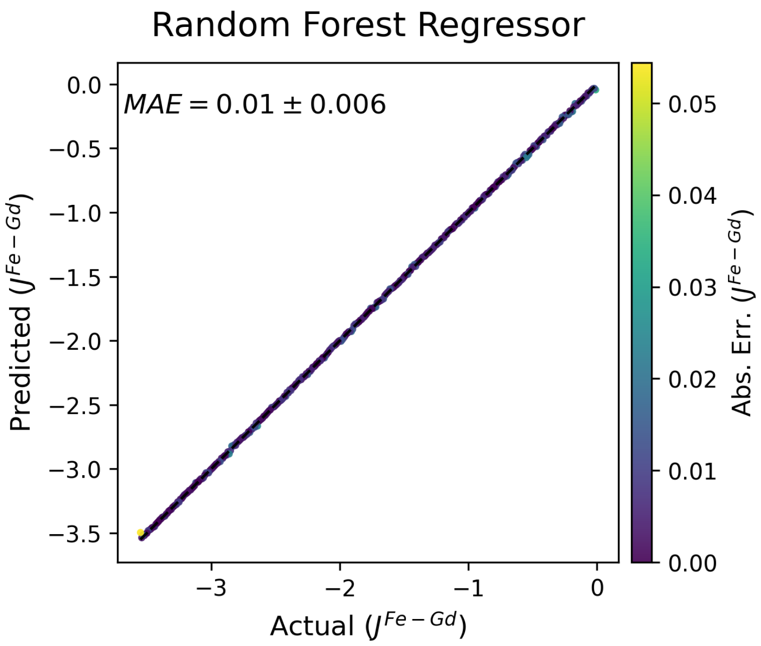
Condition for high J	Confidence
-0.03<mean(Mx)≦0.1	0.56
-0.05<mean(Mz)≦0.025	0.50

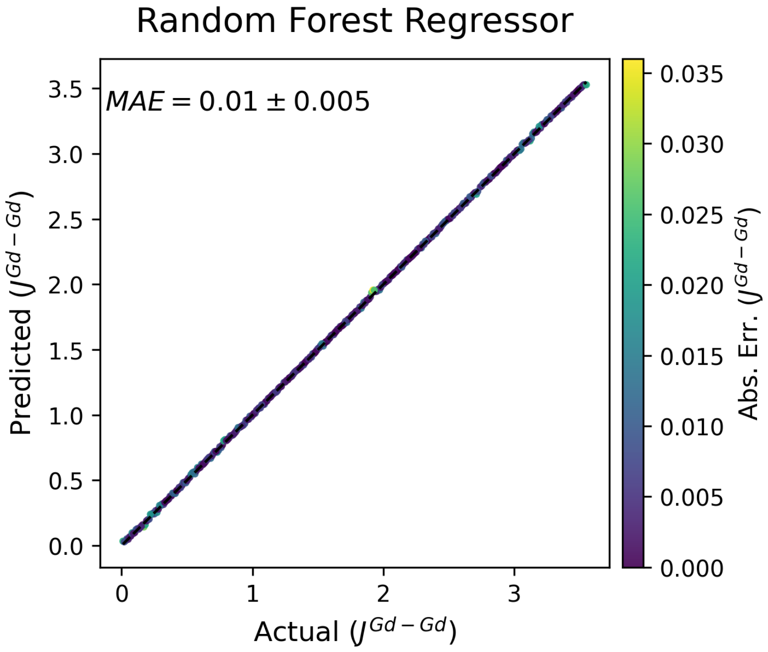
Extracting exchange interactions of FeGd

Features: max(M, Mz, My, Mx)
min(M, Mz, My, Mx)
slope
intercept

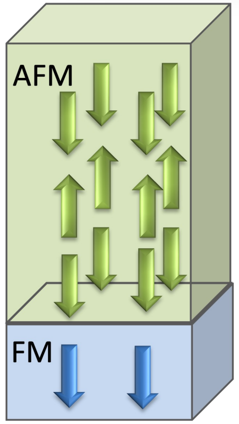


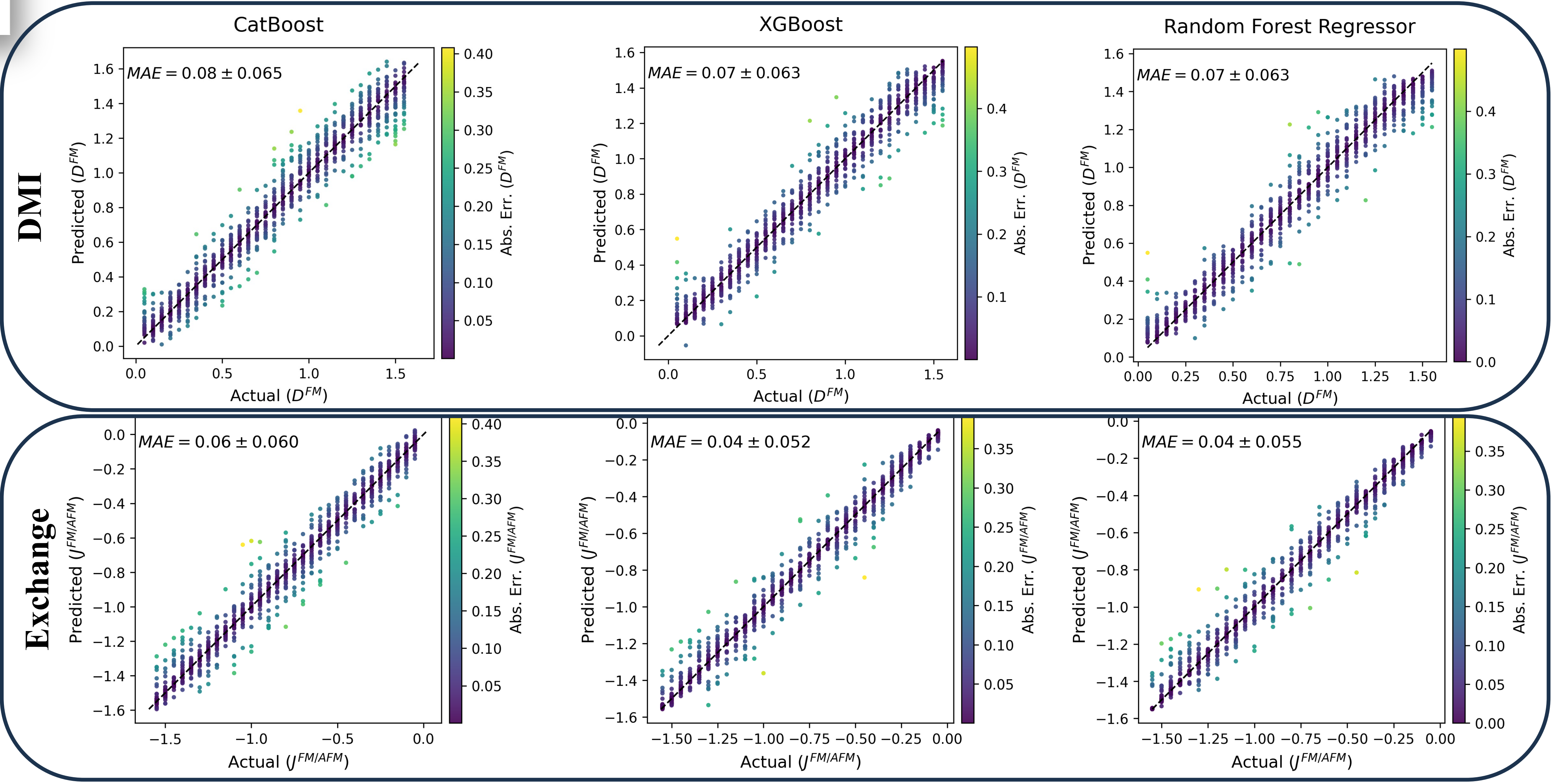






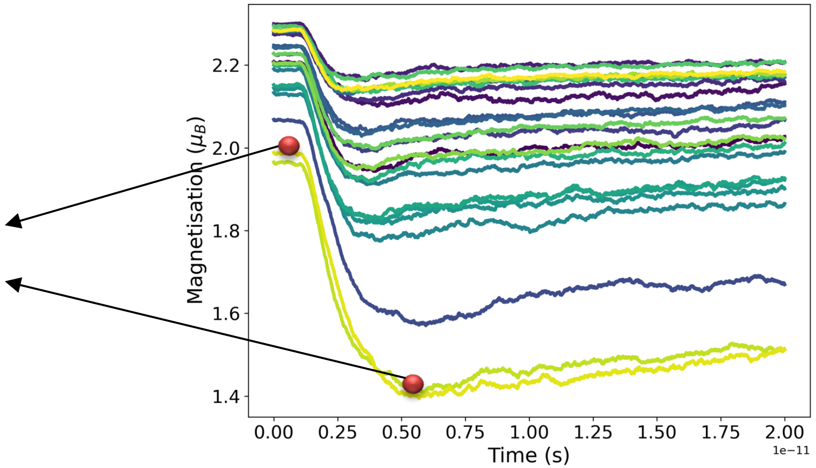
Extracting exchange and DMI interactions of FM-AFM bilayer

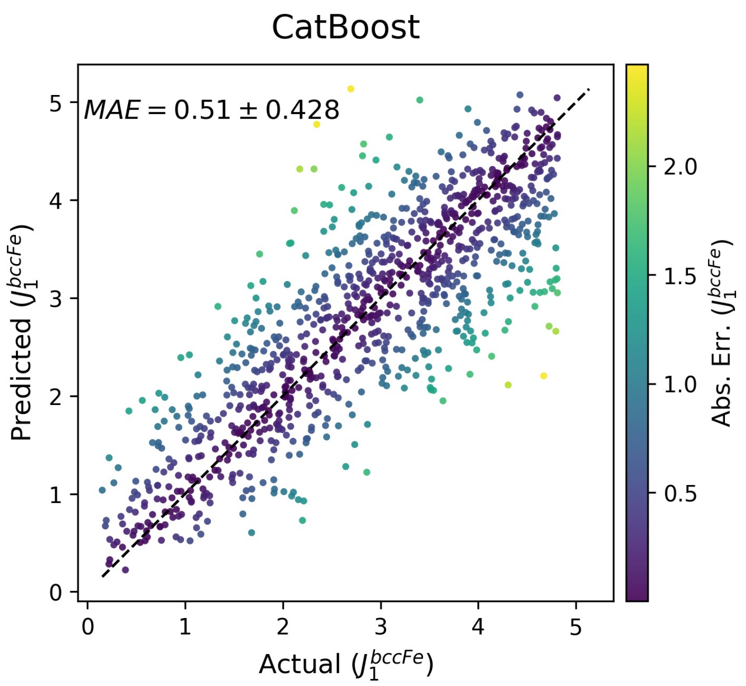


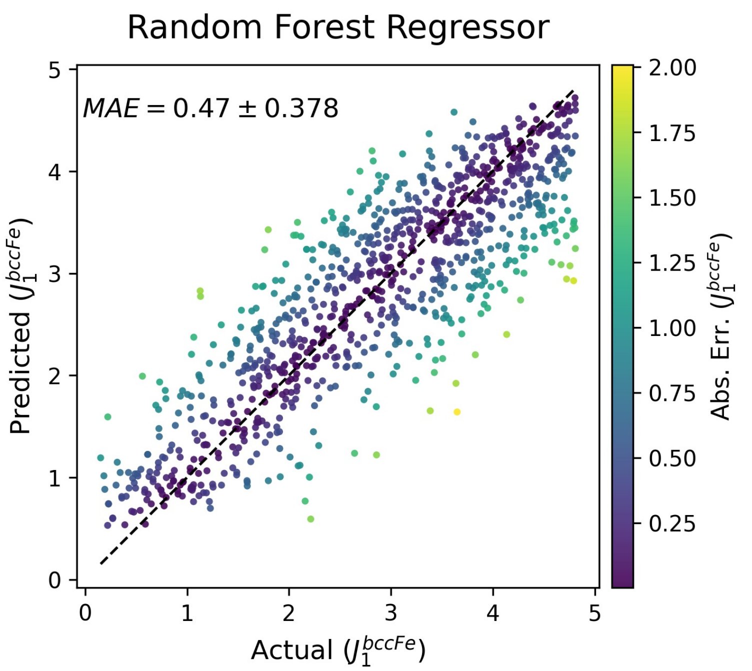


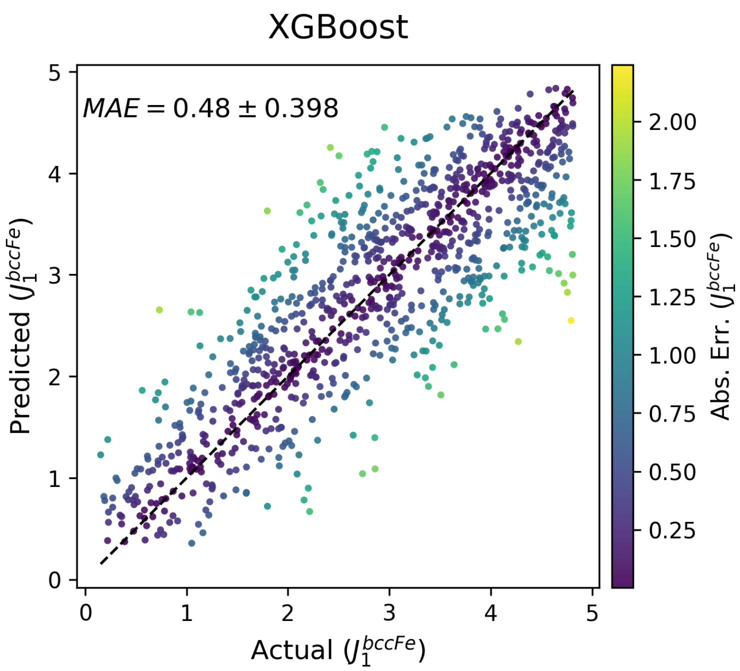
Extracting exchange interactions of bccFe

Features: max(M, Mz, My, Mx)
min(M, Mz, My, Mx)
slope
intercept









Introduction. Explainable machine learning to address the "black box" problem

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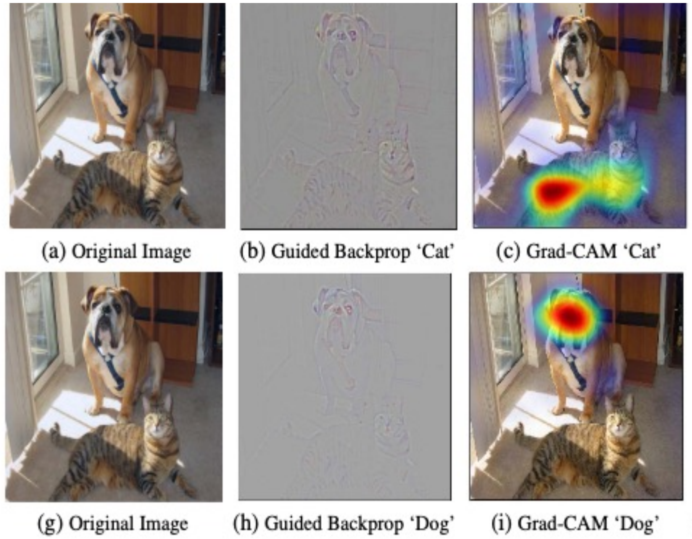
Explainability is about users understanding the output from an ML system or its underlying behaviour.

Gradient-weighted Class Activation Mapping (Grad-CAM)



Can generate visual explanations from *any* CNN-based network without requiring architectural changes or re-training.

Selvaraju et al.: Grad-CAM. In: ICCV (2017)

From Local to Global Explainability

TreeSHAP

- Local Explanations
- Prediction of a single instance.

Prediction 1 Prediction 2 Prediction 3

CEGA

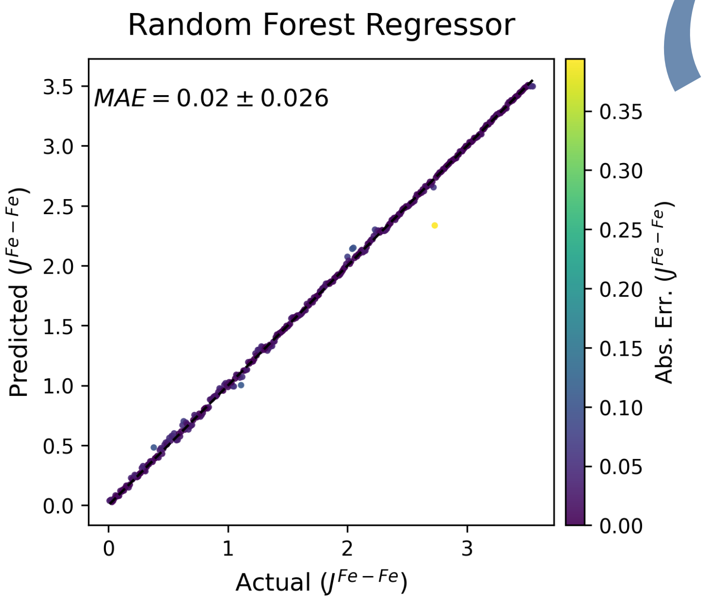
Capture the model's overall behaviour or global decision-making patterns.

Provides a global, interpretable summary of the model's decision-making process

Global Rules

Rule 1 Rule 2 Rule 3

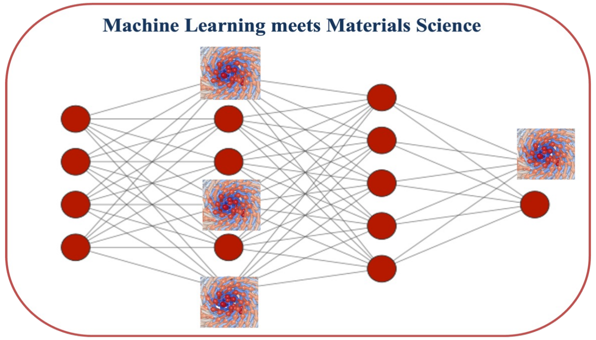
Extracting exchange interactions of FeGd



Explainability analysis:

- 49% cases, max(M_z) is used
- 53% cases max(M) is used
- 33% cases max(M_y) is used

MSE		
XGBoost	Random Forests	CatBoost
5 features: max(M, Mx, My, Mz), slope, and intercept		
0.001073	0.000677	0.009420
2 features: max(M, Mz)		
0.001626	0.001177	0.000147



Conclusions:

- ❖ Our goal is to develop a new ML method for magnetic interaction extraction, compare it to the existing ML-based method, and incorporate ML explainability, aiming for more precise methods and raising awareness and deepening understanding in the research community of the mechanism of ML algorithms.

- ❖ We have shown that ML is a useful tool to extract parameters of bccFe, FeGd, and exchange-biased bilayers from magnetisation dynamics.

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Thank you for your attention!

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