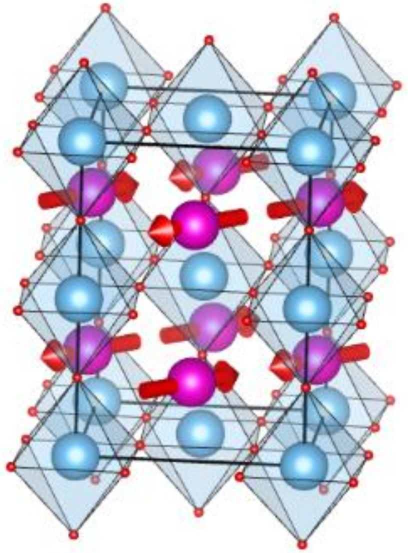
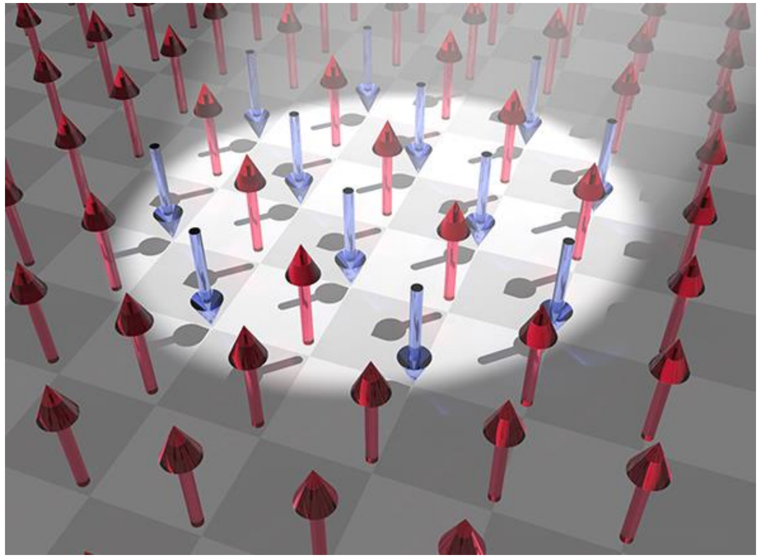
Machine Learning Magnetism: Predicting Magnetic Order from Chemical, Structural, Electronic, and Thermodynamic Descriptors.

Ahmed Fahmy, Murod Mirzhalilov, Brandon Abrego, Sayok Chakravarty

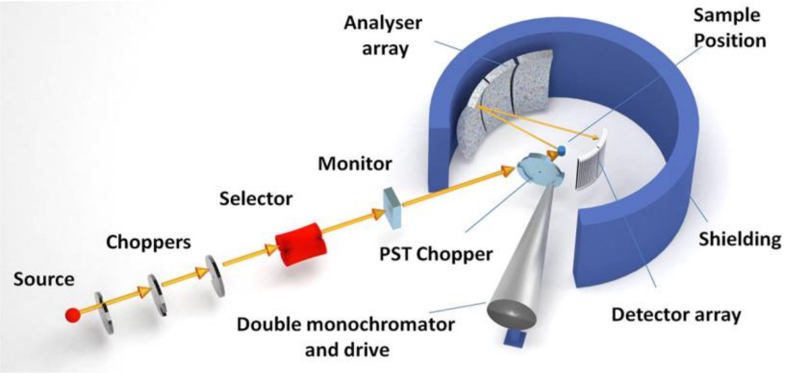




Summer 2025 Data Science Bootcamp
Erdos Institute

Predicting magnetism is essential for spintronics & quantum technology.

Schematic for neutron scattering experiments



Neutron Scattering Facility at NIST

Our Approach:

Input Descriptors:
- Chemical
- Structural
- Electrical
- Thermodynamic

Train ML models on *Materials Project* Database

Train ML models on *MAGNDATA* Database to correct bias in *Materials Project*.

Prediction Targets:
- Non-magnetic
- Ferromagnetic
- Antiferromagnetic
- Ferrimagnetic
- Propagation Vector

Neutron Scattering

✅ High accuracy
❌ Expensive, slow, and not scalable to large datasets

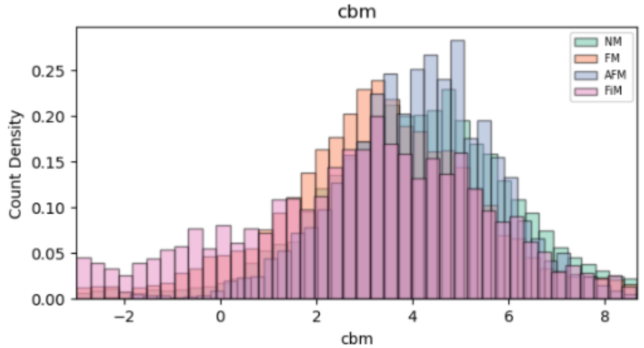
🖥 DFT Calculations

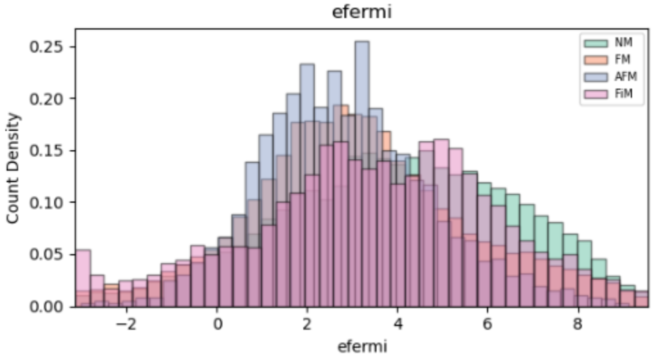
❌ Often fails for strongly correlated systems
❌ Require experimental input
❌ Computationally slow

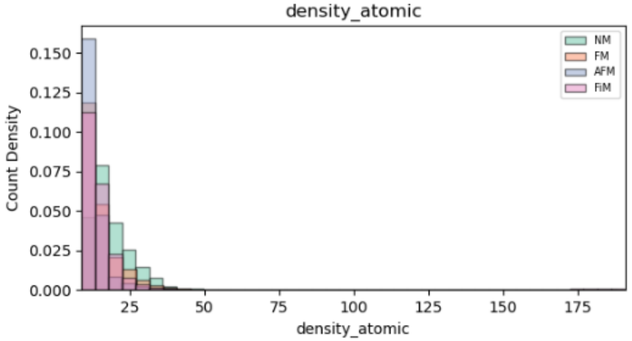
Data Collecting

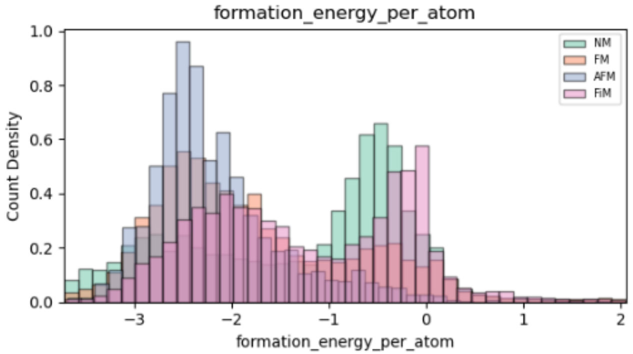
The Materials Project
materialsproject.org

- **Dataset 1 (Magnetism classification is done based on DFT-based Collinear Magnetic Order calculations)**
  - **Materials Project**: largest database of various inorganic materials with an API to import the targeted materials and their features.
- **Features**
  - Data set includes numerical and categorical features
    - Features selected to not directly correlate with magnetism (e.g. magnetic moments strength, is_magnetic, etc.)
    - Several categorical features are of high cardinality (ex. Elements)
- **Characteristics**
  - 154,803 different materials in our data set
    - 83,355 non-magnetic
    - 56,688 ferromagnetic
    - 11,345 ferrimagnetic
    - 3,415 antiferromagnetic



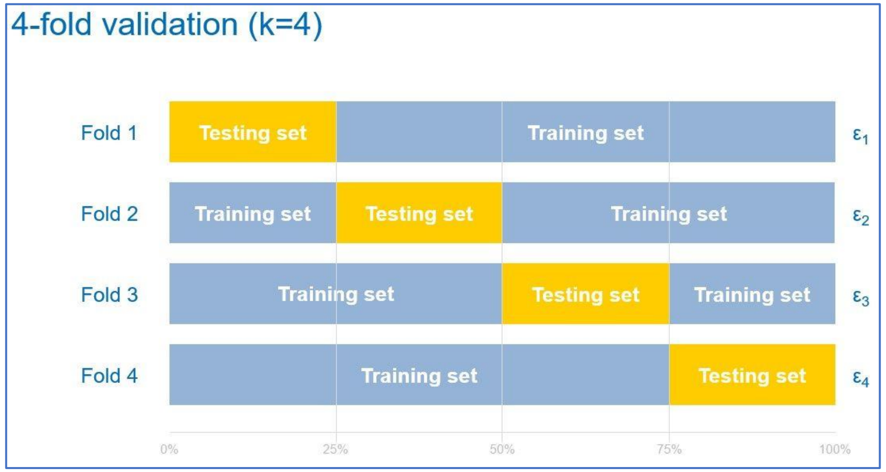


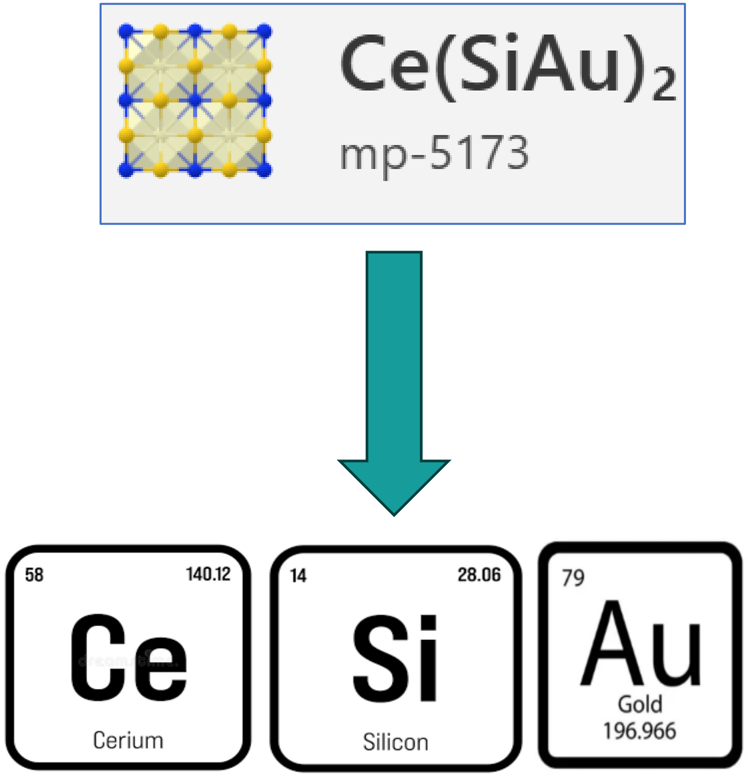




Data Preprocessing (on Materials Project dataset)

- Remove unique identifier data.
- Remove features with empty values.
- One hot encoding categorical features (e.g. crystal structure and chemical composition).
- Created a second dataset with materials with at least one magnetic element to compare with a literature recent study*.
- Prepared 2 (magnetic v.s. nonmagnetic), 3 (AFM, FM&FiM, NM), and 4 unique classes to assess the classification performance on each case.



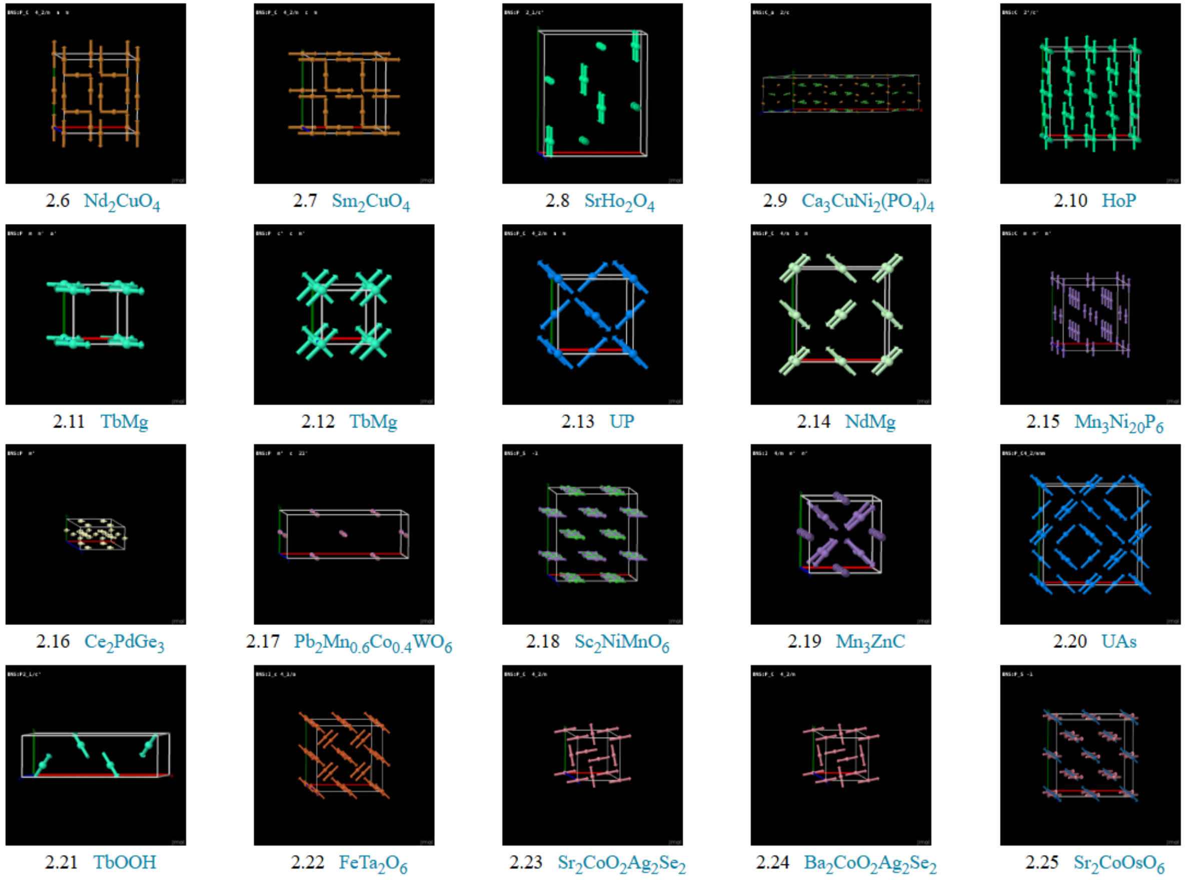


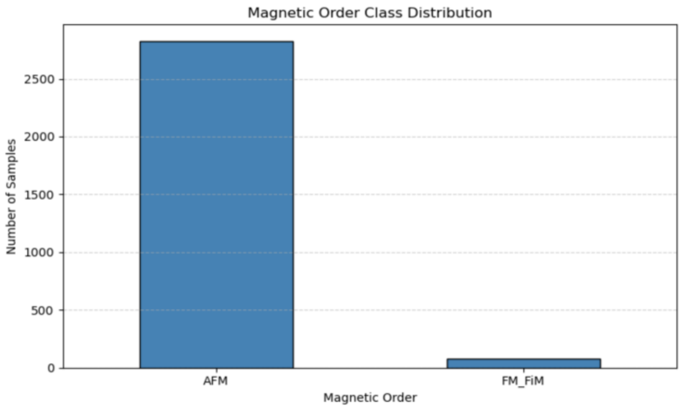
- 60%-20%-20% dataset split
- 4-fold cross validation

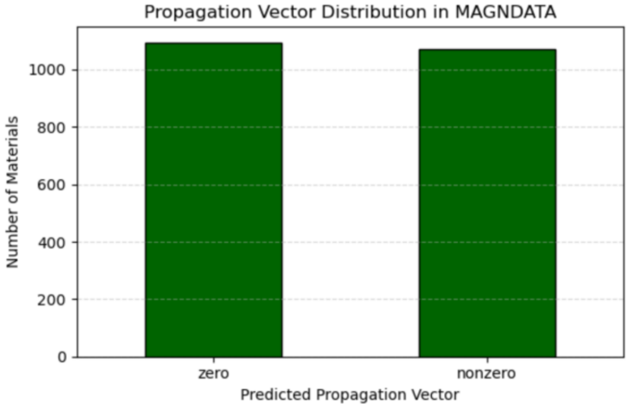
*Helena A. Merker, et al., "Machine learning magnetism classifiers from atomic coordinates", iScience (2022)

Database 2: **MAGNDATA**

- Unlike *Materials Project* (DFT calculations), MAGNDATA is the most comprehensive magnetism database based on experimental results from the state-of-the-art neutron scattering experiments.
- However, smaller set of data: 2167 commensurate magnetic materials.





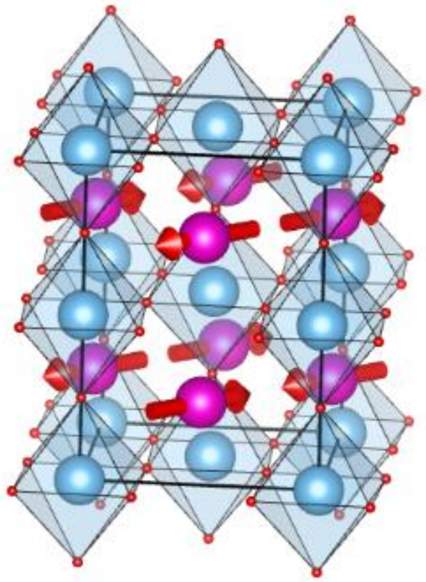


- We build a classifier for the propagation vector trained on MAGNDATA → Then we apply it the *Materials Project* to *partially correct* the FM bias in the DFT-calculations.
- Model training were chosen as 67.5% Training (with 6-fold cross validation), 22.5% Validation, 10% Testing.
- Data were collected through *web scraping*, then identified their *Materials Project* ID, and supplemented them with features from *Materials Project.*

Motivation: using coarse-grained descriptors to avoid the need to detailed structural and non-structural (e.g. electronegativity and piezoelectricity) features*.

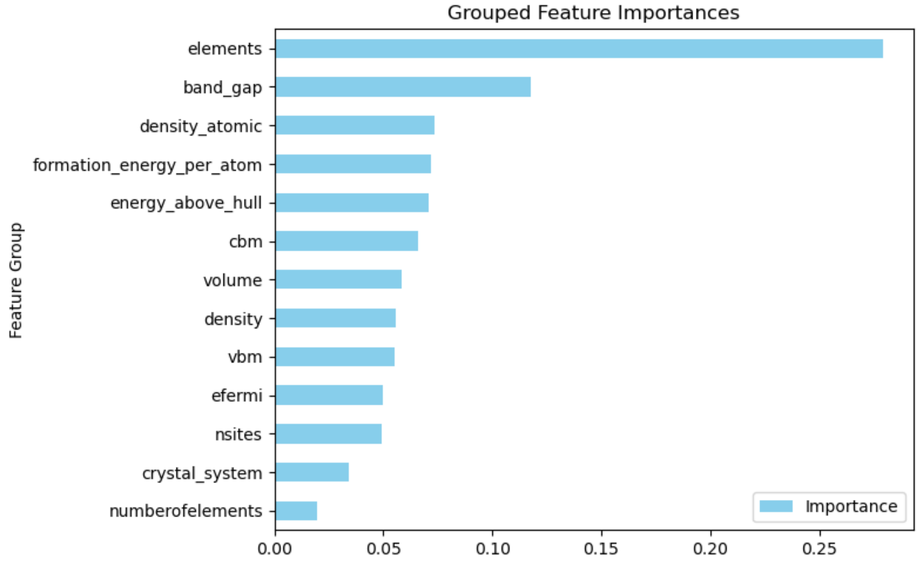
Final Descriptors

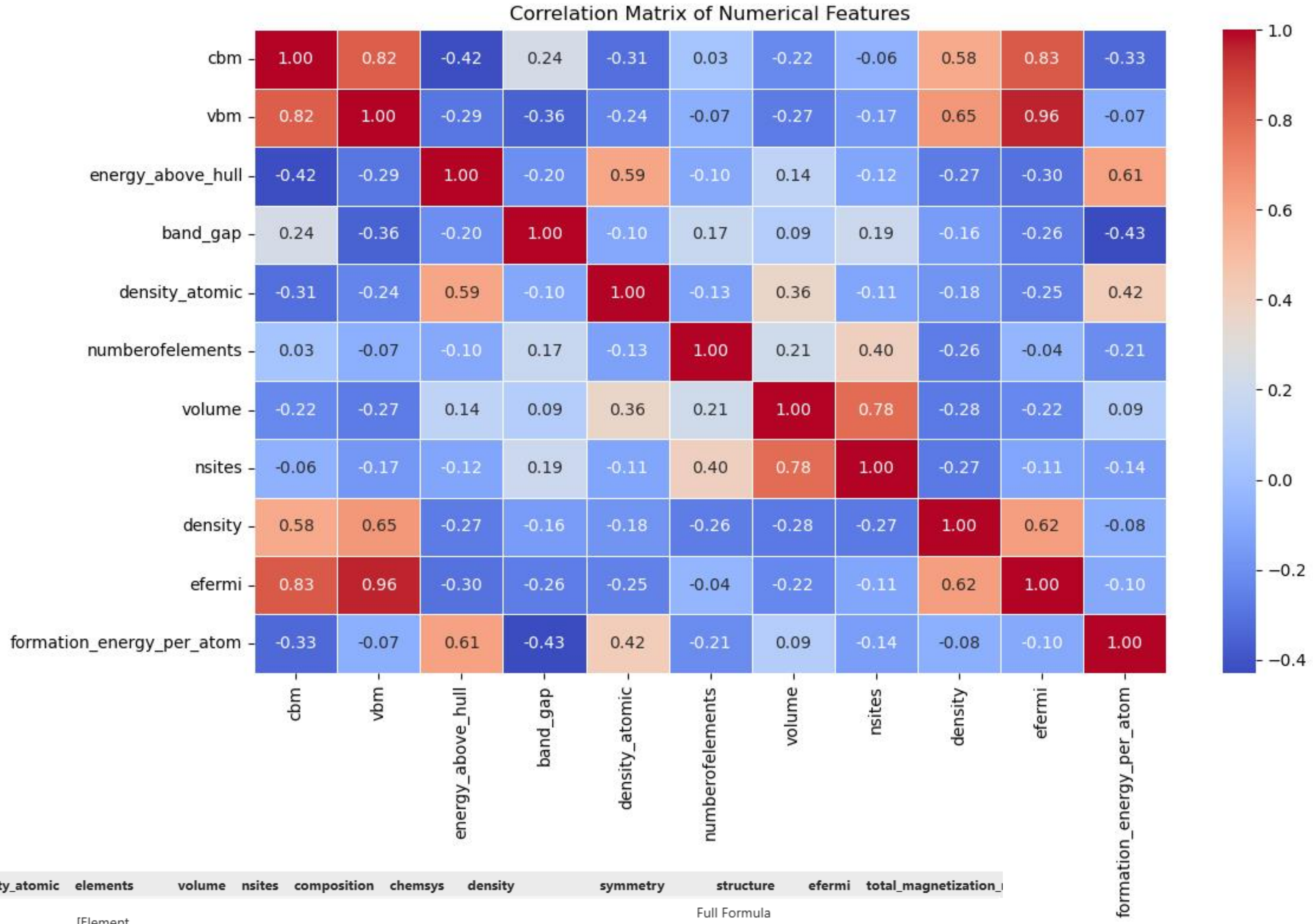
- Compositional
  - Chemical Elements
- Structural
  - Crystal Structure
  - Density
  - Atomic Density
  - Number of Unique Elements
  - Number of Sites
  - Volume of Unit Cell
- Electronic
  - Band Gap
  - Conduction Band Minimum (cbm)
  - Valence Band Maximum (vbm)
- Thermodynamic
  - Formation Energy per Atom
  - Energy above Hull



*Helena A. Merker, et al., "Machine learning magnetism classifiers from atomic coordinates", iScience (2022)

- Using Random Forest Feature Importance analysis, Principal Component Analysis, and features correlations, we find that *numerical* features are of close importance, so we keep the 11 numerical features without reduction.

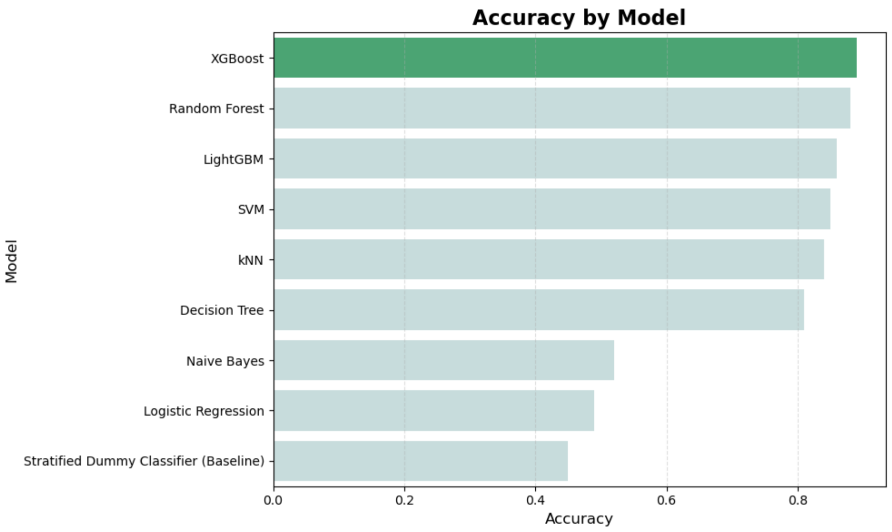


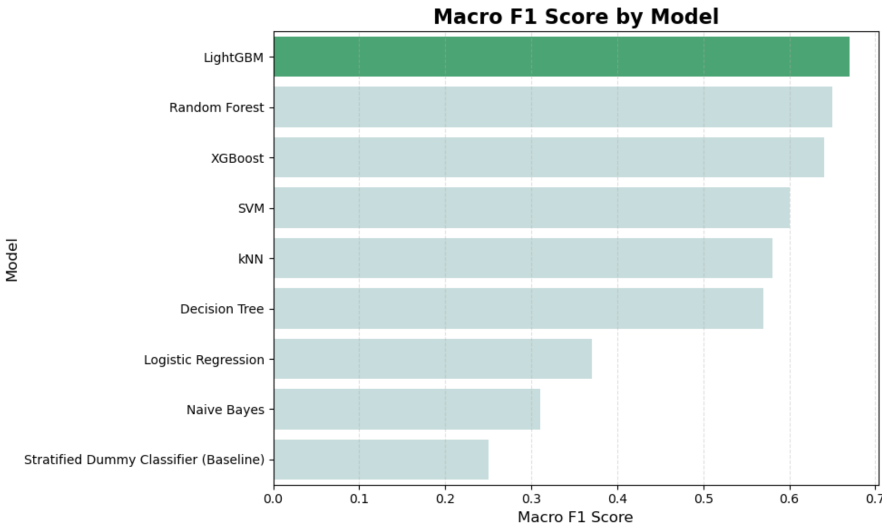


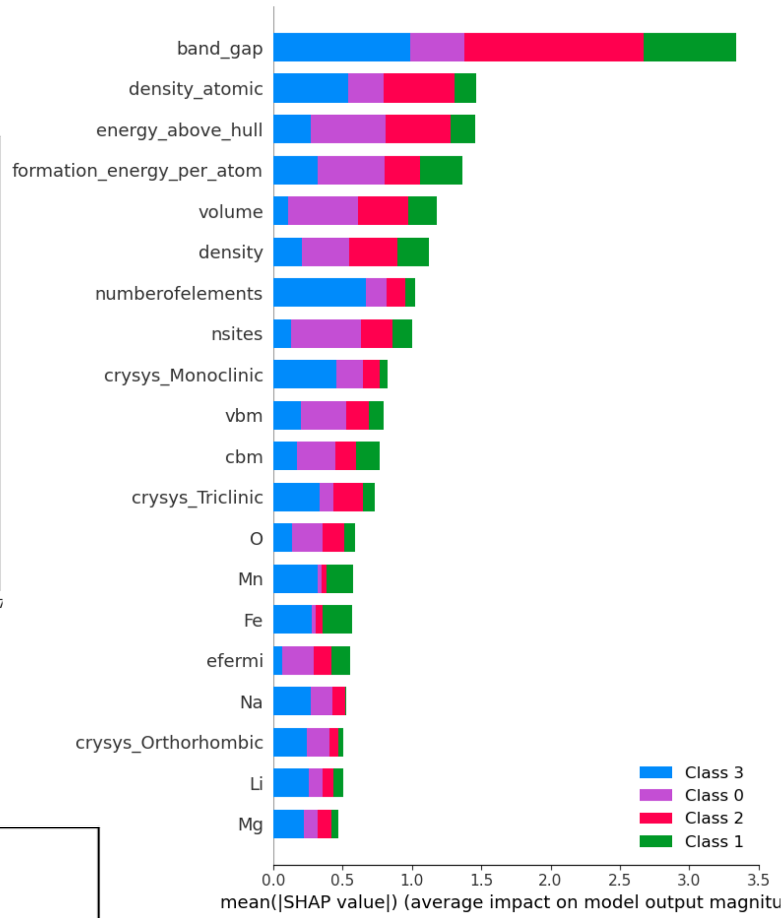
	material_id	formula	band_gap	ordering	numberofelements	density_atomic	elements	volume	nsites	composition	chemsys	density	symmetry	structure	efermi	total_magnetization_
879	mp-1106356	AlH3	3.1107	NM	2	11.309947	[Element Al, Element H]	180.959152	16	Al4 H12	Al-H	1.101355	crystal_system= <CrystalSystem.cubic: 'Cubic'> ...	Full Formula (Al4 H12)\nReduced Formula: AlH3\...	-0.348651	
45721	mp-561117	SXeO3F2	2.4934	NM	4	20.170010	[Element F, Element O, Element S, Element Xe]	1129.520558	56	S8 Xe8 O24 F16	F-O-S-Xe	2.932645	crystal_system= <CrystalSystem.ortho: 'Orthorho...	Full Formula (S8 Xe8 O24 F16)\nReduced Formula...	-2.542468	
30983	mp-1032067	Mg6CoBO8	1.8597	FM	4	9.472699	[Element B, Element Co, Element Mg, Element O]	151.563183	16	Mg6 Co1 B1 O8	B-Co-Mg-O	3.764175	crystal_system= <CrystalSystem.tet: 'Tetragonal...	Full Formula (Mg6 Co1 B1 O8)\nReduced Formula:...	6.681638	

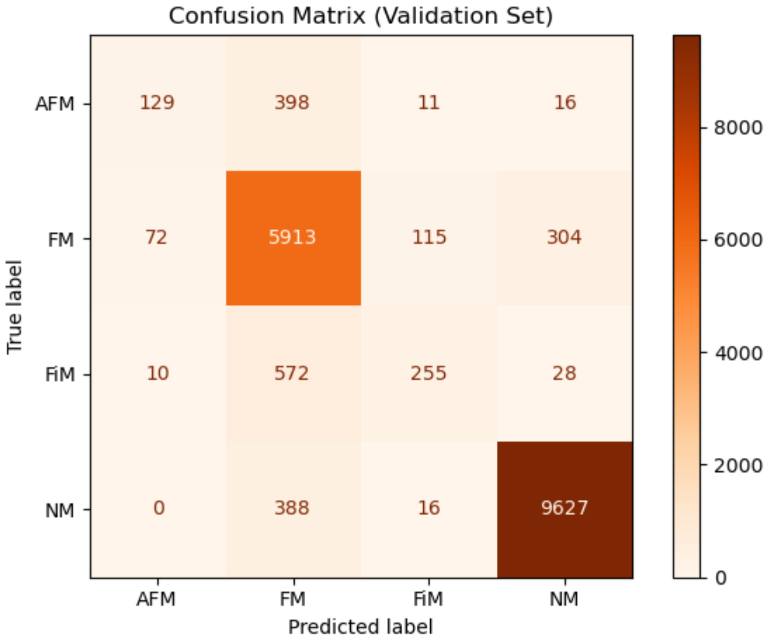
...etc

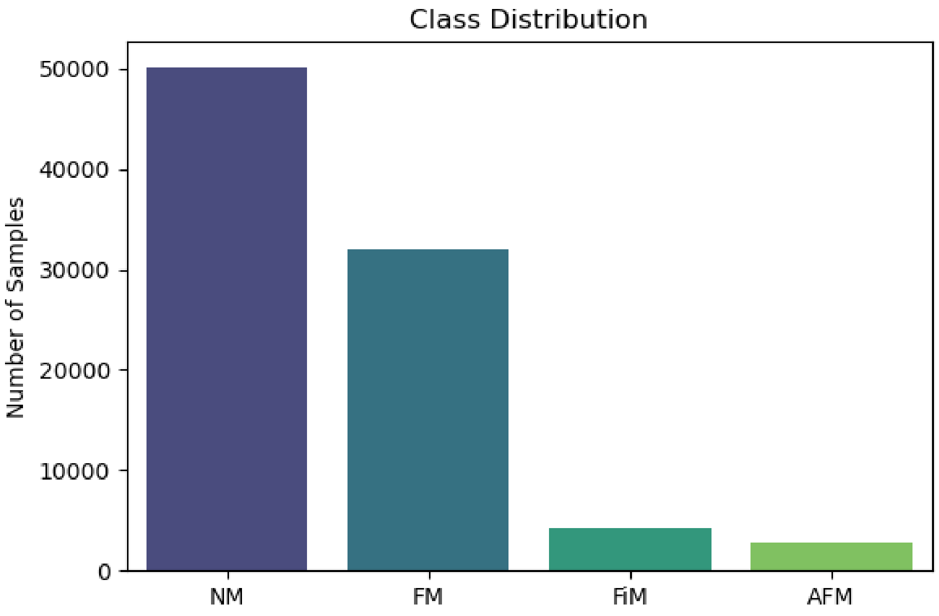
Model Comparison: *Materials Project*





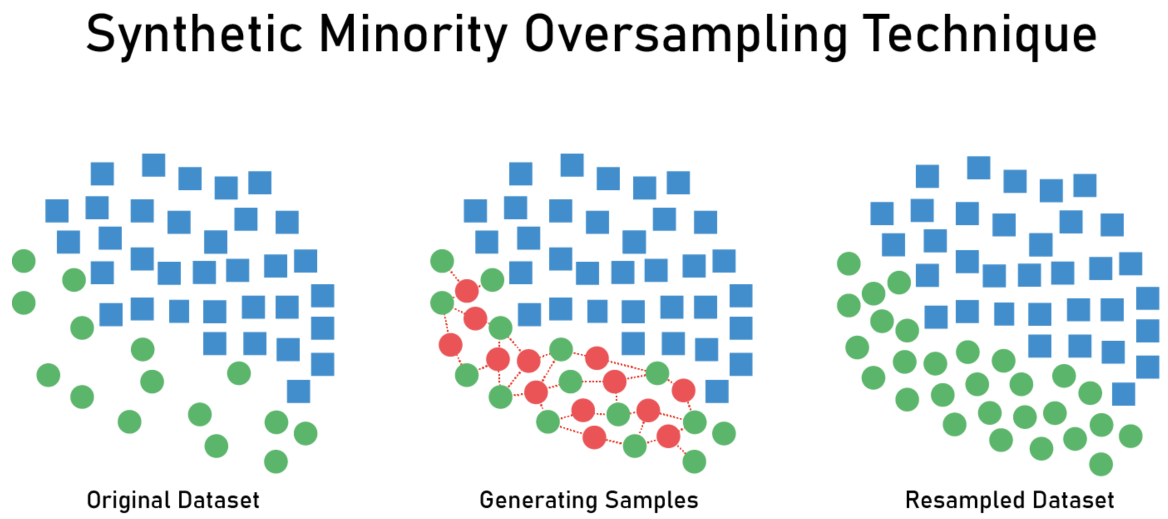






- Accuracy 89%
- Weighted F1 score 88%
- Macro F1 Avg score 64%

XGBoost + SMOTE: slight improvement on the F1 Macro scores of AFM and FiM.



Pre-SMOTE

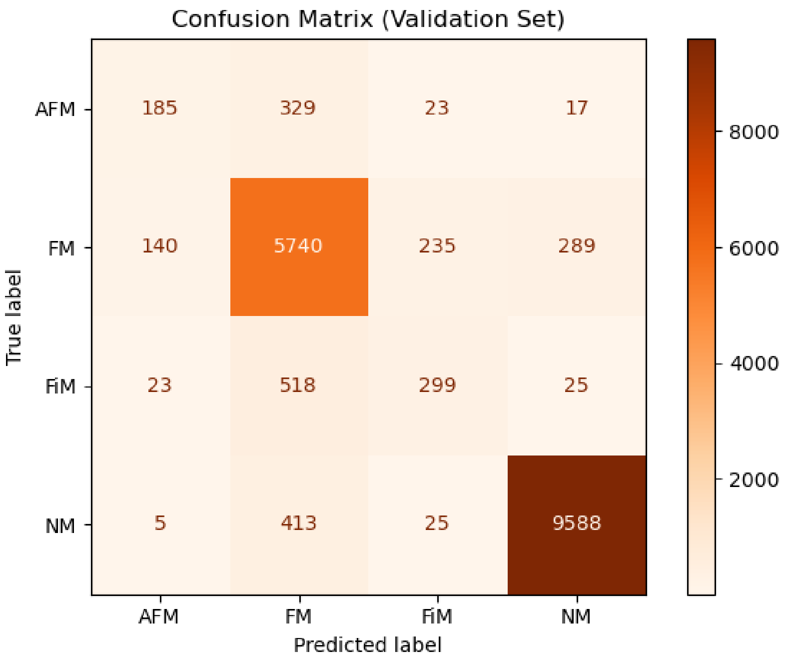
📊 Validation Classification Report:

	precision	recall	f1-score
AFM	0.61	0.23	0.34
FM	0.81	0.92	0.86
FiM	0.64	0.29	0.40
NM	0.97	0.96	0.96
accuracy			0.89
macro avg	0.76	0.60	0.64
weighted avg	0.88	0.89	0.88

Post-SMOTE

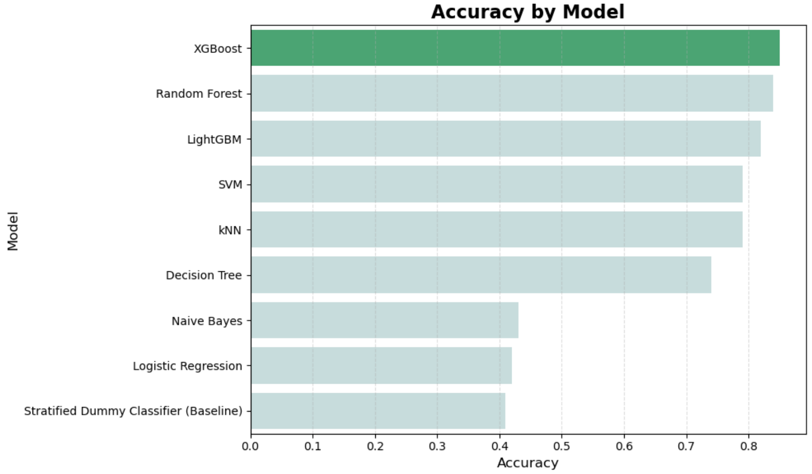
📊 Validation Classification Report:

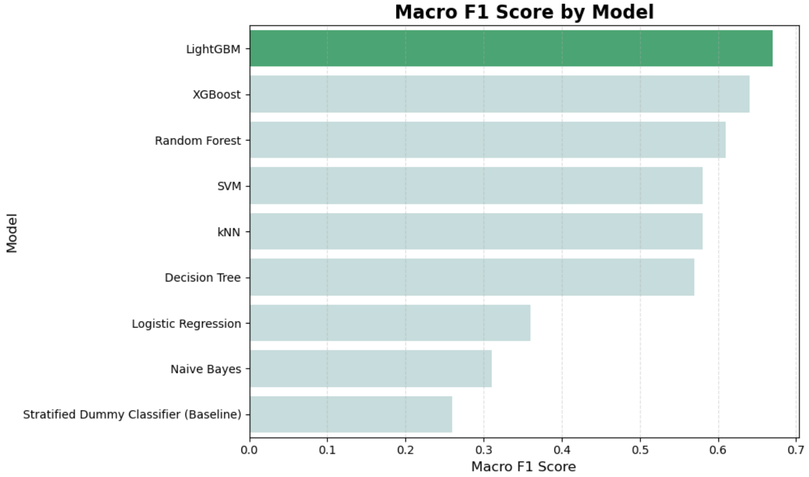
	precision	recall	f1-score
AFM	0.52	0.33	0.41
FM	0.82	0.90	0.86
FiM	0.51	0.35	0.41
NM	0.97	0.96	0.96
accuracy			0.89
macro avg	0.71	0.63	0.66
weighted avg	0.88	0.89	0.88

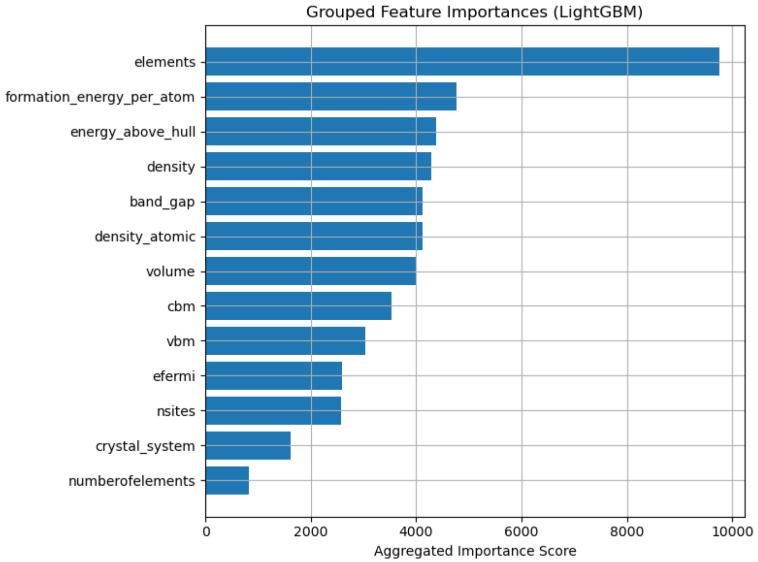


Model Comparison: *Materials Project* with Magnetic elements

```
transition_metals = {'Sc', 'Ti', 'V', 'Cr', 'Mn', 'Fe', 'Co', 'Ni', 'Cu', 'Y',
                     'Nb', 'Mo', 'Ru', 'Rh', 'Re', 'Os', 'Ir', 'Pt'}
lanthanides = {'Ce', 'Pr', 'Nd', 'Sm', 'Eu', 'Gd', 'Tb', 'Dy', 'Ho', 'Er', 'Tm', 'Yb'}
actinides = {'Th', 'U', 'Np', 'Pu'}
```

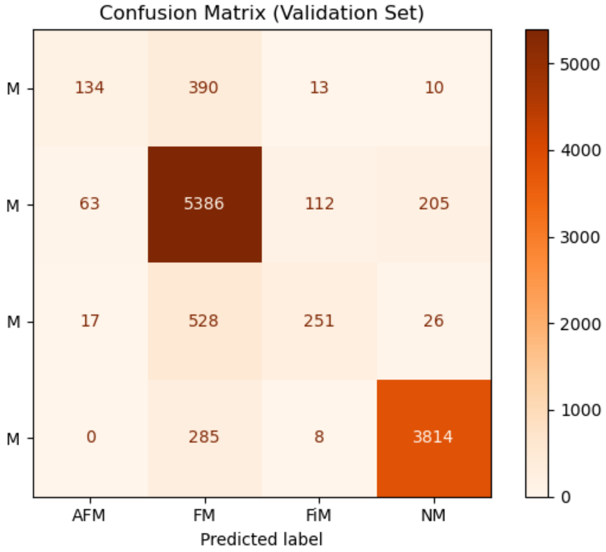


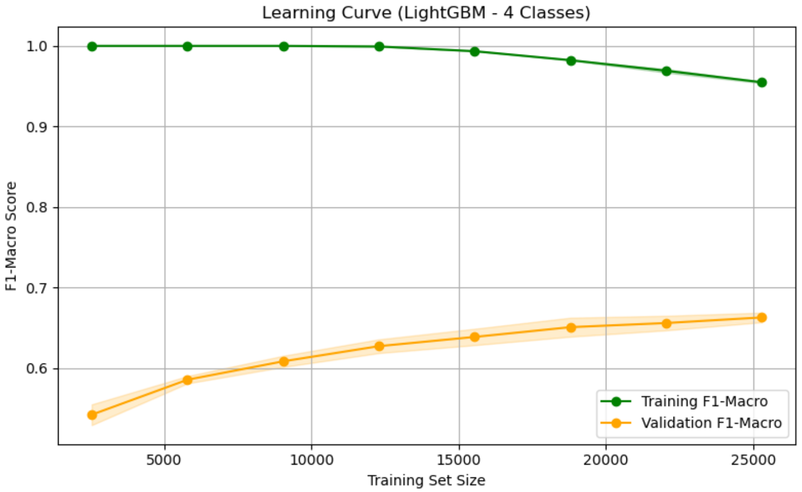




Classification Report (Validation Set)

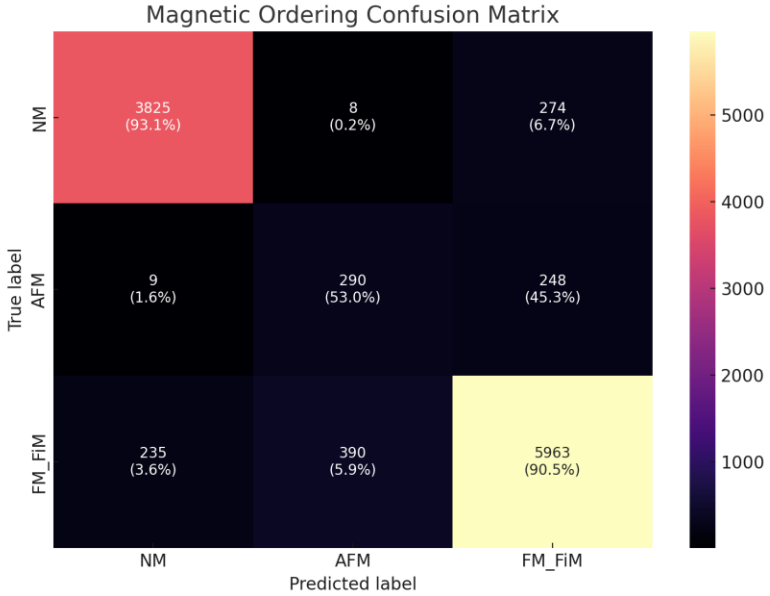
	Precision	Recall	F1-score
AFM	0.63	0.24	0.35
FM	0.82	0.93	0.87
FiM	0.65	0.31	0.42
NM	0.94	0.93	0.93
Accuracy			0.85
Macro avg	0.76	0.60	0.64
Weighted avg	0.84	0.85	0.84



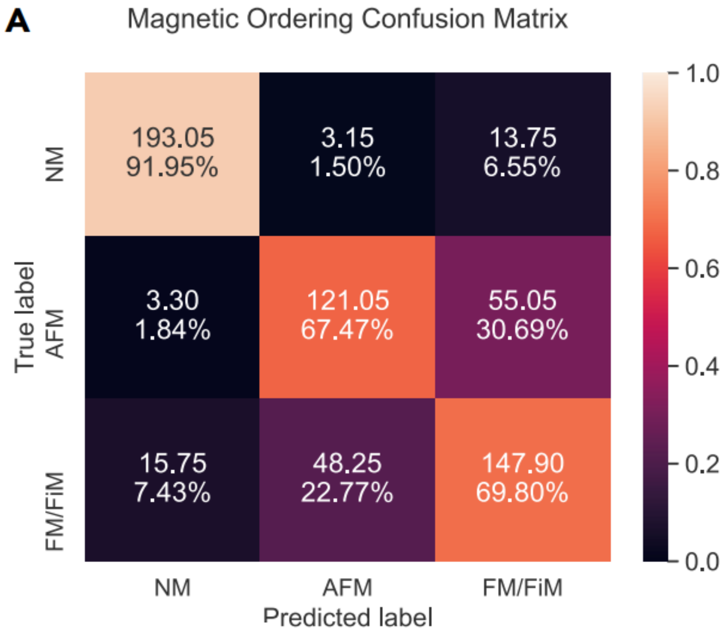


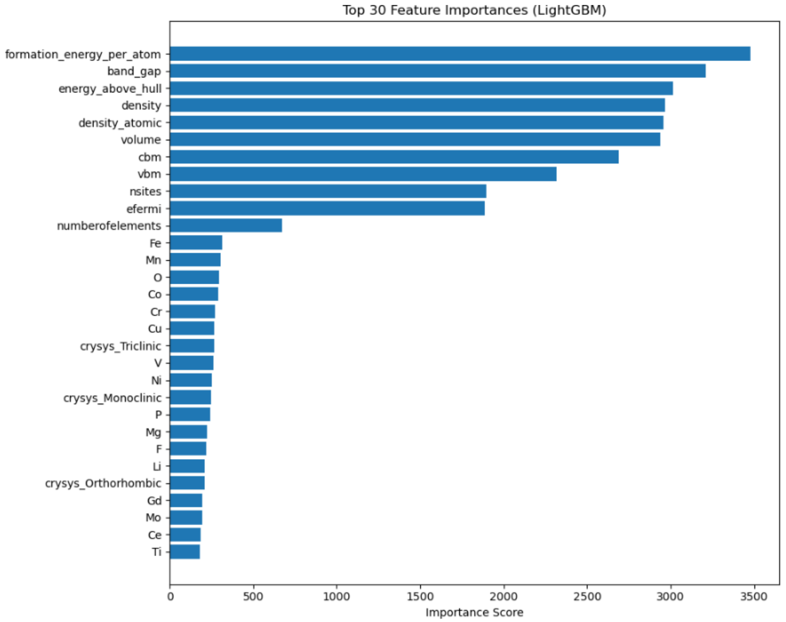
Model Comparison: *Materials Project* with Magnetic elements (merging FM and FiM)

Our LightGBM classifier



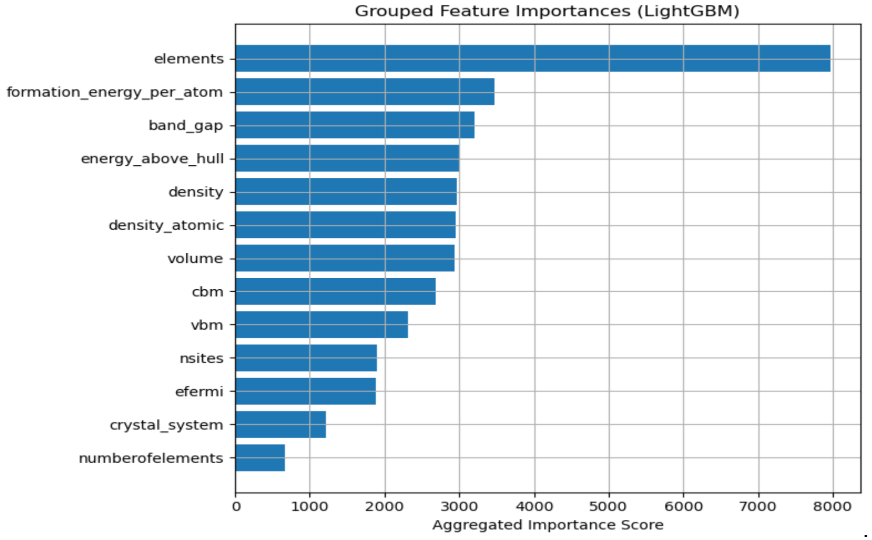
Recent research study*





📊 Validation Classification Report:

	precision	recall	f1-score	support
AFM	0.42	0.53	0.47	547
FM_FiM	0.92	0.91	0.91	6588
NM	0.94	0.93	0.94	4107
accuracy			0.90	11242
macro avg	0.76	0.79	0.77	11242
weighted avg	0.90	0.90	0.90	11242

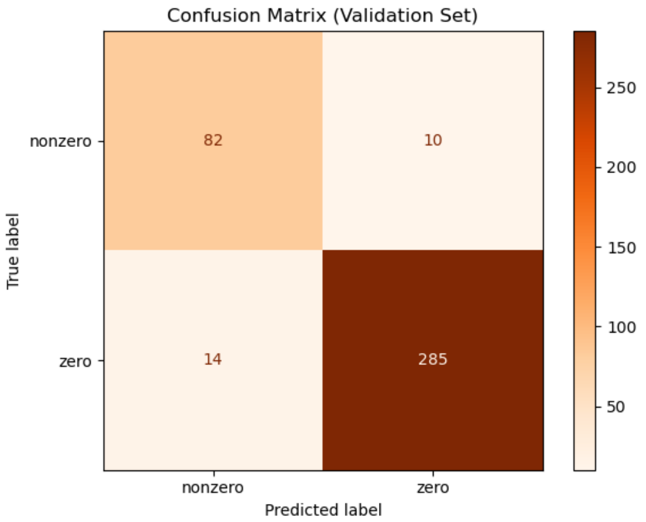


Our LightGBM outperforms recent literature* on the NM and FM/FiM classes and scores worse on the AFM class.

*Helena A. Merker, et al., "Machine learning magnetism classifiers from atomic coordinates", iScience (2022)

Model Training on MAGNDATA database to predict Propagation Vector

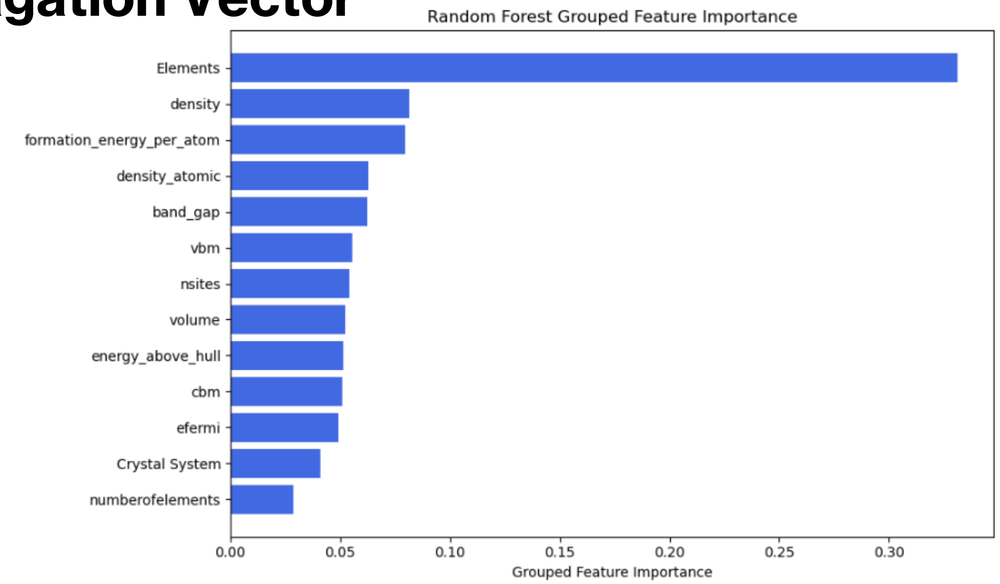
- Two classifier were trained: Random Forest and XGBoost. Result: Random Forest is higher performance on both accuracy and F1 macro avg score.
- Model training were chosen as 67.5% Training (with 6-fold cross validation), 22.5% Validation, 10% Testing.




```
📊 Validation Report:
              precision    recall  f1-score   support

     nonzero       0.85      0.89      0.87        92
        zero       0.97      0.95      0.96       299

    accuracy                           0.94       391
   macro avg       0.91      0.92      0.92       391
weighted avg       0.94      0.94      0.94       391
```



- Best classifier, after GridSearchCV, is then applied to the data of *Materials Project* (after removing the common subset of the two databases on which the training was performed).
- Predicted *12609* materials, which have 'FM' label on *Materials Project*, to have nonzero propagation vector (a contradiction: collinear FMs always have zero propagation vector) → therefore these materials are highly predicted, according to our classifier, to have non-FM label (either FiM or AFM), thereby partially address the FM bias in DFT calculations.

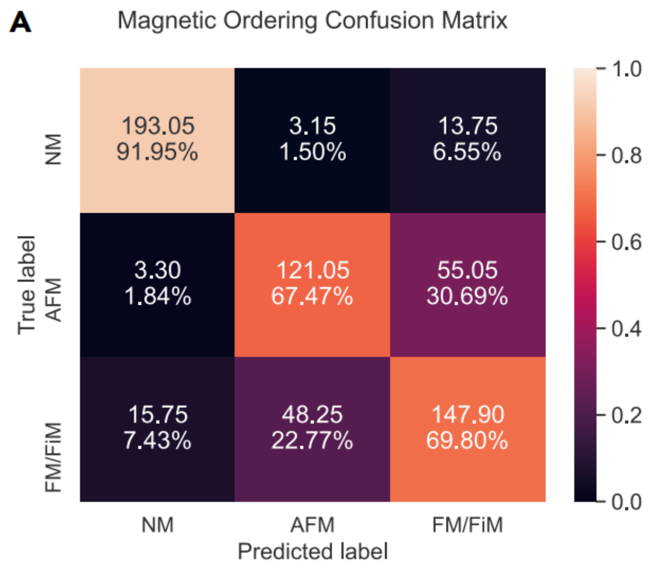
Examples out of the predicted-to-be wrongly labelled FMs on Materials Project after machine learning from MAGNDATA:

	formula	ordering	Predicted Propagation Vector
58369	CaLa2Co2Sb2(PbO6)2	FM	nonzero
29878	Ca(FeS2)2	FM	nonzero
43219	MgCo4(HgO4)2	FM	nonzero
38410	Li2FeBr4	FM	nonzero
85725	Mg6CoSiO8	FM	nonzero
44682	Mn2TeO6	FM	nonzero
41283	LiCo5O7F	FM	nonzero
70704	MgMn2(MoO4)2	FM	nonzero
8692	K2Na2Gd4Nb2O13	FM	nonzero
42306	LiZrHg2	FM	nonzero
80479	V2CdO10	FM	nonzero
42889	Mg30NbZnO32	FM	nonzero
80598	V3O5F3	FM	nonzero
87963	VO2	FM	nonzero
43840	MgMn6O11F	FM	nonzero
31544	CeMg6BO8	FM	nonzero
40950	Li9Mn2Co5O16	FM	nonzero
38332	Li2Cu2Si2O7	FM	nonzero
71692	MnCd(GaSe2)4	FM	nonzero
48859	Rb3Nb	FM	nonzero

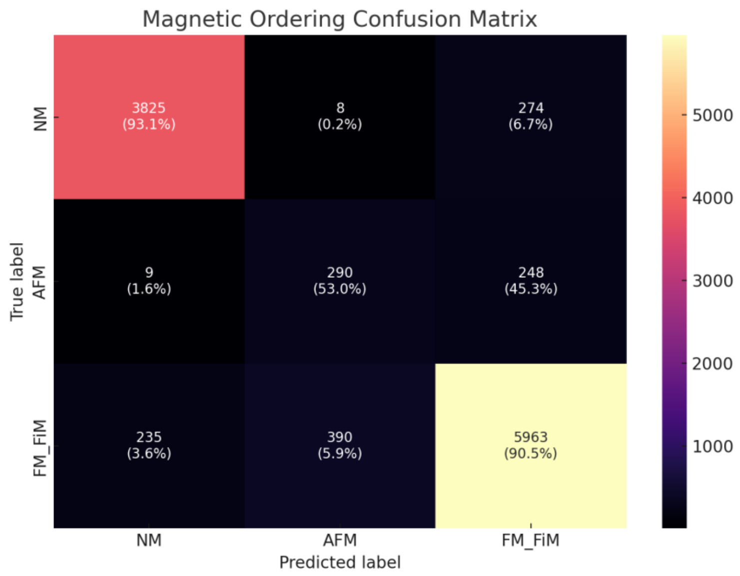
Conclusion and Future Directions

- Trained several machine learning models that can classify magnetic ordering efficiently on the *Materials Project* database.
- Trained machine learning models that can classify magnetic propagation vectors highly efficiently on the MAGNDATA database and applied it on the *Materials Project* database **to partially correct some of FM bias in the DFT calculations (for more than 12000 materials).**
- **Therefore, taking a more serious step in tackling the grand challenge of magnetism prediction.**
- Performance of LightGBM (shown on bottom right) surpasses that of a recent literature study (shown on top right) that worked on the 3 classes case.
- Future work: More exhaustive hyperparameter optimization, use of Neural Networks, and adding more detailed features to predict details of noncollinear magnetic structures .

Recent research study*



Our LightGBM classifier



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