

The Neighborhood Influence in Magnetization

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Abstract—Magnetization, a fundamental property of materials, is driven by unpaired electron spins and their exchange interactions. This study leverages the Materials Project API, a database of approximately 70,000 inorganic compounds with DFT-calculated magnetization values, to investigate the relationship between local atomic environments and magnetization. Focusing on high-magnetization compounds ($> 10 \mu\text{B}$), we analyzed neighborhood properties up to the fourth coordination shell, identifying recurring structural configurations and their chemical compositions. A Random Forest Regressor was employed to predict magnetization, achieving an R^2 score of 0.302 after hyperparameter optimization. Key findings highlight the role of coordination number, elemental diversity, and crystallographic symmetry in determining magnetic behavior, with uniform local environments correlating with higher magnetization. This work demonstrates the potential of combining structural analysis with machine learning to uncover patterns in magnetic materials, offering insights for future materials design.

Index Terms—Magnetization, Machine Learning, Random Forest Regressor, Materials Project, Inorganic Compounds, Neighborhood Properties

I. INTRODUCTION

Magnetization is a critical property of materials, originating from unpaired electron spins and their exchange interactions, which determine whether a material exhibits ferromagnetic or antiferromagnetic behavior [1]. The local atomic environment plays a pivotal role in magnetic coupling, with factors such as coordination number (the number of adjacent atoms) and bond lengths influencing electron spin alignment. Higher coordination numbers generally enhance magnetic interactions, while shorter bond lengths improve orbital overlaps, strengthening exchange coupling and increasing magnetization [2].

This study utilizes the Materials Project API, a comprehensive database of approximately 70,000 inorganic compounds with density-functional-theory (DFT)-calculated properties, to investigate trends in magnetization [3]. By focusing on high-magnetization compounds (magnetization $> 10 \mu\text{B}$), we aim to identify patterns in local atomic environments that contribute to strong magnetic behavior, particularly in transition metal compounds. The analysis examines neighborhood properties up to the fourth coordination shell, identifies recurring structural configurations, and employs machine learning to predict magnetization based on these features. This dual approach—combining structural analysis with predictive modeling—provides a robust framework for understanding and designing magnetic materials.

II. DATA COLLECTION AND PREPARATION

A. Data Source

The dataset was sourced from the Materials Project API, which provides DFT-calculated properties for approximately 70,000 inorganic compounds. Relevant fields extracted include material ID, chemical formula, total magnetization, magnetic ordering, symmetry (space group) and neighborhood configurations up to 4th places. A filtering process was applied to identify magnetic compounds by excluding non-magnetic entries (ordering labeled as “NM” or “NONMAGNETIC”) and retaining only those with a total magnetization greater than zero. This process was conducted across all 230 space groups, resulting in a collection of magnetic compounds.

To ensure uniqueness, duplicate entries were removed by tracking material IDs, yielding a final set of 70,000 unique magnetic compounds. This dataset was further refined by focusing on high-magnetization compounds with magnetization exceeding $10 \mu\text{B}$, reducing the dataset to approximately 25,000 entries. This subset emphasizes transition metal compounds, which are known for high magnetization, facilitating statistical analysis and pattern identification. After that, I generated another dataset which take every unique atom in the compound as central atom and find the neighborhood configuration and After this I got around 80000 rows dataset.

B. Neighborhood Details Extraction

For each compound, the atomic structure was retrieved to analyze the local environment around a central atom (chosen as the first site in the structure). Neighborhood details were computed up to the fourth coordination shell, with a distance tolerance of 0.1 \AA to group atoms into shells. For each shell, the following properties were recorded:

- **Average Distance:** Mean distance from the central atom to neighbors in the shell (in Ångströms).
- **Count:** Number of atoms in the shell.
- **Species:** Elemental composition of the neighbors.
- **Vectors:** Displacement vectors from the central atom to each neighbor.

The data was transformed to emphasize neighborhood properties, resulting in a new dataset of 90,000 rows. Each row was reformatted from (material_id, central atom, compound) to ((total neighbors, neighbor details, distance) \times 4), representing the first four coordination shells. For example, a row transformed from (mp-234, A, ABC) to ((2, B(2), 1.01), (5, A(3), C(2)), 3.02), ...). This structure highlights the influence

of coordination number and bond lengths on magnetization, providing a detailed view of the local atomic environment.

III. ANALYSIS OF NEIGHBORHOOD PROPERTIES

A. Transition Metal Central Atoms

The analysis began by identifying the prevalence of transition metals as central atoms, given their association with high magnetization. All 32,463 unique magnetic compounds had transition metal central atoms, confirming their dominance in magnetic materials. The most frequent transition metals included:

- Mn: 8,216 entries
- Fe: 7,431 entries
- Co: 3,695 entries
- Cr: 2,570 entries
- V: 2,084 entries

A total of 31 unique transition metals were identified, with less frequent elements like Ac (3 entries) and Tc (27 entries) also present (see Fig. 1). This distribution highlights the prevalence of elements like Mn and Fe, which are known for their strong magnetic properties due to unpaired d-electrons.

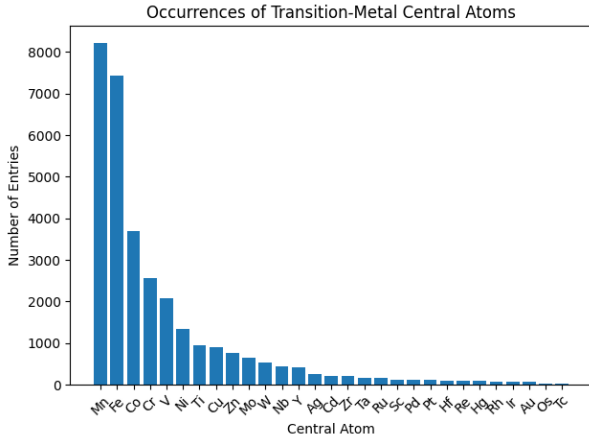


Fig. 1. Occurrences of Transition-Metal Central Atoms.

B. Space Group Analysis

The dataset was grouped by space group to examine the distribution of magnetic compounds and their neighborhood properties. The top 10 space groups by the number of materials were analyzed, focusing on the first coordination shell (Table I):

- **P1**: 4,972 materials, average 2.94 atoms, 1.11 distinct element types.
- **P2₁/c**: 2,235 materials, average 2.76 atoms, 1.04 distinct types.
- **P-1**: 2,190 materials, average 3.08 atoms, 1.07 distinct types.
- **Pnma**: 1,241 materials, average 3.09 atoms, 1.05 distinct types.
- **C2/m**: 1,062 materials, average 3.76 atoms, 1.10 distinct types.

TABLE I
TOP 10 SPACE GROUPS BY NUMBER OF MATERIALS

Space Group	Avg. Atoms (1st Shell)	Avg. Distinct Types	Num. Materials
P1	2.94	1.11	4,972
P2 ₁ /c	2.76	1.04	2,235
P-1	3.08	1.07	2,190
Pnma	3.09	1.05	1,241
C2/m	3.76	1.10	1,062
Cm	3.72	1.17	947
C2/c	2.99	1.05	738
Pm	3.18	1.06	670
C2	3.30	1.10	445
P2 ₁	2.89	1.05	396

Space groups like P1 and P2₁/c, characterized by lower symmetry, contained the largest number of magnetic compounds, with first-shell coordination numbers ranging from 2.76 to 3.76. The number of distinct element types in the first shell was generally low (1.04–1.17), indicating that the immediate neighborhood often consists of a single dominant element type, which may enhance magnetic interactions through consistent exchange coupling.

C. Central Atom and Space Group Combinations

A granular analysis was conducted by grouping the data by both central atom and space group, focusing on the average number of neighbors and distinct element types across the first four coordination shells (see Fig. 2). The top 20 combinations were selected based on the number of materials:

- Fe in P1 (497 materials): 3.5 average neighbors in the first shell, 1.1 distinct types.
- Mn in P1 (489 materials): 3.2 average neighbors, 1.1 distinct types.
- The number of distinct element types increased in higher shells (e.g., 1.2–1.8 in the fourth shell), indicating greater diversity at larger distances.

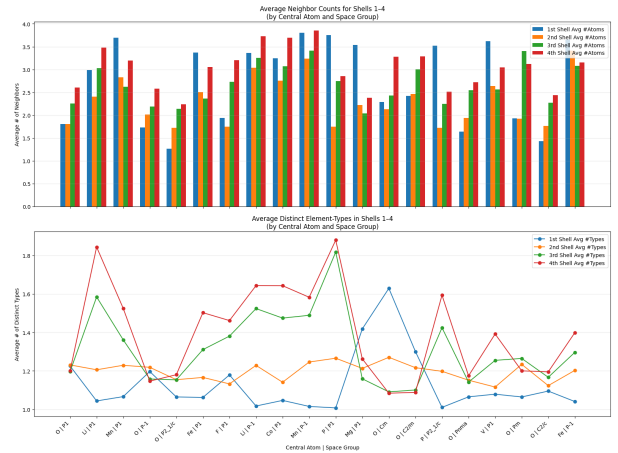


Fig. 2. Average Neighbor Counts and Distinct Element-Types in Shells 1–4.

This analysis underscores the interplay between the central atom, its crystallographic environment, and the resulting

neighborhood properties, which collectively influence magnetization.

IV. STRUCTURAL CONFIGURATION ANALYSIS

The structural configuration analysis aimed to uncover patterns in the local atomic environments of magnetic compounds, focusing on the arrangement and composition of atoms across the first four coordination shells. This analysis is crucial for understanding how the spatial and chemical organization of neighboring atoms influences magnetization, a property driven by exchange interactions between unpaired electron spins. By systematically examining recurring structural configurations and the diversity of element types within these shells, we sought to identify key factors that contribute to high magnetization, particularly in transition metal compounds.

A. Identifying Recurring Configurations

To characterize the local atomic environment, each compound's neighborhood was represented as a structural configuration, defined as a string of the form "N1—N2—N3—N4", where Ni denotes the total number of atoms in the i-th coordination shell. For example, a configuration of "1—1—1—1" indicates one atom in each of the four shells, while "4—2—2—2" indicates four atoms in the first shell and two atoms in each of the subsequent shells. This representation captures the coordination environment around a central atom, providing insight into the density and distribution of neighboring atoms.

Additionally, a "Unique_Config" was defined as a tuple (e.g., (1, 1, 1, 1)) representing the number of distinct element types in each shell. For instance, a Unique_Config of (1, 1, 1, 1) indicates that each shell contains atoms of only one element type, while (1, 1, 1, 2) indicates two distinct element types in the fourth shell. This dual representation allowed us to analyze both the structural arrangement (total atoms per shell) and the chemical diversity (distinct element types) of the local environment, both of which are critical to magnetic behavior.

The dataset, comprising 67,883 entries after preprocessing, was analyzed to identify the most frequent structural configurations. The top 50 configurations by frequency were examined to understand their prevalence and their correlation with magnetization (see Fig. 3). Key findings include:

- **Most Frequent Configurations:** The configuration "1—1—1—1" was the most frequent, appearing 684 times with an average magnetization of 24.1 μB . This configuration, characterized by minimal coordination (one atom per shell), suggests a sparse but highly uniform local environment. Other common configurations included "1—1—1—2" (553 occurrences, 23.3 μB), "4—2—2—2" (473 occurrences, 21.9 μB), and "1—1—2—2" (466 occurrences, 23.6 μB). These configurations vary in coordination density, with "4—2—2—2" indicating a denser first shell compared to "1—1—1—1".
- **Coordination and Magnetization Trends:** A notable trend emerged when comparing configurations

with different coordination numbers. Configurations with higher coordination numbers in the first shell, such as "4—2—2—2" (four atoms in the first shell), exhibited slightly lower average magnetization (21.9 μB) compared to those with lower coordination numbers, such as "1—1—1—1" (24.1 μB). This observation suggests a complex relationship between coordination density and magnetic behavior. In theoretical terms, a higher coordination number increases the number of exchange pathways, potentially strengthening magnetic interactions [1]. However, excessive coordination may introduce competing interactions or dilute the magnetic moment per atom, leading to a reduction in overall magnetization. For instance, in "4—2—2—2", the four atoms in the first shell may include non-magnetic elements or atoms with opposing spins, weakening the net magnetization.

- **Uniformity in Element Types:** Focusing on configurations with a (1, 1, 1, 1) Unique_Config—indicating one distinct element type per shell—the top 10 structural configurations were analyzed in greater detail. The "1—1—1—1" configuration again dominated, with an average magnetization of 24.1 μB , followed by "1—1—1—2" (23.3 μB) and "1—1—2—2" (23.6 μB). Other configurations in this subset, such as "8—6—12—24" (17.0 μB) and "4—2—2—4" (25.7 μB), showed a wider range of magnetization values. The high magnetization in configurations like "1—1—1—1" and "1—1—1—2" suggests that minimal diversity in element types across shells promotes consistent exchange interactions. When each shell contains atoms of the same element type, the magnetic coupling between the central atom and its neighbors is likely to be uniform, enhancing the alignment of electron spins and boosting magnetization [2]. Conversely, configurations with higher coordination numbers, such as "8—6—12—24", exhibited lower magnetization, possibly due to the increased likelihood of non-magnetic or antiferromagnetic neighbors diluting the overall magnetic moment.
- **Chemical Composition of Configurations:** The chemical composition of these configurations provides further insight. For example, in configurations like "1—1—1—1", the single atom in each shell was often a transition metal (e.g., Fe, Mn) or a ligand like oxygen (O), which is common in magnetic oxides. In contrast, denser configurations like "4—2—2—2" frequently included a mix of transition metals and non-magnetic elements (e.g., Zr, O, Cl), which may introduce competing interactions. The presence of non-magnetic elements in the coordination shells can disrupt ferromagnetic alignment, reducing the net magnetization, as observed in configurations with lower average magnetization values.
- **Structural Implications:** The prevalence of sparse configurations like "1—1—1—1" and "1—1—1—2" may reflect the crystallographic constraints of certain space groups, such as P1 and P2₁/c, which dominated the

dataset. These space groups, characterized by lower symmetry, allow for a variety of atomic arrangements but often favor simpler coordination environments around magnetic atoms. In contrast, configurations with higher coordination numbers, such as “8—6—12—24”, were more common in higher-symmetry space groups like Cmc_m, where the central atom is surrounded by a larger number of neighbors due to lattice packing effects. This interplay between structural configuration and crystallographic symmetry highlights the importance of considering both local and global structural factors in understanding magnetization.

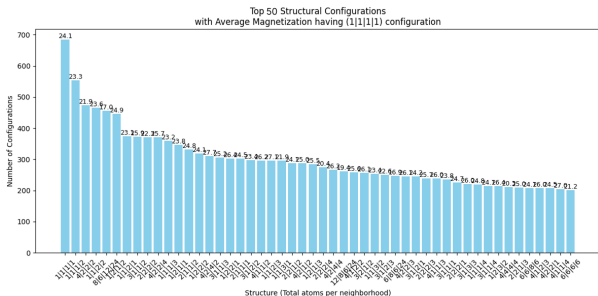


Fig. 3. Top 50 Structural Configurations with Average Magnetization having (1—1—1—1) configuration.

B. Frequency of Unique Configurations

The frequency of unique configurations, defined by the number of distinct element types in each shell, was analyzed to assess the chemical diversity of the local environment and its impact on magnetization. The Unique_Config tuple (e.g., (1, 1, 1, 1)) provides a compact representation of the elemental composition across the four shells, complementing the structural configuration analysis. The top 25 unique configurations were examined to determine their prevalence and distribution within the dataset (see Fig. 4).

- Dominance of Simple Configurations:** The Unique_Config (1, 1, 1, 1) was overwhelmingly dominant, appearing 22,378 times out of 67,883 entries, accounting for approximately 33% of the dataset. This configuration indicates that each of the four coordination shells contains atoms of only one element type, reflecting a highly uniform chemical environment. The second most frequent configuration, (1, 1, 1, 2), appeared 9,772 times (14.4%), followed by (1, 1, 2, 2) with 6,688 occurrences (9.8%). These three configurations alone account for over 57% of the dataset, indicating that the majority of magnetic compounds exhibit simple neighborhood compositions with minimal elemental diversity.
- Implications for Magnetic Behavior:** The dominance of (1, 1, 1, 1) reinforces the hypothesis that uniformity in the local environment enhances magnetic properties. In a (1, 1, 1, 1) configuration, the central atom is surrounded by neighbors of the same element type in each shell,

which may promote consistent exchange interactions. For transition metal central atoms like Fe or Mn, this uniformity often means that the neighbors are either the same transition metal (forming a metallic cluster) or a single ligand type (e.g., O in oxides), both of which can support ferromagnetic coupling [3]. The high frequency of (1, 1, 1, 2) and (1, 1, 2, 2) suggests a gradual increase in diversity in the outer shells, which may still maintain strong magnetic interactions if the additional element types are compatible with the central atom’s magnetic moment.

- Comparison with Structural Configurations:** Cross-referencing unique configurations with structural configurations provides additional insight. For instance, the (1, 1, 1, 1) Unique_Config often corresponds to structural configurations like “1—1—1—1” and “4—2—2—2”, but the magnetization trends differ. The “1—1—1—1” configuration with (1, 1, 1, 1) has a higher average magnetization (24.1 μ B) compared to “4—2—2—2” with (1, 1, 1, 1) (21.9 μ B), despite both having uniform element types. This difference highlights the interplay between coordination density and chemical composition: sparse coordination may optimize magnetic interactions by minimizing competing effects, while denser coordination may introduce subtle variations in bond lengths or angles that affect spin alignment.
- Elemental Diversity and Magnetization:** Configurations with greater elemental diversity, such as (1, 2, 2, 2) or (2, 2, 2, 2), were less frequent, appearing in fewer than 1,000 entries each. These configurations often involved a mix of transition metals and non-magnetic elements (e.g., Zr, Cl, O), which can introduce antiferromagnetic coupling or reduce the net magnetic moment. For example, a configuration like Zr(6)—Cl(12)—Cl(6)—O(24) with a (1, 1, 1, 1) Unique_Config (indicating one element type per shell but different elements across shells) had a magnetization of 24.9 μ B, lower than expected for a transition metal compound, likely due to the non-magnetic nature of Cl and O atoms diluting the magnetic contribution of Zr.
- Crystallographic Context:** The distribution of unique configurations is also influenced by the space group of the compound. Space groups like P1 and P-1, which dominated the dataset, frequently exhibited (1, 1, 1, 1) configurations due to their lower symmetry, allowing for simpler coordination environments. In contrast, higher-symmetry space groups like Cmc_m and C2/m were more likely to exhibit configurations with greater diversity, such as (1, 1, 2, 2), due to the presence of multiple equivalent sites in the lattice. This suggests that crystallographic symmetry plays a dual role: it dictates the structural arrangement of atoms (coordination numbers) and influences the chemical diversity of the neighborhood, both of which impact magnetization.
- Theoretical Insights:** From a theoretical perspective, the prevalence of simple unique configurations aligns with the principles of exchange interaction in magnetic materi-

als. The exchange interaction, which determines whether spins align ferromagnetically or antiferromagnetically, is strongest when the local environment is uniform, as variations in element types can introduce differences in exchange constants [4]. For instance, in a (1, 1, 1, 1) configuration with Fe as the central atom and O as the neighbor in all shells (e.g., in Fe oxides), the Fe-O-Fe superexchange interaction can promote ferromagnetic alignment, leading to high magnetization. In contrast, a (1, 1, 2, 2) configuration with mixed neighbors (e.g., Fe with O and Cl) may introduce competing interactions, reducing the net magnetization.

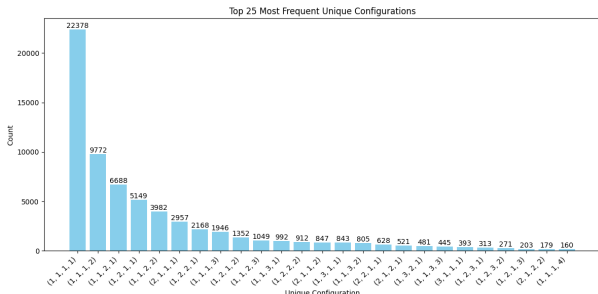


Fig. 4. Top 25 Most Frequent Unique Configurations.

C. Interplay Between Structure, Composition, and Magnetization

The structural configuration analysis reveals a nuanced interplay between coordination density, elemental diversity, and magnetization. Sparse configurations like “1—1—1—1” with uniform element types (1, 1, 1, 1) consistently exhibit higher magnetization, likely due to optimized exchange interactions in a simple, uniform environment. In contrast, denser configurations like “4—2—2—2” or “8—6—12—24” show lower magnetization, possibly due to the increased likelihood of non-magnetic neighbors or competing interactions. This trend suggests that there may be an optimal coordination number for maximizing magnetization, beyond which additional neighbors dilute the magnetic moment.

The chemical composition of the shells further modulates this effect. Configurations with transition metal neighbors (e.g., Fe, Mn) in all shells tend to have higher magnetization compared to those with mixed neighbors (e.g., transition metals and ligands like Cl or O). This is consistent with the role of d-electrons in transition metals, which contribute unpaired spins essential for magnetism. The presence of non-magnetic elements, while structurally necessary in many compounds, can weaken the overall magnetic moment by reducing the density of magnetic interactions.

The space group also plays a critical role in shaping these configurations. Lower-symmetry space groups like P1 favor sparse, uniform configurations, which correlate with higher magnetization, while higher-symmetry space groups like Cmc₂m support denser, more diverse configurations, often

with lower magnetization. This interplay highlights the importance of considering both local (neighborhood) and global (crystallographic) factors in understanding magnetic behavior.

V. METHODOLOGY: MACHINE LEARNING APPROACH

A. Preprocessing Steps

The dataset was preprocessed to ensure compatibility with machine learning:

- **Numeric Features:** Local magnetization, neighbor distances, and coordination numbers were processed using median imputation for missing values and standardized with StandardScaler.
- **Categorical Features:** Central atom and neighbor elements were one-hot encoded to convert them into binary vectors.
- **Feature Engineering:** Features included “Local Magnetization,” neighbor distances, coordination numbers, and one-hot encoded categorical variables.

B. Model Selection

A Random Forest Regressor was chosen for its robustness in handling mixed data types and reducing overfitting through ensemble averaging of 100 decision trees [5]. The model balances accuracy and interpretability, making it suitable for predicting magnetization.

C. Model Pipeline

The pipeline integrated preprocessing and prediction:

- Numeric transformer: Median imputation and StandardScaler.
- Categorical transformer: One-hot encoding.
- Model: RandomForestRegressor with warm start enabled for incremental training.

D. Hyperparameter Optimization

A manual grid search was performed over parameters:

- `n_estimators`: [100, 200, 300]
- `max_depth`: [5, 10, 15]
- **Optimal configuration:** `n_estimators=300`, `max_depth=10`, yielding an R^2 score of 0.302 on the test set.

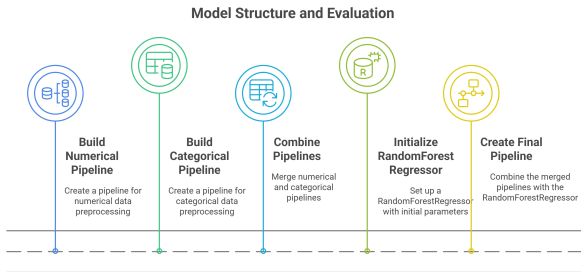


Fig. 5. Machine learning pipeline architecture showing data flow from preprocessing to prediction.

VI. RESULTS AND OBSERVATIONS

A. Model Performance

The Random Forest Regressor achieved an R^2 score of 0.302, indicating moderate predictive performance. Coordination number and neighbor distances were the most influential features, confirming their role in magnetic interactions.

B. Neighborhood Properties and Magnetization

- **Coordination Number:** Higher first-shell coordination numbers (3–4 atoms) correlated with strong magnetization, but excessive coordination reduced it.
- **Elemental Diversity:** Low diversity in the first shell (1–1.2 types) enhanced magnetization, while diversity increased in higher shells.
- **Space Group Influence:** Low-symmetry space groups (e.g., P1) favored high-magnetization configurations.

C. Structural Configurations and Magnetization Trends

Simple configurations like “1—1—1—1” with (1, 1, 1, 1) exhibited higher magnetization (24.1 μB) compared to denser ones like “4—2—2—2” (21.9 μB). Uniformity in element types across shells enhanced magnetization by promoting consistent exchange interactions.

D. Frequency of Unique Configurations

The analysis of unique configurations revealed that the (1,1,1,1) pattern dominated the dataset (33% of cases), demonstrating that uniform elemental composition across all coordination shells is a common feature in high-magnetization materials. This uniformity correlated with higher average magnetization values (24.1 μB) compared to more diverse configurations, suggesting that consistent local environments promote stronger magnetic interactions. The prevalence of these simple configurations across multiple space groups indicates their fundamental role in determining magnetic properties.

E. Transition Metal Dominance

The prevalence of Mn, Fe, and Co as central atoms aligns with their strong magnetic properties, driven by unpaired d-electrons.

VII. CONCLUSION

This study provides a comprehensive analysis of magnetization in inorganic compounds, combining structural analysis with machine learning. Neighborhood properties like coordination number and elemental diversity significantly influence magnetization, with uniform environments correlating with higher values. The Random Forest Regressor achieved moderate predictive accuracy ($R^2 = 0.302$), highlighting the potential of machine learning in materials science.

Key findings include the dominance of simple (1,1,1,1) unique configurations in high-magnetization materials, accounting for 33% of cases and demonstrating the importance of uniform elemental composition across coordination shells.

These configurations consistently showed higher magnetization values (24.1 μB) compared to more diverse arrangements, reinforcing that consistent local environments promote stronger magnetic interactions.

Future work could explore additional features (e.g., electronic structure) or advanced models to enhance predictions, guiding the design of high-magnetization materials. The insights gained from analyzing unique configurations provide a valuable framework for understanding the structural basis of magnetic behavior in inorganic compounds.

REFERENCES

- [1] J. M. D. Coey, *Magnetism and Magnetic Materials*. Cambridge, UK: Cambridge University Press, 2010.
- [2] R. Skomski and J. M. D. Coey, *Permanent Magnetism*. Bristol, UK: IOP Publishing, 1999.
- [3] A. Jain *et al.*, “The Materials Project: A materials genome approach to accelerating materials innovation,” *APL Materials*, vol. 1, no. 1, p. 011002, 2013.
- [4] P. W. Anderson, “Antiferromagnetism,” *Physical Review*, vol. 79, no. 2, pp. 350–356, 1950.
- [5] L. Breiman, “Random forests,” *Machine Learning*, vol. 45, no. 1, pp. 5–32, 2001.