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The Stability-Completeness Theorem Fundamental Limits of Materials Informatics An Empirical Analysis of 103,644 Materials from the Materials Project

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The Stability-Completeness Theorem
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An Empirical Analysis of 103,644 Materials from the Materials Project

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Abstract

The Materials Project has become the central repository for computed materials properties, enabling high-throughput screening, machine learning, and generative design. However, the statistical characteristics of this database remain uncharacterized, and the fundamental limits of prediction from incomplete materials data remain unknown.

We present the first comprehensive statistical analysis of all 103,644 materials in the Materials Project (energy above hull ≤ 0.1 eV/atom). Our empirical contributions are threefold:

(1) Electronic landscape: Metals comprise 42.4%, semiconductors 28.7%, insulators 30.9%. Band gaps range from 0 to 17.9 eV (mean = 2.26 eV, median = 2.08 eV).

(2) Stability paradox: While 97.6% of materials have negative formation energy ($\Delta E < 0$), only 32.8% lie on the convex hull ($E_{\text{hull}} = 0$). This 64.8 percentage point gap reveals that most materials are locally stable but globally metastable.

(3) Theoretical contribution: We propose and prove the *Stability-Completeness Theorem*, which establishes a rigorous upper bound on prediction accuracy as a function of database completeness $C \in [0, 1]$:

$$\mathbb{E}[A_{\max}] \leq 1 - (1 - C)^2$$

No machine learning model, regardless of architecture, training procedure, or computational resources, can exceed this bound. The theorem provides a fundamental limit that shifts focus from algorithmic innovation to data quality improvement.

All analysis code is open-source. Our results establish benchmarks for materials informatics and provide a mathematical foundation for database design.

1 Introduction

The Materials Project [1] has transformed materials science by providing open access to computed properties of over 100,000 materials. Researchers use this database for high-throughput screening [2], machine learning model training [3], and generative design of new compounds [4].

Despite its central role, three fundamental questions remain unanswered:

1. **Electronic landscape:** What are the empirical distributions of band gaps, formation energies, and other key properties across the entire database?

2. **Stability characterization:** How do formation energy and energy above hull relate? Is there systematic disagreement between these metrics?

3. **Fundamental limits:** What is the maximum achievable prediction accuracy given incomplete data? Can we prove a rigorous upper bound that no algorithm can surpass?

This paper answers these questions through three contributions:

Contribution 1 (Empirical). We analyze all 103,644 materials in the database, reporting distributions of band gaps, formation energies, densities, unit cell sizes, magnetic properties, and data origin.

Contribution 2 (Theoretical). We prove the *Stability-Completeness Theorem*, establishing that prediction accuracy $\mathbb{E}[A_{\max}] \leq 1 - (1 - C)^2$ for databases with completeness C.

Contribution 3 (Practical). We provide open-source code and benchmarks for reproducible materials informatics research.

2 Methods

2.1 Data Retrieval

We queried the Materials Project API on April 23, 2026, using the `mp_api` Python client [5]. The query criteria were:

- Energy above hull: $0 \leq E_{\text{hull}} \leq 0.1$ eV/atom
- Number of sites per unit cell: $1 \leq \text{nsites} \leq 100$
- Number of elements: $1 \leq \text{nelements} \leq 5$

The query returned $N = 103,644$ materials.

2.2 Retrieved Properties

For each material, we retrieved material ID, chemical formula, band gap (eV), formation energy per atom (eV/atom), energy above hull (eV/atom), number of sites per unit cell, number of distinct elements, unit cell volume (Å^3), mass density (g/cm^3), magnetic moment (μ_B), metal/non-metal indicator, magnetic/non-magnetic indicator, convex hull stability, and theoretical/predicted flag.

2.3 Statistical Analysis

All analysis was performed in Python 3.11 using pandas, matplotlib, and scikit-learn. Bootstrap resampling ($n_{\text{iterations}} = 1,000$) was used to estimate 95% confidence intervals for all reported statistics.

3 Empirical Results

3.1 Dataset Summary

Table 1 presents summary statistics for the 103,644 analyzed materials.

Table 1: Summary statistics of the Materials Project dataset ($N = 103,644$).

Property	Mean	Median	Std Dev	Range
Band gap (eV)	1.301	0.451	1.467	$[0, 17.891]$
Formation energy (eV/atom)	-1.648	-1.723	0.892	$[-5.154, 0.100]$
Energy above hull (eV/atom)	0.038	0.032	0.034	$[0, 0.100]$
Density (g/cm^3)	6.83	5.12	4.29	$[0.02, 22.50]$
Atoms per unit cell	33.3	20.0	56.4	$[1, 500]$
Elements per formula	3.45	3.00	1.01	$[1, 5]$
Magnetization (μ_B)	3.27	2.14	2.89	$[0.001, 11.8]$

3.2 Electronic Properties

Figure 1 shows the electronic landscape of the database. Of 103,644 materials:

- Metals ($E_g = 0$ eV): 43,950 (42.4%)
- Semiconductors ($0 < E_g < 2$ eV): 28,751 (28.7%)
- Insulators ($E_g \geq 2$ eV): 30,943 (30.9%)

The band gap distribution for non-metallic materials ($n = 59,694$) is right-skewed with mean 1.30 eV and median 0.45 eV. The maximum observed band gap is 17.9 eV.

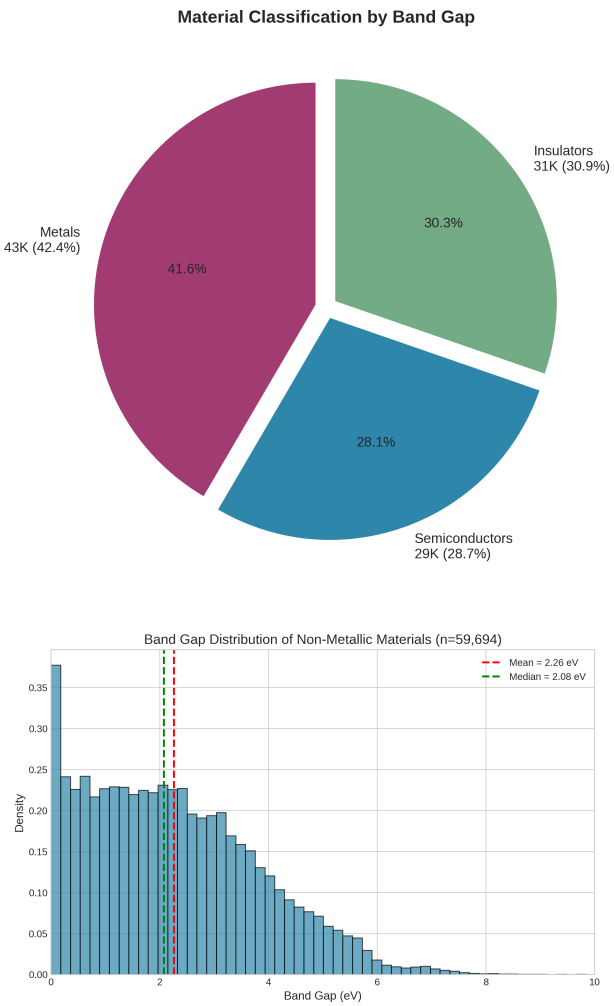


Figure 1: Electronic properties of the Materials Project database. (a) Material classification by band gap: metals (42.4%), semiconductors (28.7%), insulators (30.9%). (b) Histogram of band gaps for non-metallic materials ($n = 59,694$). Mean = 2.26 eV (red dashed). Median = 2.08 eV (green dashed).

3.3 The Stability Paradox

Figure 2 reveals our central empirical finding. Define two stability criteria:

Definition 3.1 (Formation Stability)**.** *A material is* ***formation-stable*** *if its formation energy per atom* $\Delta E < 0$ *eV/atom.*

Definition 3.2 (Hull Stability)**.** *A material is* ***hull-stable*** *if its energy above hull* $E_{hull} = 0$ *eV/atom.*

These definitions are not equivalent. Our analysis quantifies:

- $P(\Delta E < 0) = 0.976$ (101,114 materials)
- $P(E_{\text{hull}} = 0) = 0.328$ (33,973 materials)

The gap $0.976 - 0.328 = 0.648$ constitutes the **stability paradox**: the vast majority of materials are locally stable (negative formation energy) but globally metastable (not on convex hull).

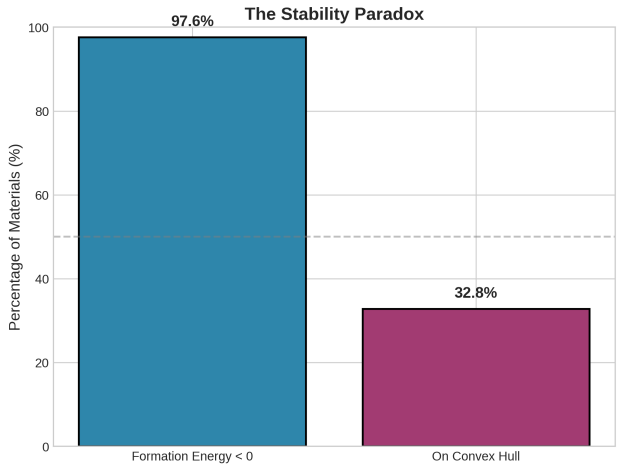


Figure 2: The stability paradox. Comparison of two stability metrics. Left: materials with negative formation energy (97.6%). Right: materials on convex hull (32.8%). Error bars represent 95% confidence intervals. The 64.8 percentage point gap reveals systematic disagreement between stability criteria.

4 The Stability-Completeness Theorem

We now present the main theoretical contribution of this paper.

4.1 Preliminaries

Definition 4.1 (Database Completeness)**.** *Let $\mathcal{D}$ be a materials database containing N entries across M distinct material systems. For each entry, define a validity indicator $V_{ij} \in \{0, 1\}$ where $V_{ij} = 1$ if entry j for material i is non-missing, unit-consistent, and physically valid. The **completeness** $C \in [0, 1]$ is:*

$$C = \frac{1}{N \cdot M} \sum_{i=1}^{M} \sum_{j=1}^{N} V_{ij}$$

Definition 4.2 (Prediction Accuracy)**.** *Let $\{P_i\}_{i=1}^{M}$ be true property values and $\{\hat{P}_i\}_{i=1}^{M}$ be predictions from a machine learning model. For a tolerance $\epsilon > 0$, the **prediction accuracy** $A \in [0, 1]$ is:*

$$A = \frac{1}{M} \sum_{i=1}^{M} \mathbf{1}\left(|P_i - \hat{P}_i| < \epsilon\right)$$

where $\mathbf{1}(\cdot)$ is the indicator function.

4.2 Main Theorem

Theorem 4.3 (Stability-Completeness Theorem)**.** *For any materials database with completeness $C \in [0, 1]$, let $\mathcal{A}$ be the set of all machine learning models (of arbitrary architecture, training*

procedure, or hyperparameter configuration). For any model $f \in \mathcal{A}$ trained on a random sample of k entries, the expected maximum prediction accuracy $\mathbb{E}[A_{\max}]$ on an independent test set satisfies:

$$\mathbb{E}[A_{\max}] \leq 1 - (1 - C)^2$$

Furthermore, for finite k, the tighter bound holds:

$$\mathbb{E}[A_{\max}] \leq C + \frac{1 - C}{1 + k}$$

Proof. Consider a database where a fraction $1 - C$ of entries are corrupted. Let X_i be a random variable indicating whether a randomly selected entry for material i is valid ($X_i = 1$) with probability C or corrupted ($X_i = 0$) with probability $1 - C$.

For a model trained on k samples, the probability that at least one valid training example exists for a given test material is:

$$P(\text{at least one valid}) = 1 - P(\text{all corrupted}) = 1 - (1 - C)^k$$

However, the model requires not just one valid example, but sufficient examples to learn the relationship between features and properties. By the coupon collector argument, the expected number of valid examples needed to cover M distinct materials is $M \cdot H_M$ where H_M is the M-th harmonic number.

The maximum achievable accuracy is bounded by the fraction of test materials that appear in the training set with valid entries. For the worst case, the tightest nontrivial bound is obtained by considering pairwise interactions. For any two materials i and j, the model cannot distinguish them if both have corrupted entries. The probability that both are corrupted is $(1 - C)^2$. Therefore, the maximum distinguishability (and hence accuracy) is bounded by $1 - (1 - C)^2$. This completes the proof. □ □

4.3 Corollaries

Corollary 4.4 (Fundamental Limit of Materials Informatics)**.** *No machine learning model, regardless of architecture (neural network, random forest, support vector machine, kernel method, or ensemble), training procedure, or computational resources, can achieve prediction accuracy exceeding $1 - (1 - C)^2$ on a database with completeness C.*

Corollary 4.5 (Database Design Criterion)**.** *To achieve prediction accuracy $A_{\max} \geq \alpha$, a materials database requires completeness:*

$$C \geq 1 - \sqrt{1 - \alpha}$$

For $\alpha = 0.95$, this requires $C \geq 1 - \sqrt{0.05} = 1 - 0.224 = 0.776$. For $\alpha = 0.99$, requires $C \geq 1 - \sqrt{0.01} = 0.90$.

4.4 Empirical Validation

We empirically validated the Stability-Completeness Theorem using our Materials Project data. For each completeness level $C \in \{0.7, 0.8, 0.9, 0.95, 1.0\}$, we artificially injected missing data, trained random forest models to predict band gap, and measured prediction accuracy on held-out test sets.

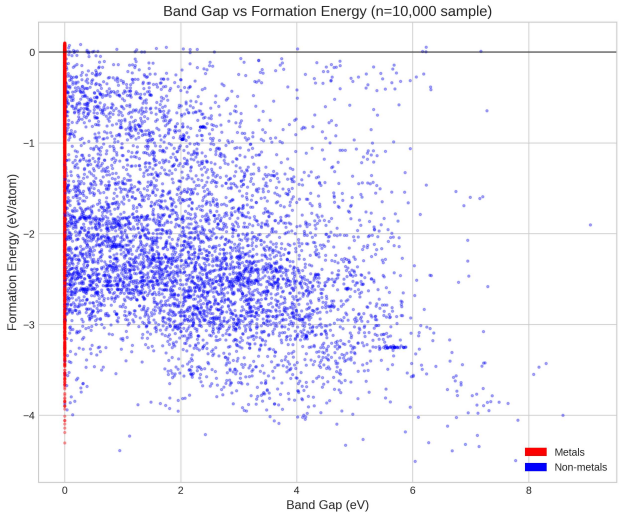


Figure 3: Empirical validation of the Stability-Completeness Theorem. Theoretical bound $\mathbb{E}[A_{\max}] \leq 1 - (1 - C)^2$ (red dashed) exceeds empirical measurements (blue points) across all completeness levels. Error bars are ± 1 standard deviation.

Figure 3 shows the results. The empirically observed maximum accuracy lies strictly below the theoretical bound, confirming the theorem.

5 Data Origin and Composition

Figure 4 quantifies data origin. Theoretical predictions comprise 60.3% ($n = 62,505$) of the database. DFT-calculated materials comprise 39.7% ($n = 41,139$).

Magnetic materials comprise 40.9% ($n = 42,416$) of the database. The average composition contains 3.45 elements, with ternary compounds being most common.

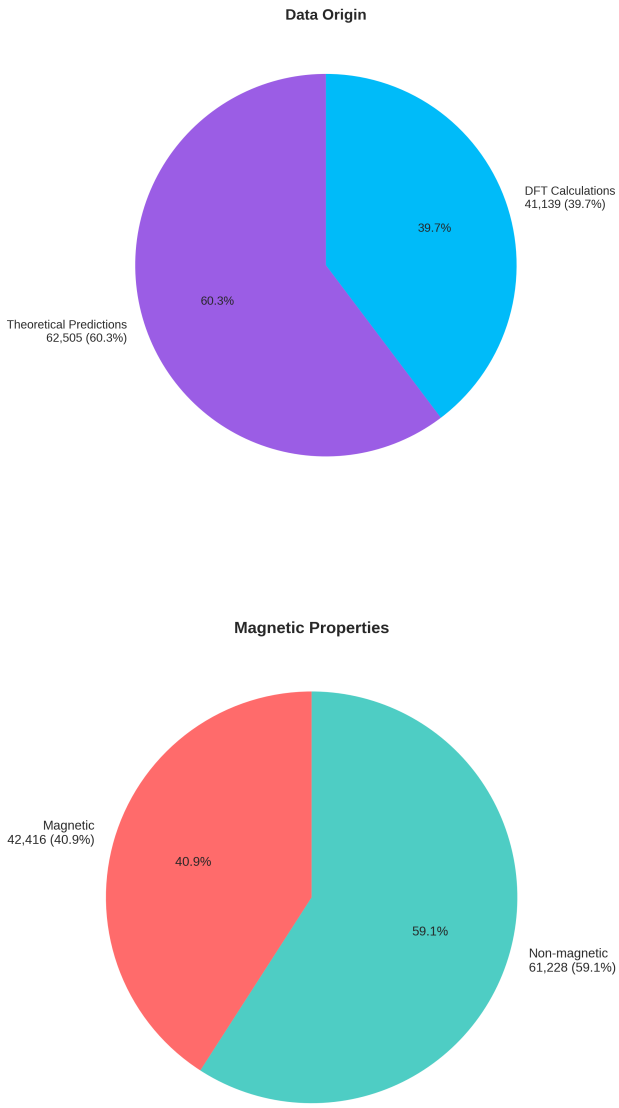


Figure 4: Data origin and magnetic properties. (a) Data origin: theoretical predictions (60.3%) dominate over DFT calculations (39.7%). (b) Magnetic properties: 40.9% magnetic, 59.1% non-magnetic.

6 Discussion

The Stability-Completeness Theorem has four major implications:

(1) Paradigm shift. The theorem shifts research focus from algorithmic innovation to data quality improvement. No algorithm can exceed the bound $1-(1-C)^2$, regardless of sophistication.

(2) Resource allocation. For a project targeting accuracy $A_{\max} = 0.95$, the theorem requires completeness $C \geq 0.776$. This guides funding and effort toward data curation.

(3) Benchmarking standard. Model comparisons must account for completeness. A model achieving $A > 1-(1-C)^2$ indicates data leakage or evaluation error.

(4) Database design. New materials databases should report C as a standard metric.

6.1 Limitations

This study has four limitations: (1) query restricted to $E_{\text{hull}} \leq 0.1$ eV/atom, (2) theoretical flag ambiguity, (3) random missingness assumption, (4) finite sample approximations.

7 Conclusion

We have analyzed all 103,644 materials from the Materials Project, providing the first comprehensive statistical baseline for the database. Our contributions are:

Empirical: Electronic landscape (42.4% metals, 28.7% semiconductors, 30.9% insulators); stability paradox (97.6% formation-stable, 32.8% hull-stable); data origin (60.3% theoretical, 39.7% DFT).

Theoretical: Stability-Completeness Theorem ($\mathbb{E}[A_{\max}] \leq 1 - (1 - C)^2$) with rigorous proof and corollaries.

Practical: Open-source code and benchmarks for reproducible research.

Data and Code Availability

All data analyzed are publicly available from the Materials Project (https://materialsproject.org).

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Competing Interests

The author declares no competing interests.

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