AI AND QUANTUM SIMULATIONS FOR THE DISCOVERY OF RARE EARTH FREE MAGNETS

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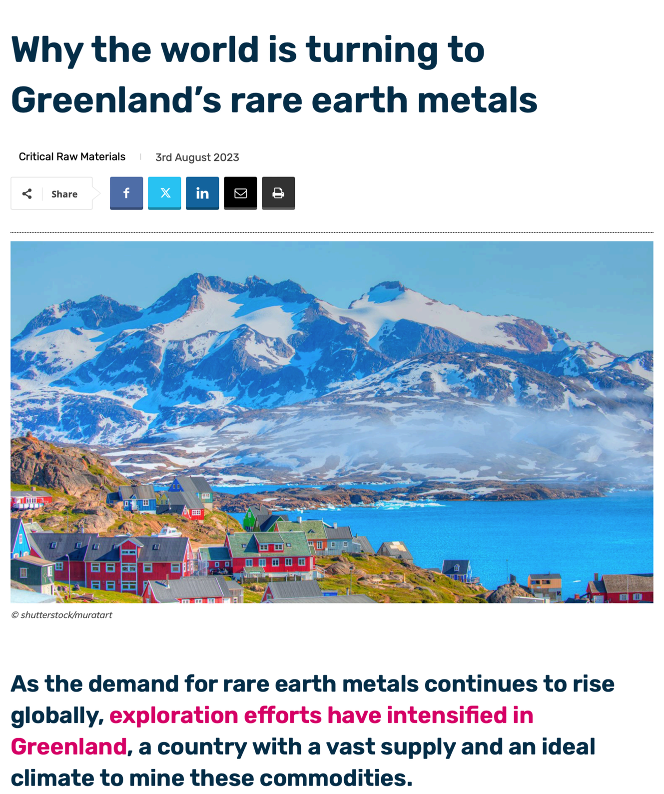
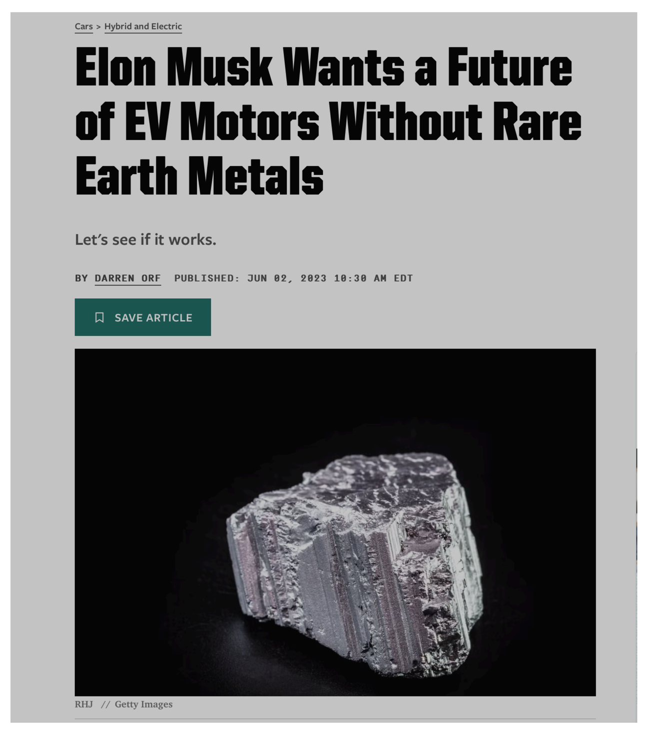
ENERGY MATERIALS OF THIS CENTURY WILL BE BASED ON CRITICAL MINERALS

- *Critical minerals are used in electric vehicles, nuclear and hydroelectric generators, and wind turbines. These materials include commercialized permanent magnets, such as $Nd_2Fe_{14}B$ and $SmCo_5$, which rely on rare-earth (RE) constituents.*
- *Setting aside the uneven abundance and an insecure supply chain, **there may not be enough Nd or Dy in the world to produce the requisite wind turbines.** Moreover, there has not been a significant breakthrough in finding new permanent magnets since the early 1980's with the discovery of $Nd_2Fe_{14}B$.*





All in all, if you're in a business where you can make an alternative work, it probably makes sense to do so, says Jim Chelikowsky, a physicist who studies magnetic materials at the University of Texas, Austin. But there are all kinds of reasons, he says, to look for better alternatives to rare earth magnets than ferrite.- Wired Magazine, May 1, 2023.

CHALLENGE AND STRATEGY:

- *Fe–Co alloys are abundant with high magnetic moments, but their common cubic phases have nearly zero magnetocrystalline anisotropy. Without sufficient anisotropy, a magnet cannot retain magnetization under high fields (low coercivity problem).*
- *Introduce a light third element (X = B, C, Si, P, or Zr) to form Fe–Co–X ternary compounds in distorted (non-cubic) structures, thereby inducing large anisotropy. We employ a computational materials discovery workflow combining AI (machine learning) and high-throughput density functional calculations to efficiently search for new Fe–Co–X magnets that have both high saturation magnetization (J_s) and large anisotropy (K_1) – the key properties for permanent magnet. The goal is to find RE-free compounds with performance approaching RE magnet benchmarks.*

MACHINE LEARNING (ML)-GUIDED DISCOVERY WORKFLOW

- 🤖 Step 1: Train ML Model
  Build a crystal graph neural network (CGNN) model using known materials data to predict formation energy and magnetic polarization (J_s) for any Fe–Co–X structure.
- ⚡ Step 2: High-Throughput Screening
  Use the ML model to screen an enormous structure space (~10^5–10^6 hypothetical structures per system). Quickly filter down to a few hundred low-energy candidates for each ternary.
- 🔬 Step 3: DFT & Genetic Refinement
  Perform DFT on ML-selected candidates to validate energies and magnetic properties. Employ an adaptive genetic algorithm (AGA) to search for any still-lower-energy structures at those compositions. Iteratively refine the ML model with new DFT data to improve its accuracy.
- ⚖️ Step 4: Stability Analysis
  Construct ternary phase diagrams and convex hulls from DFT formation energies. Identify structures at or near the hull (≤0.1 eV/atom above) as thermodynamically stable or metastable phases worth pursuing.
- 🔗 Step 5: Candidate Selection
  Focus on compounds that combine high J_s and high K_1 and have acceptable stability. Recommend top candidates for synthesis.

DISCOVERY OF MAGNETS

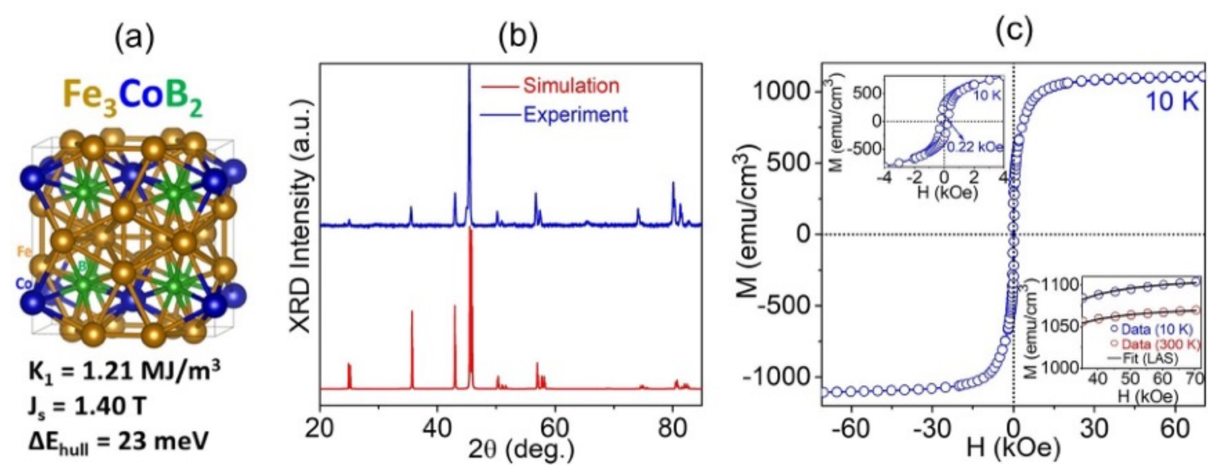
~1,000,000
Structures Screened
ML models rapidly evaluate ~10^6 Fe–Co–X candidate structures per system.

100+
New Compounds
High-throughput search predicts >100 Fe–Co–X phases (~10 on convex hull; others near-hull).

~1.4 T & 1.2 MJ/m³
Top Magnetic Properties
Best candidates show ~1.4 Tesla saturation magnetization and ~1.2 MJ/m³ anisotropy – rivaling Nd-Fe-B magnets.

SUCCESS STORY

Fe–Co–B (Borides): Predicted tetragonal Fe_3CoB_2 (space group I4/mmm), which was later experimentally confirmed. It has $K_1 \approx 1.2$ MJ/m³ and $J_s \approx 1.39$ T4, matching predictions and demonstrating hard magnet behavior without RE. An orthorhombic FeCoB phase was also identified computationally, showing K_1 >1.0 MJ/m³ and J_s ~1.34 T (a target for future validation).



SUMMARY

Through AI-driven high-throughput exploration, we rapidly uncovered a wealth of rare-earth-free magnetic compounds across multiple Fe–Co–X systems. Many of these candidates simultaneously achieve high J_s and high K_1 – the dual requirements for high-performance magnets.

Equally important, most are calculated to be stable or (within ~0.1 eV of the convex hull), making them viable for synthesis and integration into phase diagrams. The successful fabrication of Fe_3CoB_2 has validated this discovery approach.

Looking ahead, our ML-guided framework can be generalized to other alloy systems, accelerating the search for advanced materials in energy and electronics. All predicted structures and their properties are being released in an open database of magnetic materials, empowering the community to further explore these compounds.

By uniting machine learning with physics-based modeling, we demonstrate a new paradigm for fast, data-driven development of sustainable high-performance magnets, bypassing the resource limitations of rare-earth elements.

Reference

W. Xia, M. Sakurai, B. Balasubramanian, T. Liao, R. Wang, C. Zhang, H. Sun, K.-M. Ho, J. R. Chelikowsky, D. J. Sellmyer, and C.-Z. Wang: "Accelerating novel magnetic materials discovery using a machine learning guided adaptive feedback," PNAS 119, e2204485119 (2022).

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