MAGNITO

The Possibility of New Ultra-Strong Complex Magnet Materials

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Program Director

Advanced Research Projects Agency – Energy (ARPA-E)

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Executive Orders

Establishing the National Energy Dominance Council

UNLEASHING AMERICA'S OFFSHORE CRITICAL MINERALS AND RESOURCES

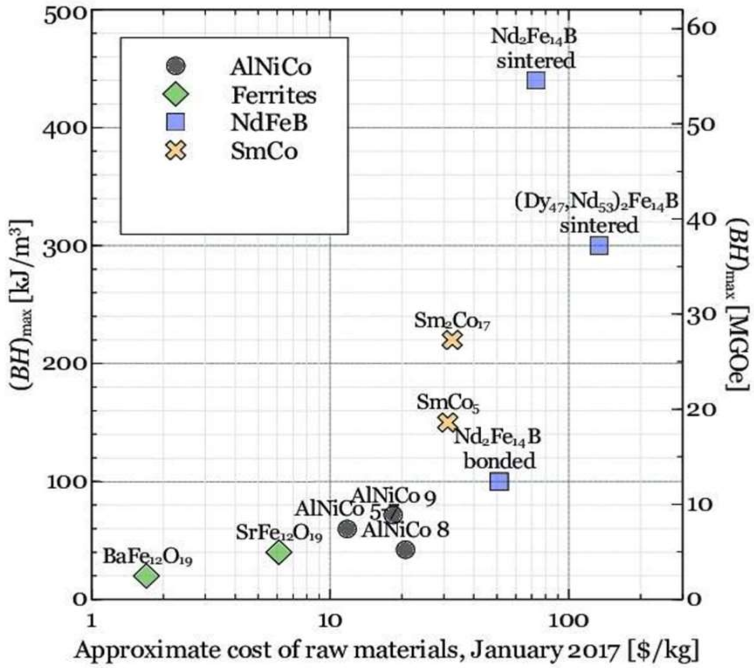
Immediate Measures to Increase American Mineral Production

ENSURING NATIONAL SECURITY AND ECONOMIC RESILIENCE THROUGH SECTION 232 ACTIONS ON PROCESSED CRITICAL MINERALS AND DERIVATIVE PRODUCTS

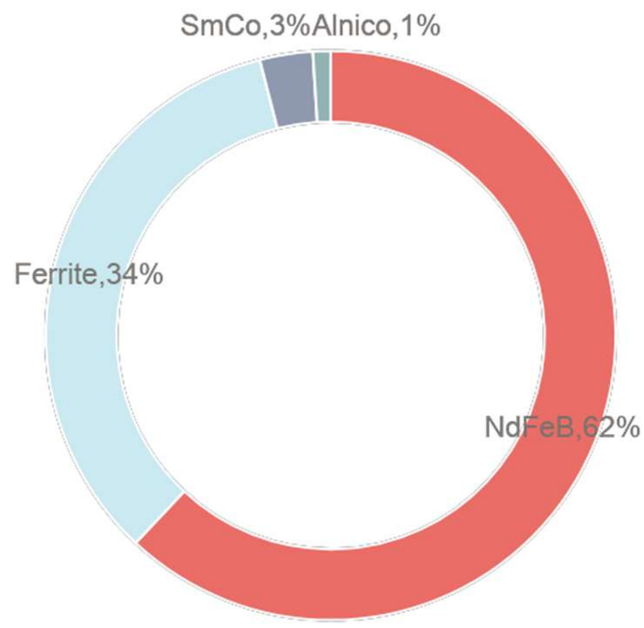
"Our national and economic security are now acutely threatened by our reliance upon hostile foreign powers' mineral production. It is imperative for our national security that the United States take immediate action to facilitate domestic mineral production to the maximum possible extent."

Strongest Magnets have the Largest Market Share

Cost and Performance Spectrum



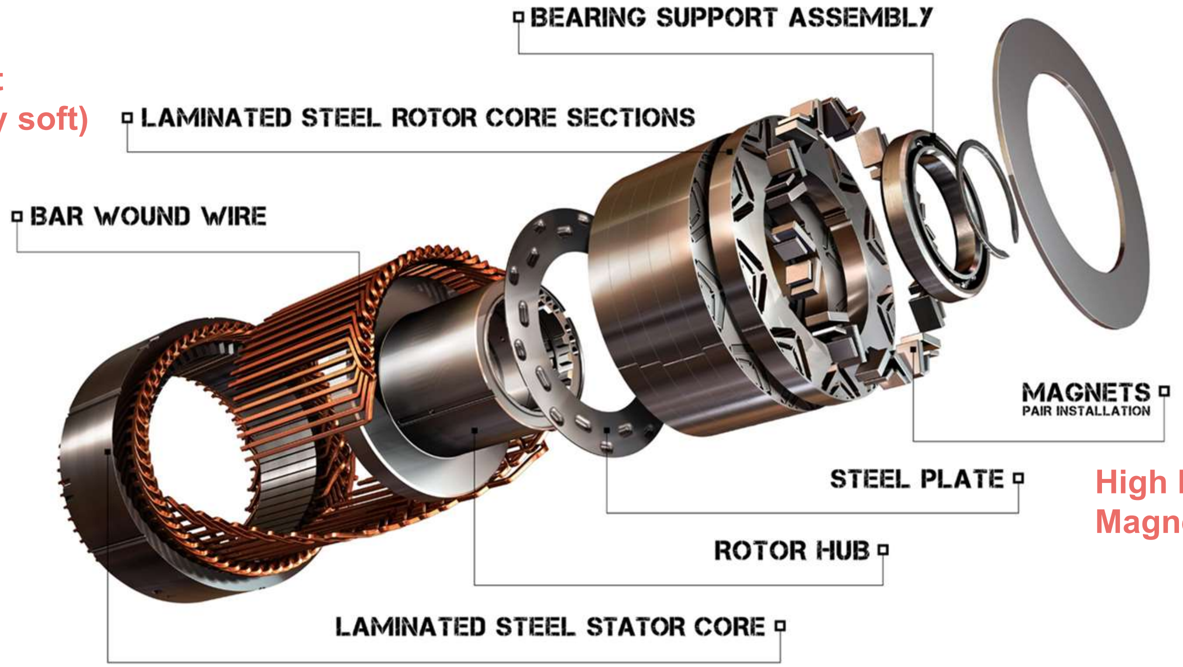
Market Share ($30B)



O. Gutfleisch, et al, Magnetic Materials and Devices for the 21st Century: Stronger, Lighter, and More Energy Efficient, Advanced Materials, August 2011, 20:1-22.

Permanent Magnet Motor-Generator: Hard, Soft and ??

High M_s Magnet
(not necessarily soft)

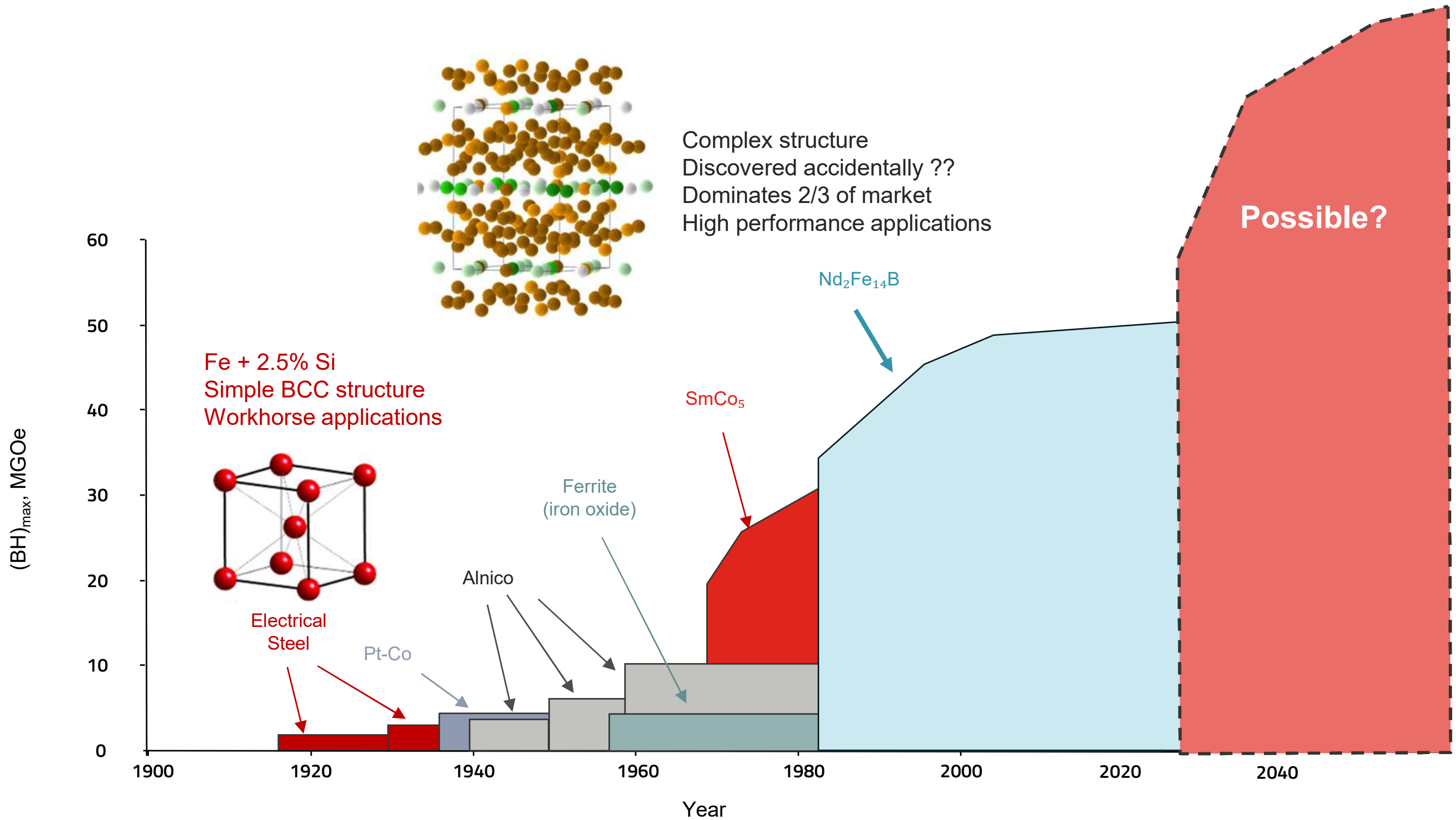


High BH_{max} Hard Magnet

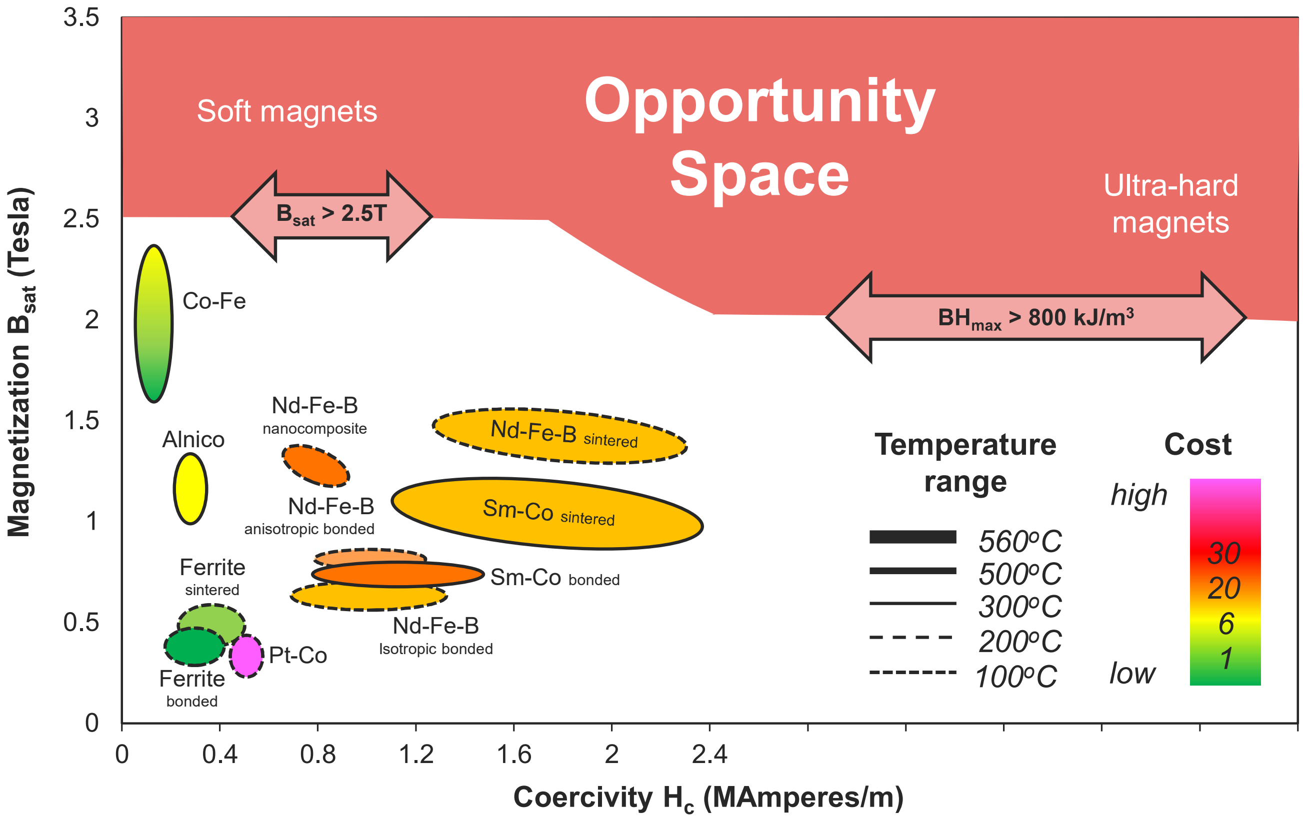
High M_s Soft Magnet

Interior permanent magnet (IPM) motor

No New Magnets Developed for Over 40 Years



What Metrics Would Revolutionize Magnets ?

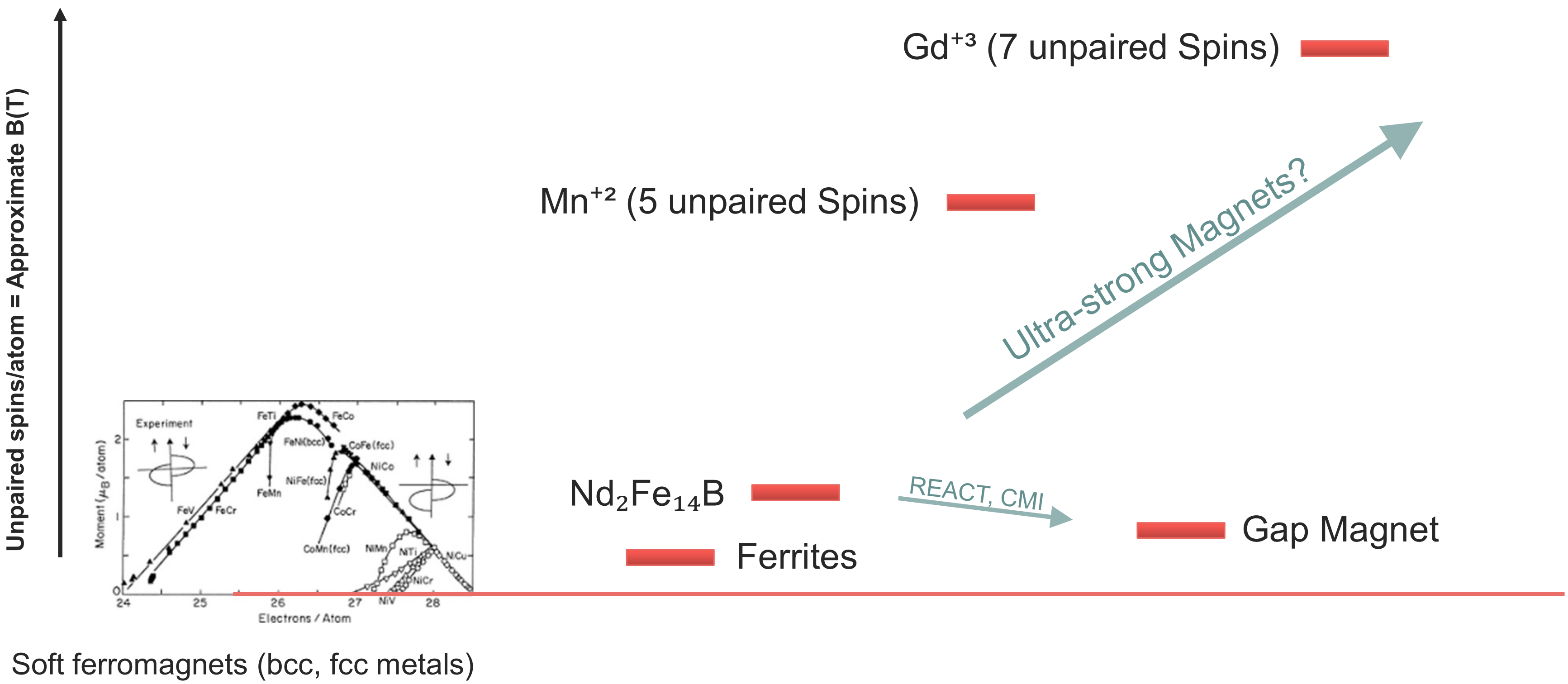


Higher B Field
than any soft or hard magnet
B_{sat} > 2.5 T

2× increase in BH_{max}
> 800 kJ/m³ (100MGOe)
will require B_{sat} > 2 T

Inset from Enclyclopedia Magnetica https://www.e-magnetica.pl/doku.php/s

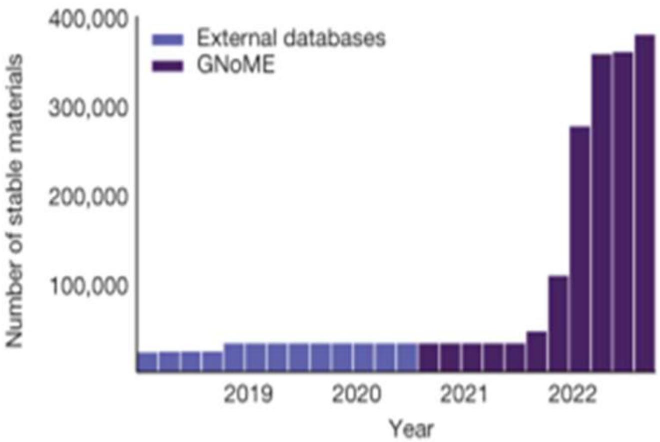
What is Possible ?

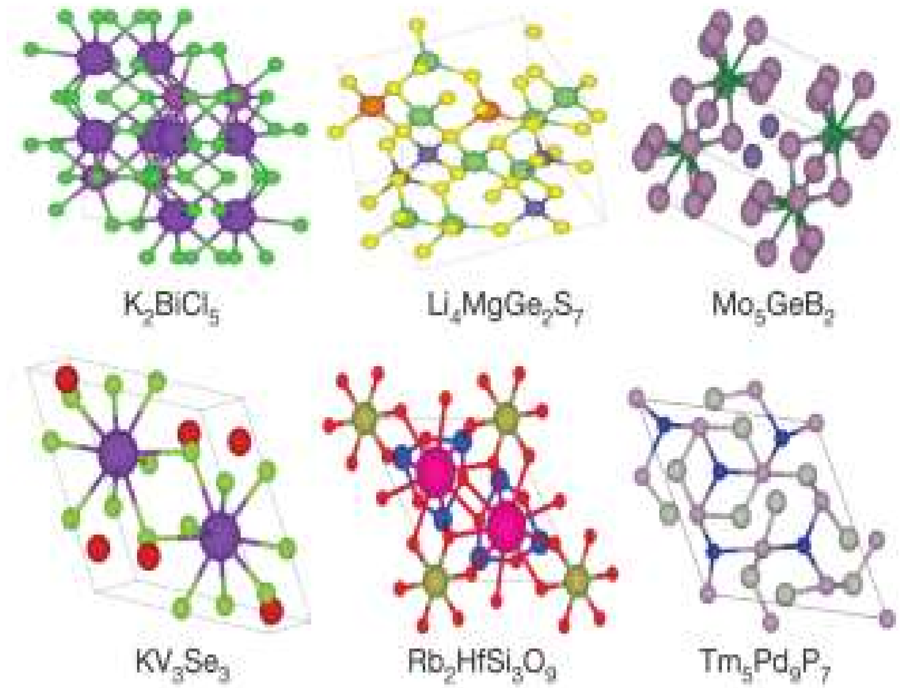


Inset figure from H. Bhatkar, et. al, “Elemental moment variation of bcc FexMn1−x on MgO(001),” *Journal of Magnetism and Magnetic Materials*, 42 (2017), pp 46-50.

Computational Materials Discovery

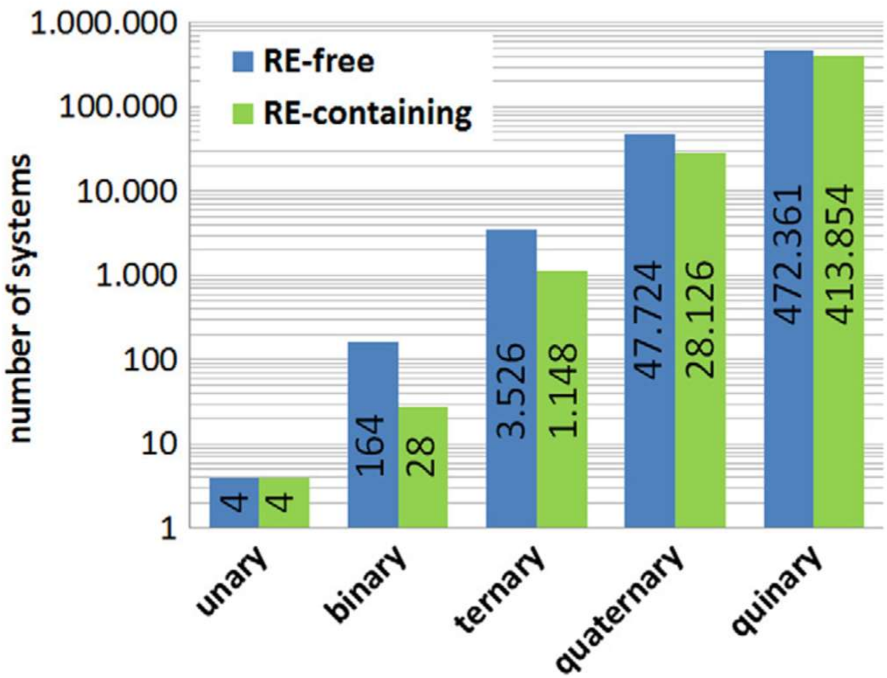
Google DeepMind
2 million new materials





A. Merchant, S. Batzner, S.S. Schoenholz. *et al.* *Nature* **624**, 80–85 (2023)

Potential for New Compounds and Structures



	Unique Combinations	*Standard*	*Missing*	*Interesting*	*Unlikely*
Chemical filter	-	Allowed	Allowed	Forbidden	Forbidden
Materials Project	-	Known	Unknown	Known	Unknown
Binary (A_wB_x)	225,879	3,627 (1.6 %)	9,837 (4.4 %)	6,354 (2.8 %)	206,061 (91.2 %)
Ternary ($A_wB_xC_y$)	77,637,589	24,713 (0.03 %)	10,754,728 (13.9 %)	12,153 (0.01 %)	66,845,995 (86.1 %)
Quaternary ($A_wB_xC_yD_z$)	16,902,534,325	16,455 (0.00 %)	2,909,418,527 (17.2 %)	962 (0.00 %)	13,993,098,381 (82.8 %)

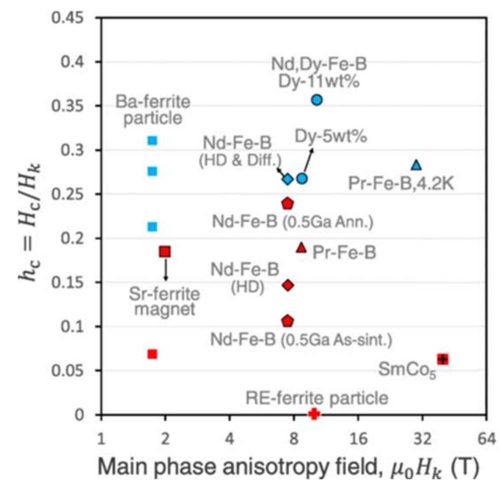
about 100k relevant 4 element systems for Magnets, maybe 1% examined

D. Goll, et al, “Novel Permanent Magnets by High-Throughput Experiments,” *JOM*, 67 (2015)

H. Park, et al, “Mapping inorganic crystal chemical space,” *Faraday Discussions*, 256 (2025)

Magnetic Properties we can Calculate: B_{sat}, T_c, H_a

- Saturation Moment B_{sat}
  - relatively easy for high throughput (maybe DMFT for RE)
    - Given a magnet order (e.g. Ferromagnetic or AntiFerromagnetic)
  - Complex Antiferromagnetic order is a challenge for high throughput
- Curie Temperature T_c
  - Demonstrated but not high throughput
- Anisotropy Field H_a
  as Upper bound for Coercivity (and BH_{max})
  - Requires greater accuracy calculations
    but could be high throughput
  - From Magneto-Crystalline Anisotropy Energy (MAE)
  - $H_c < ¼ H_a$ (Brown Paradox)
  - KKR-CPA + open core + SIC appears to work for RE+disorder

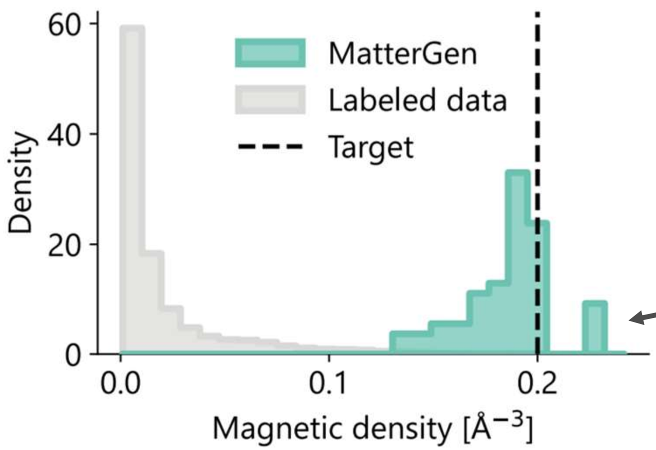


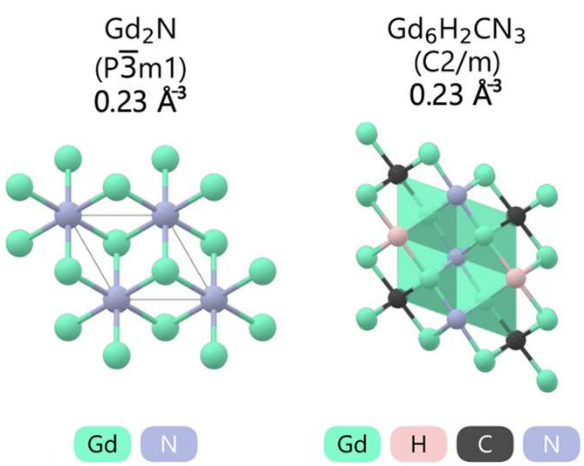
H. Zhang *Electron. Struct.* **3** 033001 (2021)
Hono et al, *Phys. Rev. B* 105, 174432 (2022)

Add Calculation of Magnetization and Target High B

Microsoft MatterGen
140 new high B materials

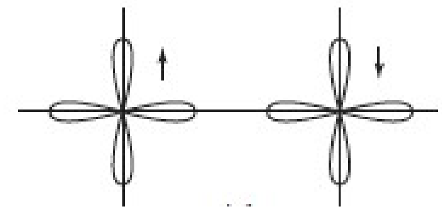
Density Functional Theory (DFT)
Calculate magnetization B



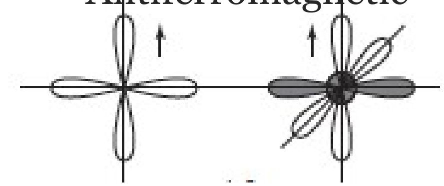


New Structure – Bonding Strategies ?

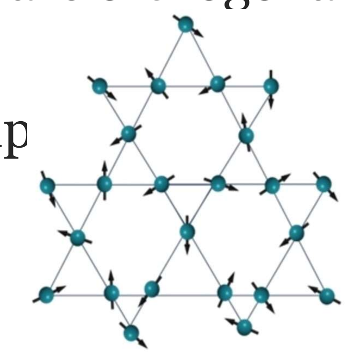
- Can High Spin Ions make Ferromagnets ?
  - High Spin (e.g. Mn^{2+} 5 unpaired spins) often in Insulators
    - crystal field splitting ?
  - High Spin Mn^{2+} is usually Antiferromagnetic
- Direct Exchange explained by Goodenough-Kanamori Rules
  - Strong Antiferromagnetic coupling between overlapping half
  - Weak Ferromagnetic coupling when orbitals are orthogonal
- Strategy – Find 3D structure
  - prevents or frustrates Antiferromagnetic coup
  - maximizes Ferromagnetic coupling
  - Anisotropic for Coercivity



Overlapping Orbitals Antiferromagnetic



Orthogonal Orbitals Ferromagnetic

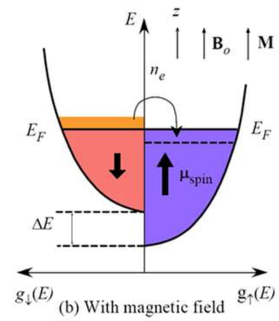


Spin Frustrated Kagome Lattice

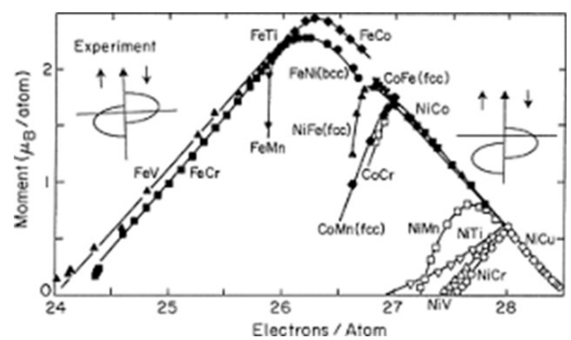
D. Khomskii, Transition Metal Compounds, 2014

Physics – Exchange Coupling of Metals

- DFT (+DMFT) predicts result but does not give strategy
  - Various structures, electron count, pressures can be calculated to ML a strategy?
- Direct Exchange coupling between spins
  - Depends on electron count (Slater-Pauling)
    - chemical doping
  - What leads to strong exchange splitting (Stoner Magnetism)?
    - giving high number of unpaired spins per atom
    - High DOS, is there an ideal, engineered DOS?
- Conduction electron mediated (indirect) exchange
  - e.g., RKKY is oscillatory
  - Depends on interatomic distance
    - physical and chemical pressure
- MAE – from Anisotropic structure



Exchange Splitting
Stoner magnetism

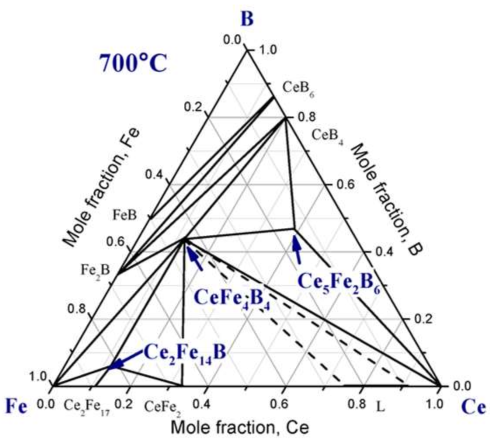


Slater-Pauling B_{sat} vs Electron Count

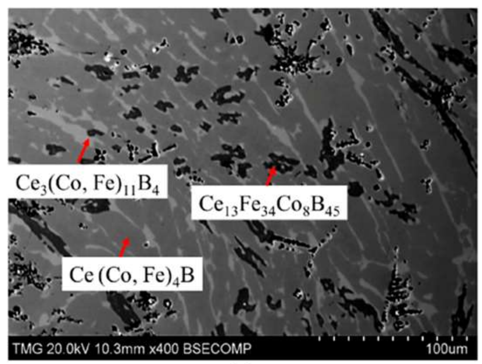
Inset figures from H. Bhatkar, et. al, “Elemental moment variation of bcc FexMn1−x on MgO(001),” *Journal of Magnetism and Magnetic Materials*, 42 (2017), pp 46-50.

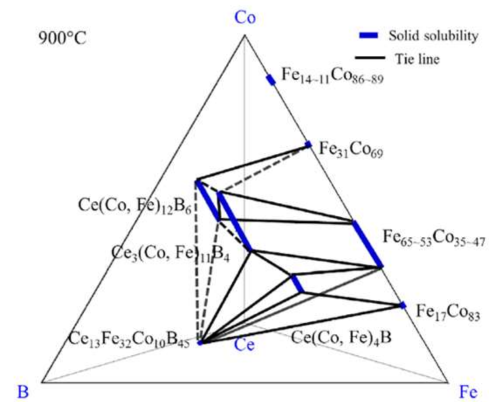
Experimental Systematic Phase Diagram Searches

Equilibrium phase diagram enables systematic searching



Ce-Fe-B Ternary diagram at 700C



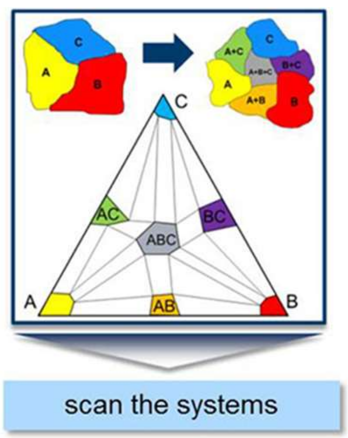


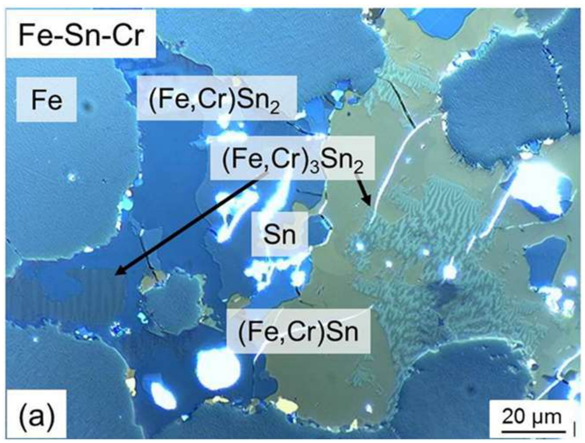
Projection of Ce-Fe-Co-B Quaternary

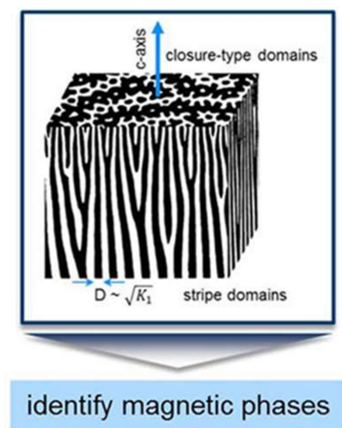
Medraj et al, *Materials*, 10, 16 (2017);
Ikeda et al., *Materials*, 18, 295 (2025), *Materia Japan* 64, p23 (2025) [10.2320/materia.64.23]

High Throughput Experiments and Characterization

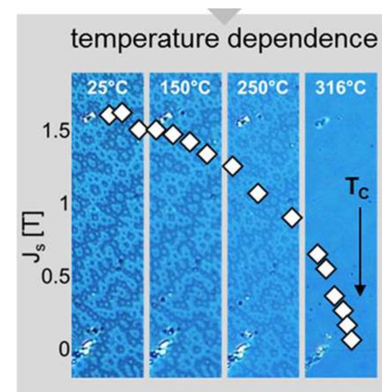
- Using diffusion couple with incomplete reaction
  - Thin films also possible but eventually we need ~cm^3 materials
- SEM or optical microscopy for phase identification
- Kerr Microscopy for magnetic property estimation, B_s, T_c, Anisotropy







Anisotropy from domain spacing

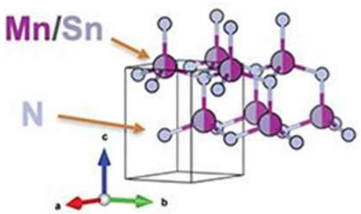


Saturation and Tc from Kerr Intensity

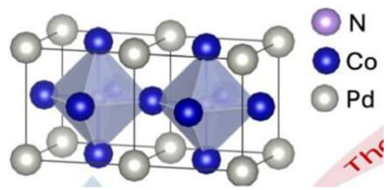
Goll et al, *JOM*, 67, 1336 (2015); *Scripta Mat.*146, 355 (2018); *J. Phys. Cond. Mat.* 26 064208 (2014)

Examples of New Complex Magnet Materials

- Nitrides

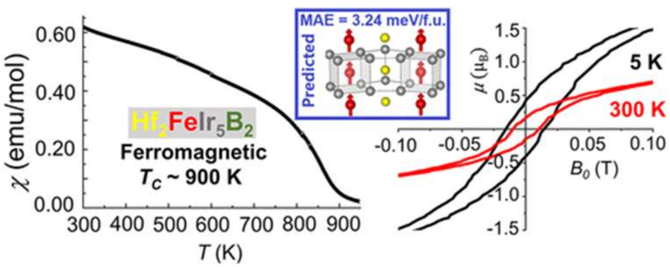


$MnSnN_2$

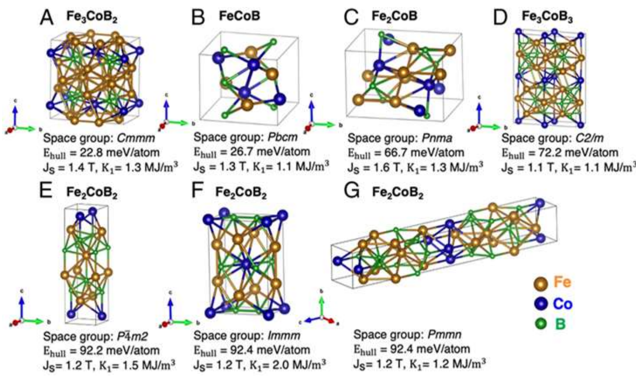


Co_3PdN

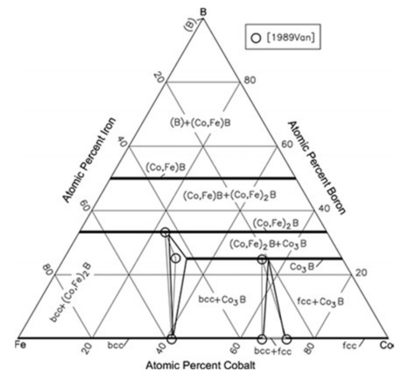
- Borides $Hf_2MIr_5B_2$ (M = Fe, Mn)



- Fe3CoB2 discovered using ML

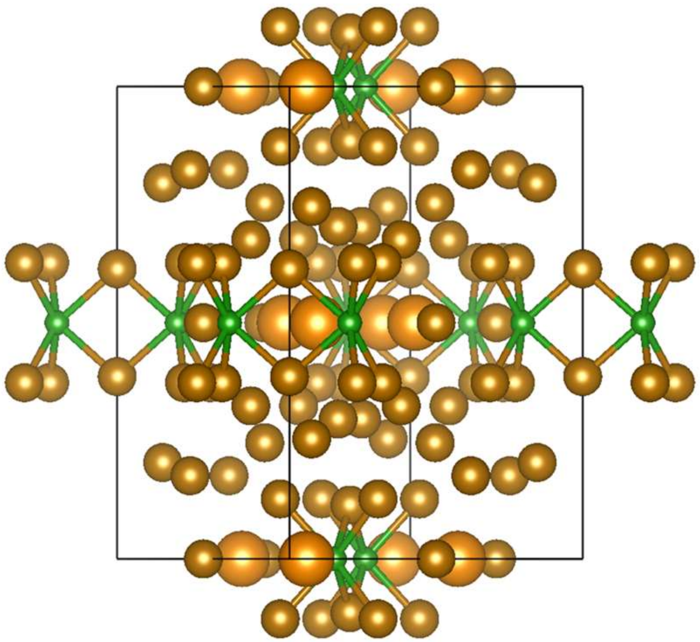


- Fe-Co-C, Fe-Co-Si



$Nd_2Fe_{14}B$ as Example and Test Case for Search

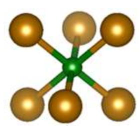
- 3 distinctly different elements
- 3 different structure environments (not just alloy)
  - Fe as a high B_s but soft phase
  - Strong Fe_6B bonds – enforce anisotropic structure?
    Help exchange splitting of Fe?
  - Rare Earth for Magneticrystalline Anisotropy?
- Stable phase (multiple synthesis routes possible)
  - Commercialized within months of discovery
- If your search wouldn't find $Nd_2Fe_{14}B$ is it broad enough?
  - only searching random alloy of binary compound ?
  - or interstitial structure of known binary alloy?



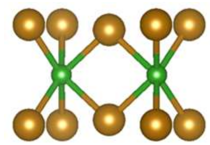
$Nd_2Fe_{14}B$

Solid State Sub-nitride, -boride Chemistry of Fe-based Magnets

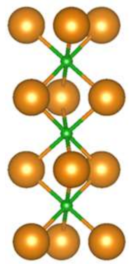
- Fe, Co, Ni and Rare Earth elements make the best Ferromagnets
  - Any d-shell or f-shell element with unpaired spins
- Interstitial Boron, Carbon, Nitrogen
  - Sub nitrides, borides, carbides, Si, P …
  - Metal-Intersitial bond good for exchange? Crystal field splitting ?
- Anisotropic structure good for hard magnets
  - Usually 3 or more different atomic sites



Fe_6N in α”-$Fe_{16}N_2$

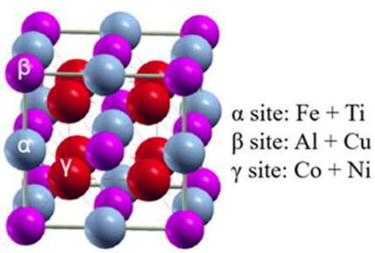


Fe_6B in $Nd_2Fe_{14}B$

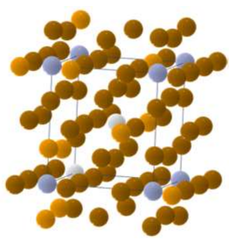


$NaBa_3N$

High symmetry magnets with low coercivity

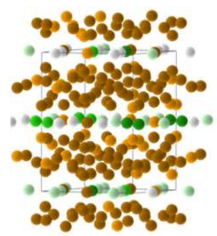


AlNiCo 8

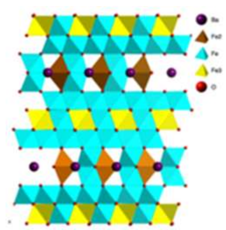


Fe_8N α”-$Fe_{16}N_2$

Strongly directional magnets with high coercivity



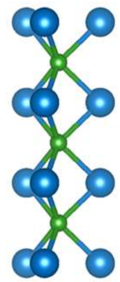
$Nd_2Fe_{14}B$

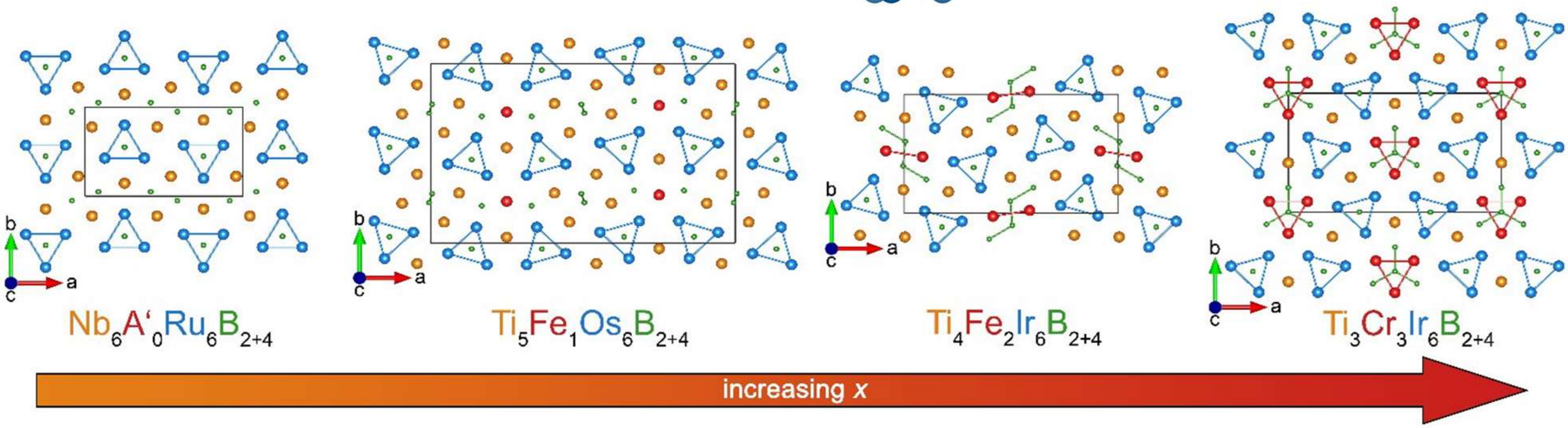


$SrFe_{12}O_{19}$

Example of Structural Motifs

Boron Trigonal Prism chains

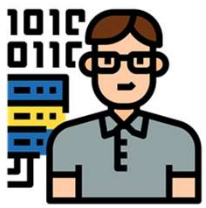




- **Structure-building block principles to discover new structures containing magnetic elements:**
- **New ferromagnets have been discovered in all structures already.   x = number of A'**

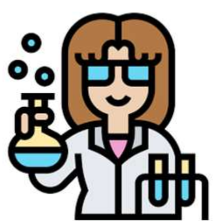
B. Fokwa et al, *Acc. Chem. Res.* 50, 2317 (2017)

Teaming is Likely Necessary



Computational Structure Discovery
High Throughput Stability

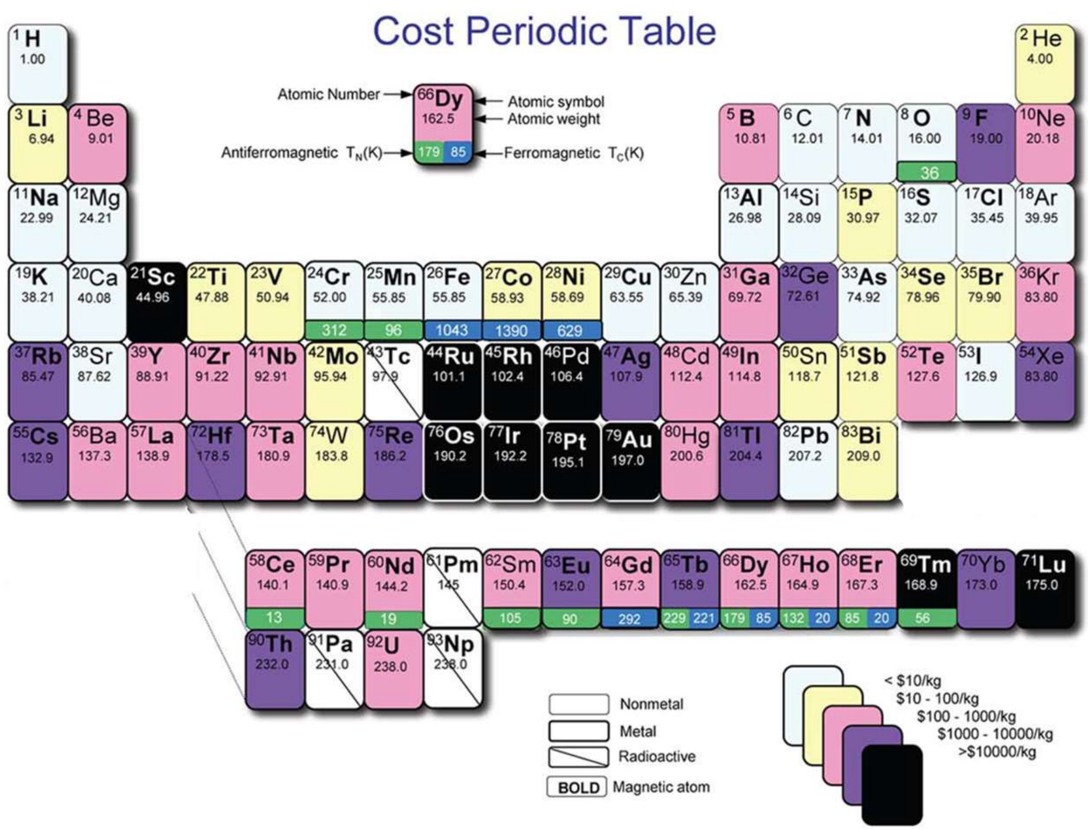
Computational Physics B_{sat}, T_c, H_a
Physics Strategies: High B_{sat} Ferromagnetism



Synthesis and Characterization
Chemical Strategies

Microstructure, Processing and
Application Engineering

Cost Considerations Should Be Appropriate For Target Application



J.M.D. Coey "Hard Magnetic Materials: A Perspective" IEEE Transaction on Magnetics, vol. 47, no. 12, December 2011

Manufacturability – Typical Applications Require ~cm^3 Pellets

Commercial neo magnets

Typical sintered pellets

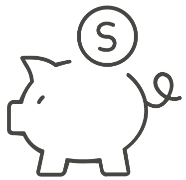
Thin Films or small quantities of nanopowder will need
to show viable path for manufacturability

Proposed Program Metrics

Performance Metrics	State of the art	Target
M1. Strength of magnet material		
a) Magnetic flux density B_{sat} or	2.2 Tesla	> 2.5 Tesla
b) Maximum energy product $(BH)_{max}$	400 kJ/m^3	> 800 kJ/m^3
M2. Manufacturability	-	1 cm^3 total pellets
M3. Curie temperature	-	>200°C
M4. Cost	-	< $1,000/kg

These metrics are aggressive targets intended to exclude incremental approaches.

Proposed program structure: $20M
6-10 projects
$500K - $3M per project



Double
power density

Reduce reliance on
critical materials

Meeting the Metrics – Example of possible path to success

- Midterm Goal 1: Calculated B_{sat} > 2.5 T or $B_{sat} \times H_A /16$ > 800kJ/m³ and T_C >200°C in new material
  - H_C can be expected to reach $H_A/4$, With limit of $B_{sat} /\mu o$
  - BH_{max} approximately $B_{sat} \times H_{CB} /4$

    since $\mu o H_{CB}$ is at most B_{sat}, need B_{sat} > 2T
- Midterm Goal 2: Measured B_{sat} > 2.5 T or $B_{sat} \times H_A /16$ > 800kJ/m³ and T_C >200°C in ~1cm³ of new material
- Final Goal: B_{sat} > 2.5 T or BH_{max} > 800kJ/m³ and T_C >200°C, 1cm³ of solid material

definitions: (experiment or computational)

- **B_{sat} Saturation Magnetization at 300K, extrapolation to H=0Tesla, converted to B in Tesla**
- **T_C Curie Temperature where B_{sat}(Temp) vanishes**
- **BH_{max} at 300K, reported in kJ/m³**
- **H_A anisotropy field at 300K of major axis, reported in MA/m or $\mu_0 H_A$ in Tesla**

If It Works, It Will Matter !

Robots

Generators

Drones
Electric aircraft

Industrial motors

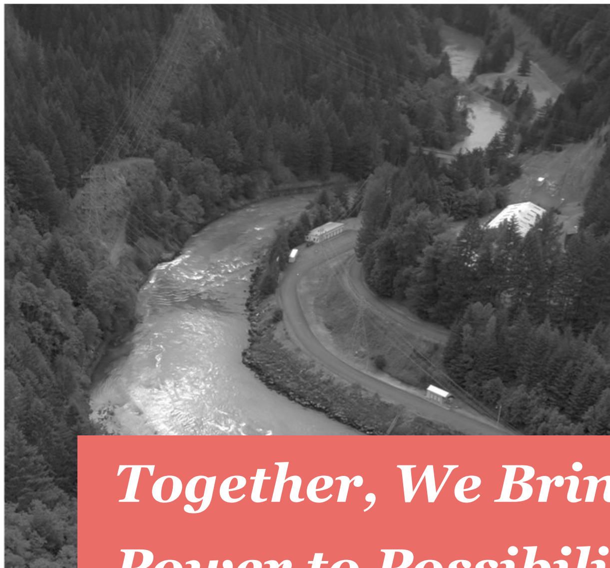
Medical
equipment

Consumer
electronics

Maglev trains

Other possibilities?

ARPA-E Engages a Wide Range of Stakeholders to Disrupt the Status Quo



Together, We Bring Power to Possibility.

We operate at the nexus of academia, industry, investment, and government.