

innovating nanoscience



End-to-end materials discovery with electronic structure theory and machine learning

Stefano Sanvito (sanvitos@tcd.ie)

School of Physics and CRANN, Trinity College Dublin, IRELAND

The question

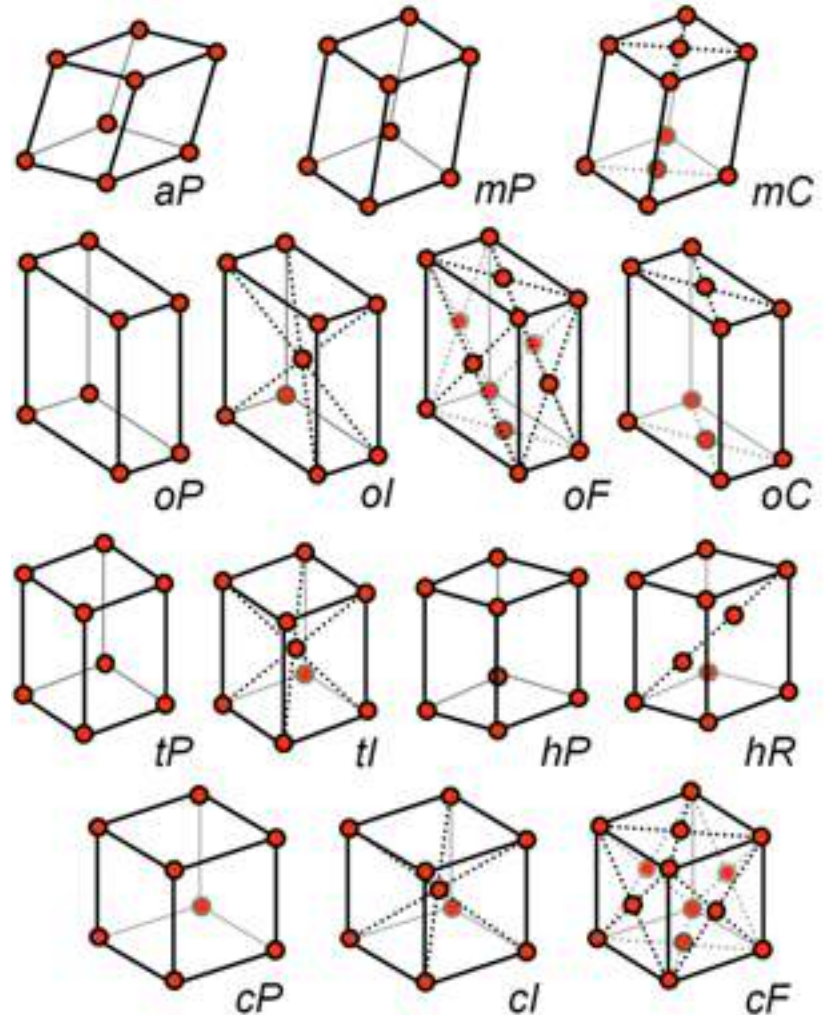
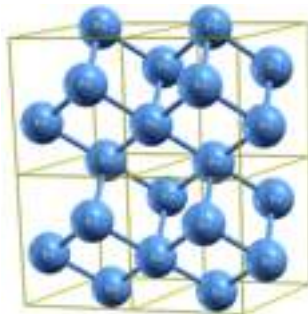
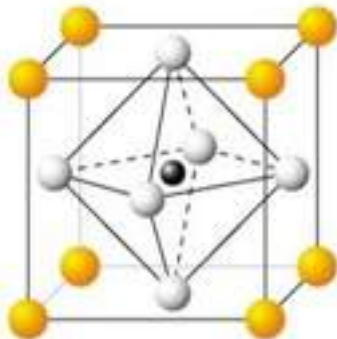


How many inorganic materials can you name?

Fe, $\text{Fe}_{1-x}\text{C}_x$, Si, U, $\text{Nd}_2\text{Fe}_{14}\text{B}$, $\text{YBa}_2\text{Cu}_3\text{O}_7$...

Only about 150,000

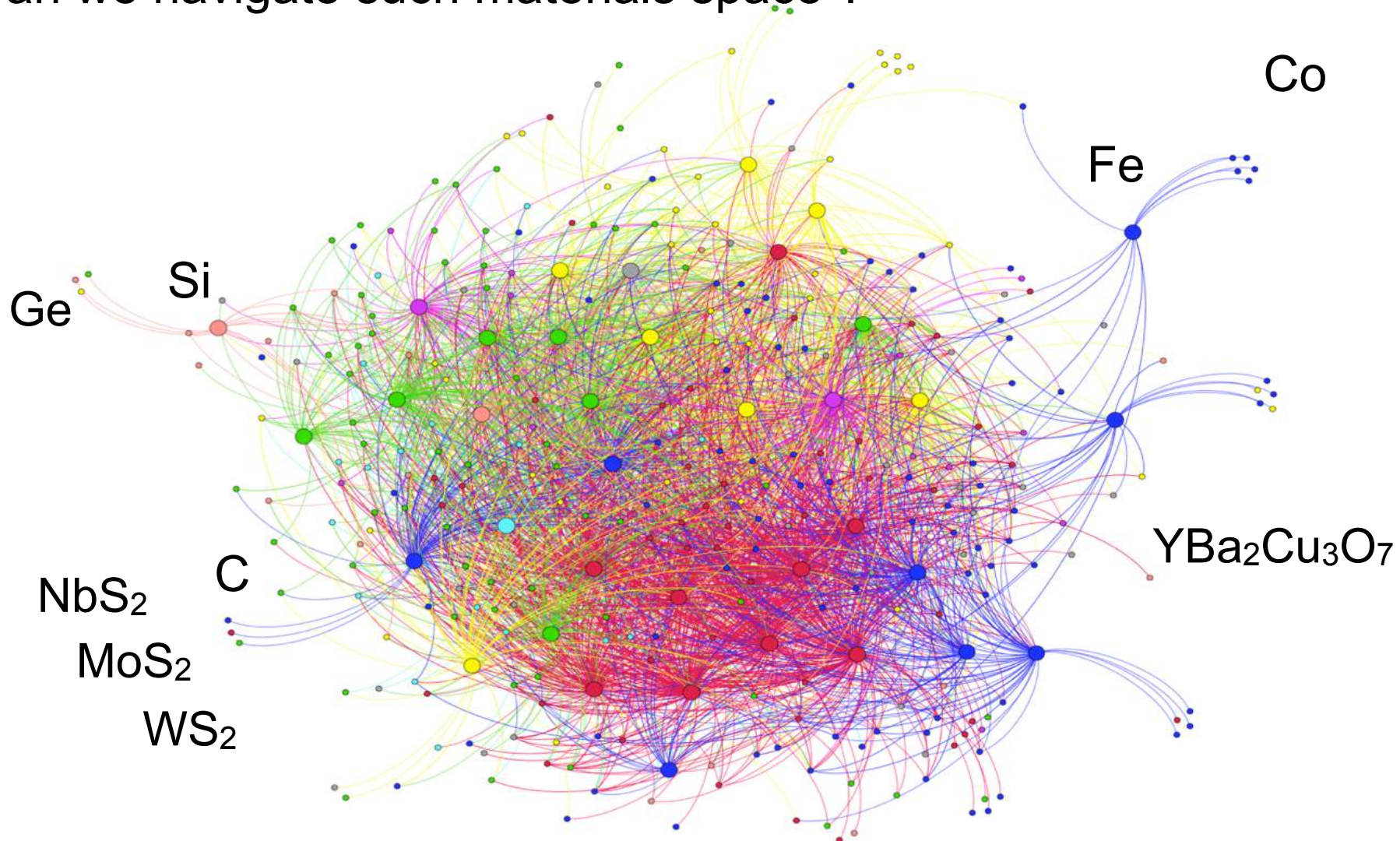
<http://www.rockoff.org/2008/06/24/2008-06-24-01>

[illegible]

Internet of materials



Can we find out what we are looking for ?
Can we navigate such materials space ?



The question

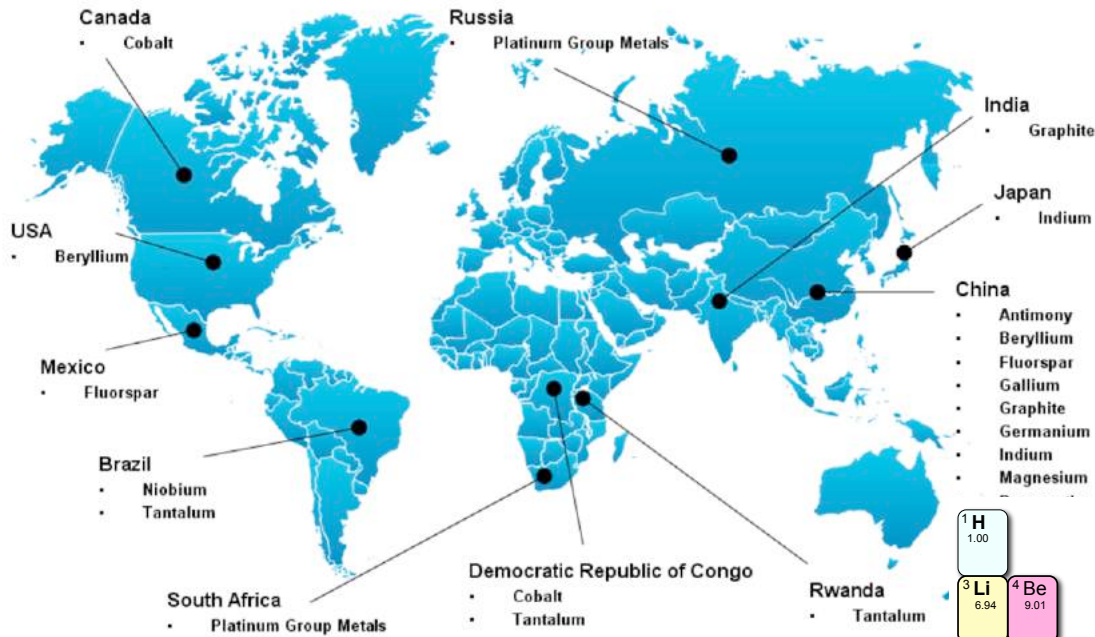


Suppose you have a new magnetic application
.... what is its ideal material(s) ?

Fe, Co, Ni, $\text{Nd}_2\text{Fe}_{14}\text{B}$, LaMnO_3 , Fe_3O_4

~4,000

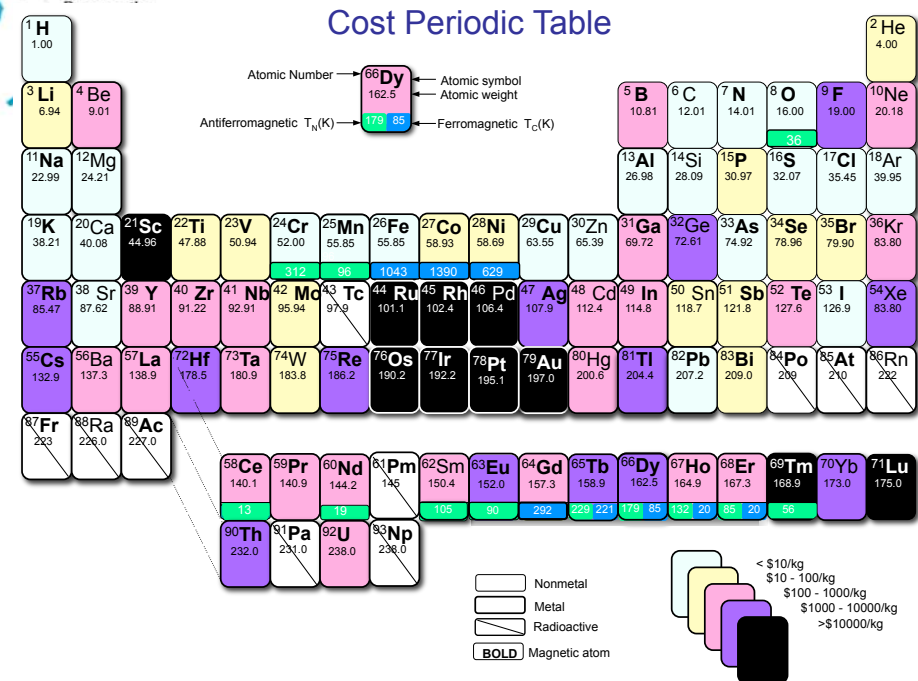
Finding new magnets: why ?



*US permanent magnets market
~15B\$ (2016)*

~22.6B\$ (2021)

Novel rare-earth-free permanent magnets

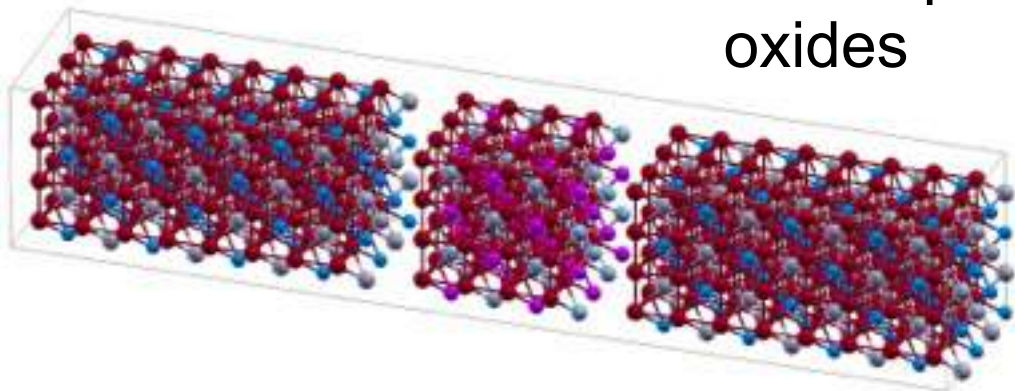


Finding new magnets: why ?

Data storage industry has multiple requirements

MRAM / STT Oscillators

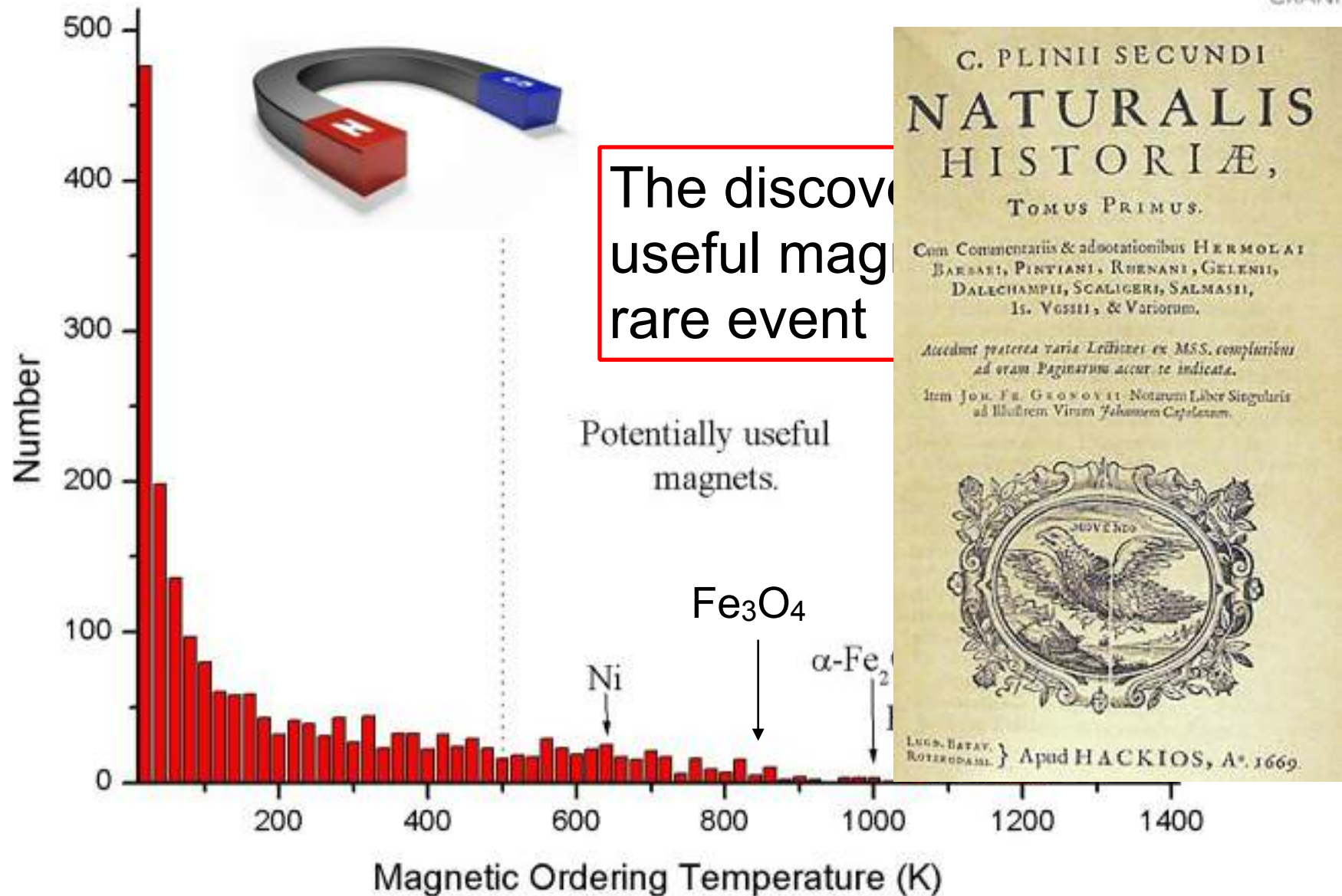
- ❑ High T_C ($>600\text{K}$)
- ❑ High spin polarization ($P \sim 100\%$)
- ❑ Low Gilbert damping
- ❑ Low saturation magnetization
- ❑ Compatible with epitaxial growth of oxides



Magnetism is rare



CRANN



Magnetism is complicated



PERIODIC TABLE OF THE ELEMENTS

PERIODIC TABLE OF THE ELEMENTS

GROUP 1 1A 2 2A 3 3B 4 4B 5 VB 6 VIB 7 VIIB 8 VIII 9 VIII 10 VIII 11 IB 12 IIB 13 IIIA 14 IVA 15 VA 16 VIA 17 VIIA 18 VIIIA

RELATIVE ATOMIC MASS (A_r)

GROUP IUPAC

ATOMIC NUMBER

SYMBOL

ELEMENT NAME

Legend:

- Metal
- Semimetal
- Nonmetal
- Alkali metal
- Alkaline earth metal
- Transition metals
- Lanthanide
- Actinide
- Chalcogens element
- Halogens element
- Noble gas

STANDARD STATE (25 °C; 101 kPa)

Ne - gas Fe - solid Ga - liquid

Hydrogen (H) is highlighted in yellow.

Chromium (Cr), Manganese (Mn), and Iron (Fe) are highlighted with a red box.

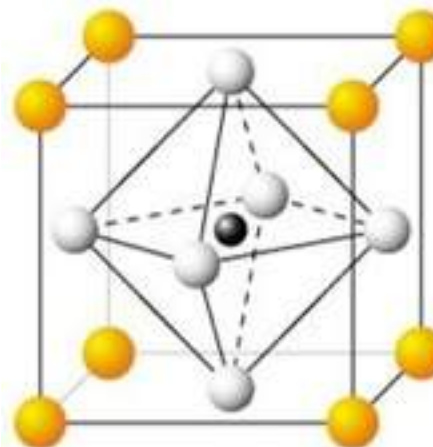
LANTHANIDE

ACTINIDE

Editor: Aditya Vashan (aditya@nottme.com)

SrCrO_3 $T_N = -230^\circ\text{C}$	SrMnO_3 $T_N = -10^\circ\text{C}$	SrFeO_3 $T_N = -140^\circ\text{C}$
--	---	--

SrMoO_3	SrTcO_3 $T_N = 500^\circ\text{C}$	SrRuO_3 $T_C = -100^\circ\text{C}$
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The magnetic genome project



with Stefano Curtarolo, Duke

The magnetic genome project



nature
materials

REVIEW ARTICLE

PUBLISHED ONLINE: 20 FEBRUARY 2013 | DOI: 10.1038/NMAT3548

The high-throughput highway to computational materials design

Stefano Curtarolo^{1,2*}, Gus L. W. Hart^{1,3}, Marco Buongiorno Nardelli^{2,4,5}, Natalio Mingo^{2,6}, Stefano Sanvito^{2,7} and Ohad Levy^{1,2,8}

Finding *descriptors*



Materials selection

Search the database for 1) new materials, 2) physical insights

Database Creation (AFLOW)



Rational materials storage

Creating searchable database where to store information

Virtual Materials Growth

- 1) Simulating existing materials
- 2) Simulating new materials

Robust electronic structure method:
density functional theory (VASP)



The magnetic genome project

nature
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The AFLOW consortium

www.aflowlib.org



S. Curtarolo, W. Setyawan, S. Wang, J. Xue, K. Yang, R.H. Taylor, L.J. Nelson, G.L.W. Hart, S. Sanvito, M. Buongiorno-Nardelli, N. Mingo, O. Levy, *Comp. Mat. Sci.* **58**, 227 (2012)

The magnetic genome project



Virtual Materials Growth (existing materials)

Only ~150,000 are known to us

ICSD: Inorganic Crystal Structure Database

- 1,616 crystal structures of the elements
- 28,354 records for binary compounds
- 55,436 records for ternary compounds
- 54,144 records for quarternary and quindenary
- About 113,000 entries (75.6%) have been assigned a structure type.
- There are currently 6,336 structure prototypes.
- **Lots of redundancy**

The magnetic genome project



Virtual Materials Growth (existing materials)

Duke calculated single elements, binary, ternary and some quaternary (about 60,000)

Calculations:

- AFLOW manages the run (large code)
- DFT done with VASP (pseudo-potential, plane-wave)
- Calculations at the DFT GGA-PBE level
- Relaxation performed → new space group worked out
- Basic electronic structures collected (including: spin-polarization, effective mass, magnetic moment, etc.)

Heusler alloys

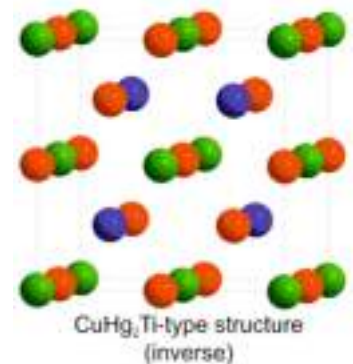
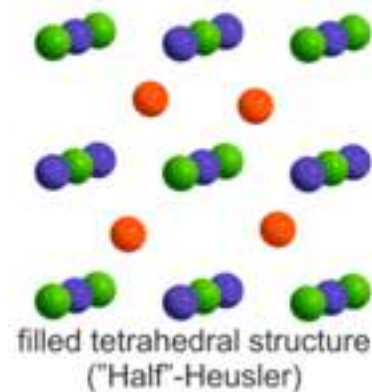
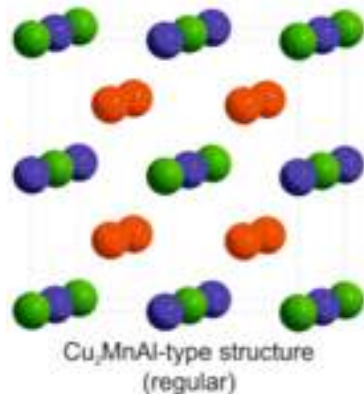
~250
known ...

~1000
claimed ...

~90
magnetic ...

X_2YZ Heusler compounds

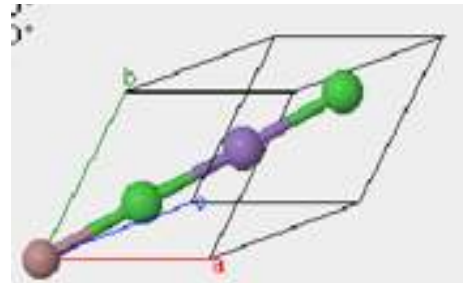
H 2.20																	He	
Li 0.98	Be 1.57											B 2.04	C 2.55	N 3.04	O 3.44	F 3.98	Ne	
Na 0.93	Mg 1.31											Al 1.61	Si 1.90	P 2.19	S 2.58	Cl 3.16	Ar	
K 0.82	Ca 1.00	Sc 1.36	Ti 1.54	V 1.63	Cr 1.66	Mn 1.55	Fe 1.83	Co 1.88	Ni 1.91	Cu 1.90	Zn 1.65	Ga 1.81	Ge 2.01	As 2.18	Se 2.55	Br 2.96	Kr 3.00	
Rb 0.82	Sr 0.95	Y 1.22	Zr 1.33	Nb 1.60	Mo 2.16	Tc 1.90	Ru 2.20	Rh 2.28	Pd 2.20	Ag 1.93	Cd 1.69	In 1.78	Sn 1.96	Sb 2.05	Te 2.10	I 2.66	Xe 2.60	
Cs 0.79	Ba 0.89			Hf 1.30	Ta 1.50	W 1.70	Re 1.90	Os 2.20	Ir 2.20	Pt 2.20	Au 2.40	Hg 1.90	Tl 1.80	Pb 1.80	Bi 1.90	Po 2.00	At 2.20	Rn
Fr 0.70	Ra 0.90																	
		La 1.10	Ce 1.12	Pr 1.13	Nd 1.14	Pm 1.13	Sm 1.17	Eu 1.20	Gd 1.20	Tb 1.10	Dy 1.22	Ho 1.23	Er 1.24	Tm 1.25	Yb 1.10	Lu 1.27		
		Ac 1.10	Th 1.30	Pa 1.50	U 1.70	Np 1.30	Pu 1.28	Am 1.13	Cm 1.28	Bk 1.30	Cf 1.30	Es 1.30	Fm 1.30	Md 1.30	No 1.30	Lr 1.30		



Heusler alloys



CRANN



~236,000/0.5M calculated !!

hydrogen 1 H 1.0079																	helium 2 He 4.0026				
lithium 3 Li 6.941	beryllium 4 Be 9.0122															boron 5 B 10.811	carbon 6 C 12.011	nitrogen 7 N 14.007	oxygen 8 O 15.999	fluorine 9 F 18.998	neon 10 Ne 20.180
sodium 11 Na 22.990	magnesium 12 Mg 24.305															aluminum 13 Al 26.982	silicon 14 Si 28.086	phosphorus 15 P 30.974	sulfur 16 S 32.065	chlorine 17 Cl 35.453	argon 18 Ar 39.948
potassium 19 K 39.098	calcium 20 Ca 40.078	scandium 21 Sc 44.956	titanium 22 Ti 47.867	vanadium 23 V 50.942	chromium 24 Cr 51.996	manganese 25 Mn 54.938	iron 26 Fe 55.845	cobalt 27 Co 58.933	nickel 28 Ni 58.693	copper 29 Cu 63.546	zinc 30 Zn 65.39	gallium 31 Ga 69.723	germanium 32 Ge 72.61	arsenic 33 As 74.922	selenium 34 Se 78.96	bromine 35 Br 79.904	krypton 36 Kr 83.80				
rubidium 37 Rb 85.468	strontium 38 Sr 87.62	yttrium 39 Y 88.906	zirconium 40 Zr 91.224	niobium 41 Nb 92.906	molybdenum 42 Mo 95.94	technetium 43 Tc [98]	ruthenium 44 Ru 101.07	rhodium 45 Rh 102.91	palladium 46 Pd 106.42	silver 47 Ag 107.87	cadmium 48 Cd 112.41	indium 49 In 114.82	tin 50 Sn 118.71	antimony 51 Sb 121.76	tellurium 52 Te 127.60	iodine 53 I 126.90	xenon 54 Xe 131.29				
cesium 55 Cs 132.91	barium 56 Ba 137.33	lanthanum 57 La 138.91	hafnium 72 Hf 178.49	tantalum 73 Ta 180.95	tungsten 74 W 183.84	rhenium 75 Re 186.21	osmium 76 Os 190.23	iridium 77 Ir 192.22	platinum 78 Pt 195.08	gold 79 Au 196.97	mercury 80 Hg 200.59	thallium 81 Tl 204.38	lead 82 Pb 207.2	bismuth 83 Bi 208.98	polonium 84 Po [209]	astatine 85 At [210]	radon 86 Rn [222]				
francium 87 Fr [223]	radium 88 Ra [226]															unquadecium 114 Uuq [289]					
		57-70 ★																			
		89-102 ★ ★																			
				actinium 89 Ac [227]	thorium 90 Th 232.04	protactinium 91 Pa 231.04	uranium 92 U 238.03	neptunium 93 Np [237]	plutonium 94 Pu [244]	americium 95 Am [243]	curium 96 Cm [247]	berkelium 97 Bk [247]	californium 98 Cf [251]	eskeium 99 Es [252]	fermium 100 Fm [257]	mendelevium 101 Md [258]	nobelium 102 No [259]				

~236,000/0.5M calculated !!

* Lanthanide series

** Actinide series

lanthanum 57 La 138.91	cerium 58 Ce 140.12	praseodymium 59 Pr 140.91	neodymium 60 Nd 144.24	promethium 61 Pm [145]	samarium 62 Sm 150.36	europium 63 Eu 151.96	gadolinium 64 Gd 157.25	terbium 65 Tb 158.93	dysprosium 66 Dy 162.50	holmium 67 Ho 164.93	erbium 68 Er 167.26	thulium 69 Tm 168.93	ytterbium 70 Yb 173.04
actinium 89 Ac [227]	thorium 90 Th 232.04	protactinium 91 Pa 231.04	uranium 92 U 238.03	neptunium 93 Np [237]	plutonium 94 Pu [244]	americium 95 Am [243]	curium 96 Cm [247]	berkelium 97 Bk [247]	californium 98 Cf [251]	eskeium 99 Es [252]	fermium 100 Fm [257]	mendelevium 101 Md [258]	nobelium 102 No [259]

Database

Rational materials storage

www.aflowlib.org



The screenshot displays the Aflowlib database search interface. At the top, there is a search bar labeled "Search Aflowlib" with a close button (X) and a green "Search" button indicating 150522 compounds. Below the search bar are tabs for "icad", "elements", "binaries", and "Heuslers". The main area features a periodic table of elements. A tooltip for element "X" is visible, showing fields for Atomic #, element, [electrons], [density], [T_M], [lattice], [crystal], and [Debye]. To the right of the periodic table are logical operators: "and", "not", "or", "xor", and parentheses. Below the periodic table, there are filters for "All Metals", "Alkali Metals", "Alkaline Earths", "Transition Metals", "Lanthanides", "Other Metals", "Nonmetals", "Group 3A", "Group 4A", "Group 5A", "Chalcogens", and "Halogens". At the bottom, there are buttons for "Chemistry", "Crystal", "Electronics", "Thermodynamics", "Magnetics", "Scintillation", "Mechanical", and "Calculation".

S. Curtarolo, W. Setyawan, S. Wang, J. Xue, K. Yang, R.H. Taylor, L.J. Nelson, G.L.W. Hart, S. Sanvito, M. Buongiorno-Nardelli, N. Mingo, O. Levy, *Comp. Mat. Sci.* **58**, 227 (2012)



ELECTRONIC PROPERTIES

Band Gap: 0.000 eV (metal)

Magnetic Moment: 7.382 μ_B

Electron Mass(FIX): XXX (m_0)

Spin Polarization (E_F): 0.666

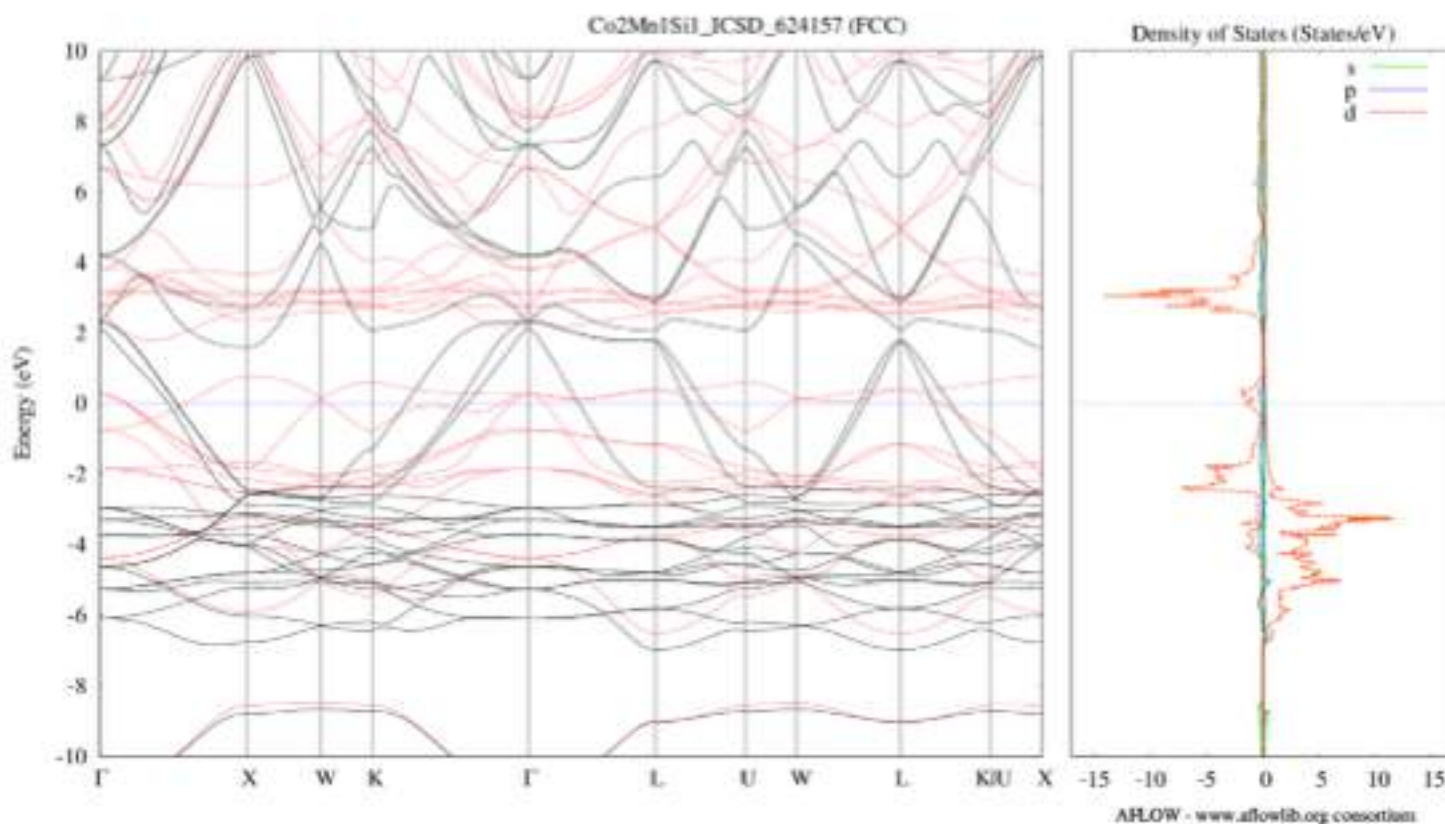
Fit Band Gap: 0.000 eV

Magnetic Moment/atom: 1.845 μ_B /atom

Hole Mass(FIX): XXX (m_0)

Spin Decomposition per atoms: {1.758,1.758,4.019,-0.054} μ_B

Band Structure:



The magnetic genome project

nature
materials

REVIEW ARTICLE

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Finding *descriptors*

The high-throughput highway to computational materials design

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Back to the magnets



S. Sanvito et al., *Accelerated discovery of new magnets in the Heusler alloy family*, Science Advances **3**, e1602241 (2017)

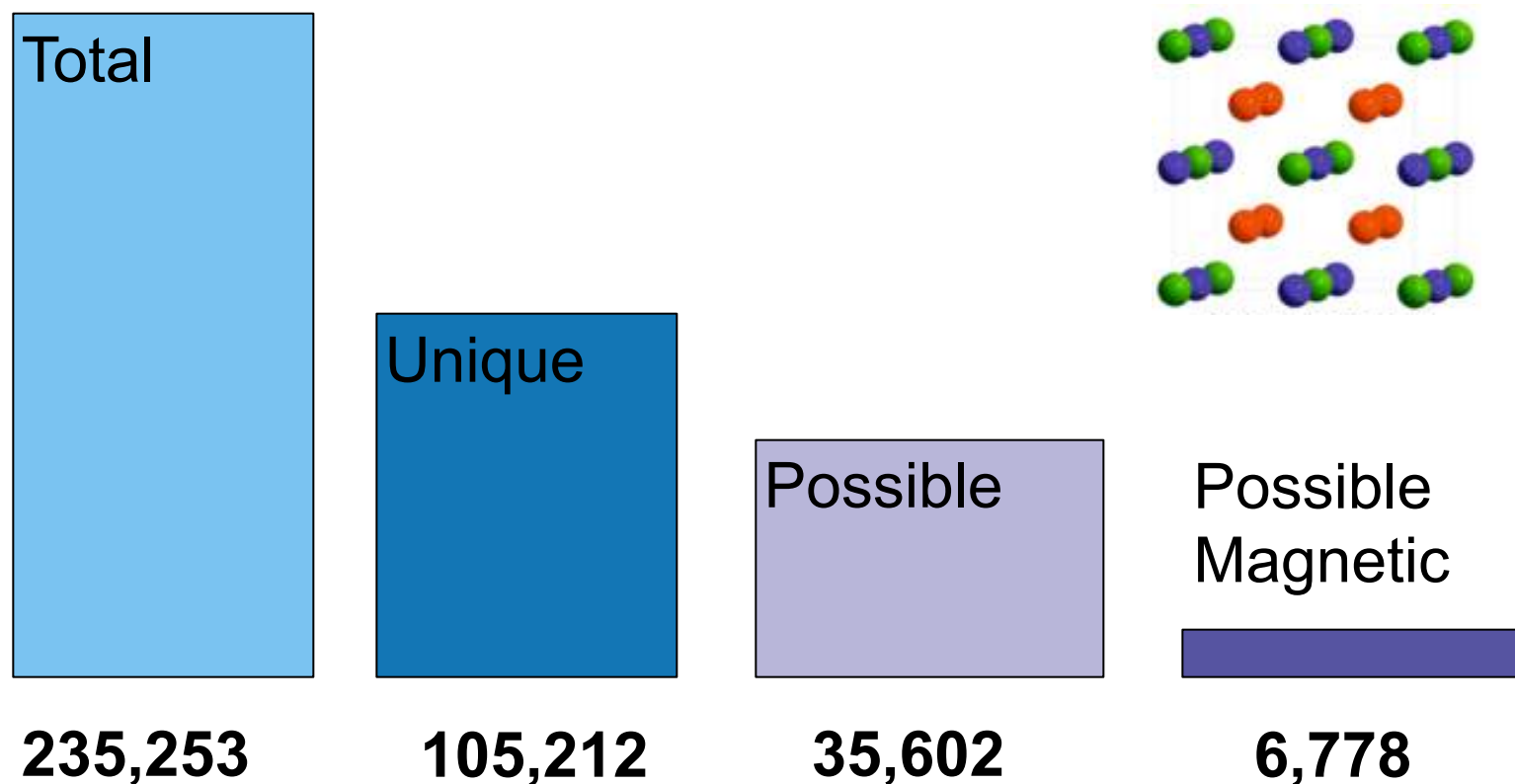
A look at the full database



Property: Can be made ?

Descriptor 0:
Enthalpy of formation

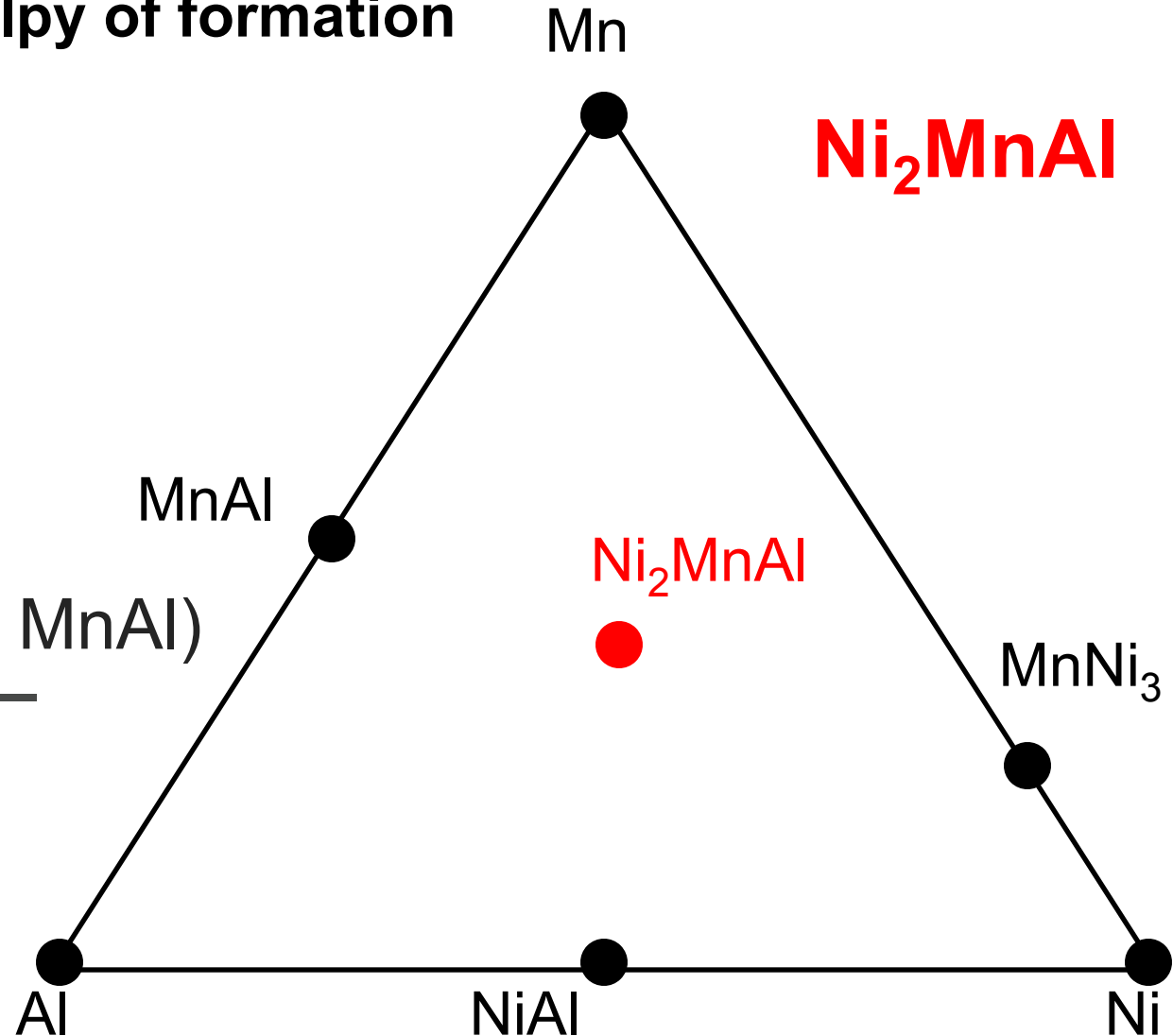
Energy (Ni_2MnAl) < Energy ($2\text{Ni} + \text{Mn} + \text{Al}$)



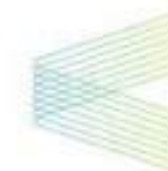
Stability analysis



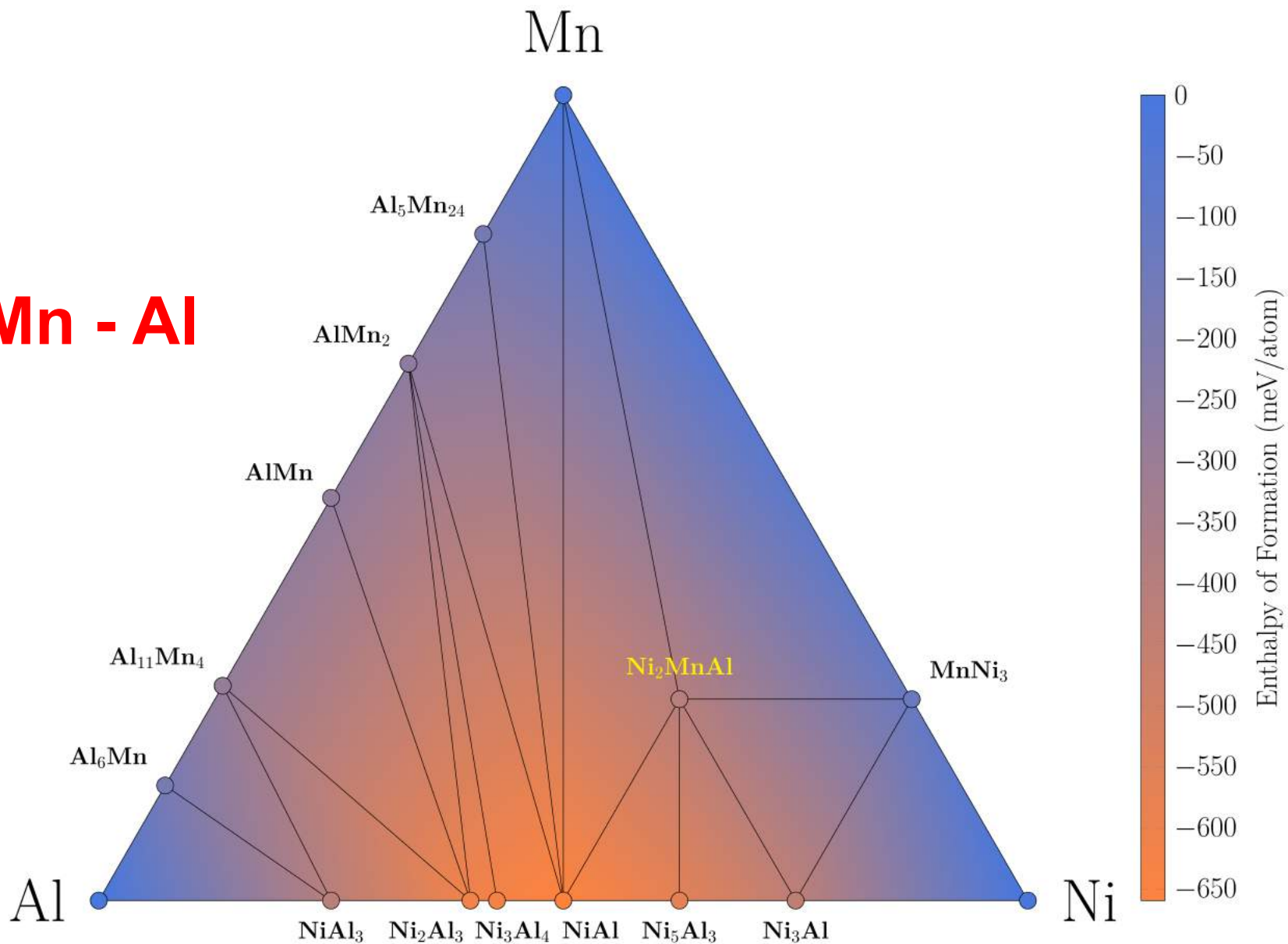
Descriptor 1: Enthalpy of formation



Stability analysis



Ni - Mn - Al



TM³



Look at the transition metal intermetallics

36,540

hydrogen 1 H 1.0079 hydrogen																		helium 2 He 4.0026 helium					
lithium 3 Li 6.941 lithium	beryllium 4 Be 9.0122 beryllium																	boron 5 B 10.811 boron	carbon 6 C 12.011 carbon	nitrogen 7 N 14.007 nitrogen	oxygen 8 O 15.999 oxygen	fluorine 9 F 18.998 fluorine	neon 10 Ne 20.180 neon
sodium 11 Na 22.990 sodium	magnesium 12 Mg 24.305 magnesium																	aluminum 13 Al 26.982 aluminum	silicon 14 Si 28.086 silicon	phosphorus 15 P 30.974 phosphorus	sulfur 16 S 32.065 sulfur	chlorine 17 Cl 35.453 chlorine	argon 18 Ar 39.948 argon
potassium 19 K 39.098 potassium	calcium 20 Ca 40.078 calcium	scandium 21 Sc 44.956 scandium	titanium 22 Ti 47.867 titanium	vanadium 23 V 50.942 vanadium	chromium 24 Cr 51.996 chromium	manganese 25 Mn 54.938 manganese	iron 26 Fe 55.845 iron	cobalt 27 Co 58.933 cobalt	nickel 28 Ni 58.693 nickel	copper 29 Cu 63.546 copper	zinc 30 Zn 65.39 zinc	gallium 31 Ga 69.723 gallium	germanium 32 Ge 72.61 germanium	arsenic 33 As 74.922 arsenic	selenium 34 Se 78.96 selenium	bromine 35 Br 79.904 bromine	krypton 36 Kr 83.80 krypton						
rubidium 37 Rb 85.468 rubidium	strontium 38 Sr 87.62 strontium	ytrium 39 Y 88.906 ytrium	zirconium 40 Zr 91.224 zirconium	niobium 41 Nb 92.906 niobium	molybdenum 42 Mo 95.94 molybdenum	technetium 43 Tc [98] technetium	ruthenium 44 Ru 101.07 ruthenium	rhodium 45 Rh 102.91 rhodium	palladium 46 Pd 106.42 palladium	silver 47 Ag 107.87 silver	cadmium 48 Cd 112.41 cadmium	indium 49 In 114.82 indium	tin 50 Sn 118.71 tin	antimony 51 Sb 121.76 antimony	tellurium 52 Te 127.60 tellurium	iodine 53 I 126.90 iodine	xenon 54 Xe 131.29 xenon						
cesium 55 Cs 132.91 cesium	barium 56 Ba 137.33 barium	57-70 *	lutetium 71 Lu 174.97 lutetium	hafnium 72 Hf 178.49 hafnium	tantalum 73 Ta 180.95 tantalum	tungsten 74 W 183.84 tungsten	rhenium 75 Re 186.21 rhenium	osmium 76 Os 190.23 osmium	iridium 77 Ir 192.22 iridium	platinum 78 Pt 195.08 platinum	gold 79 Au 196.97 gold	mercury 80 Hg 200.59 mercury	thallium 81 Tl 204.38 thallium	lead 82 Pb 207.2 lead	bismuth 83 Bi 208.98 bismuth	polonium 84 Po [209] polonium	astatine 85 At [210] astatine	radon 86 Rn [222] radon					
francium 87 Fr [223] francium	radium 88 Ra [226] radium	89-102 * *	lawrencium 103 Lr [262] lawrencium	rutherfordium 104 Rf [261] rutherfordium	dubnium 105 Db [262] dubnium	seaborgium 106 Sg [266] seaborgium	bohrium 107 Bh [264] bohrium	hassium 108 Hs [269] hassium	meitnerium 109 Mt [268] meitnerium	unnilium 110 Uun [270] unnilium	ununium 111 Uuu [271] ununium	unbibium 112 Uub [272] unbibium											

* Lanthanide series

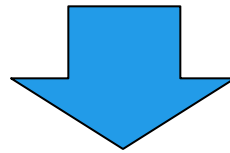
lanthanum 57 La 138.91	cerium 58 Ce 140.12	praseodymium 59 Pr 140.91	neodymium 60 Nd 144.24	promethium 61 Pm [145]	samarium 62 Sm 150.36	europium 63 Eu 151.96	gadolinium 64 Gd 157.25	terbium 65 Tb 158.93	dysprosium 66 Dy 162.50	holmium 67 Ho 164.93	erbium 68 Er 167.26	thulium 69 Tm 168.93	ytterbium 70 Yb 173.04
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* * Actinide series

In summary ...

36,540 possible $\rightarrow$ 248 stable

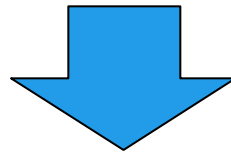
22 magnetic $\rightarrow$ 8 Robust (Δ^{30} criterion)



Extrapolating

236,000 possible $\rightarrow$ 1550 stable

138 magnetic $\rightarrow$ 50 Robust



For real

52 magnetic

Critical temperature magnetism



Descriptor 2: Critical temperature

Known Heusler
ferromagnets

Co_2XY

Fe_2MnY

Ni_2MnY

Generalized regression model based on
valence, volume, spin decomposition



Prediction of T_C

Mn_2XY

Rh_2MnY

Cu_2MnY

Pd_2MnY

Au_2MnY

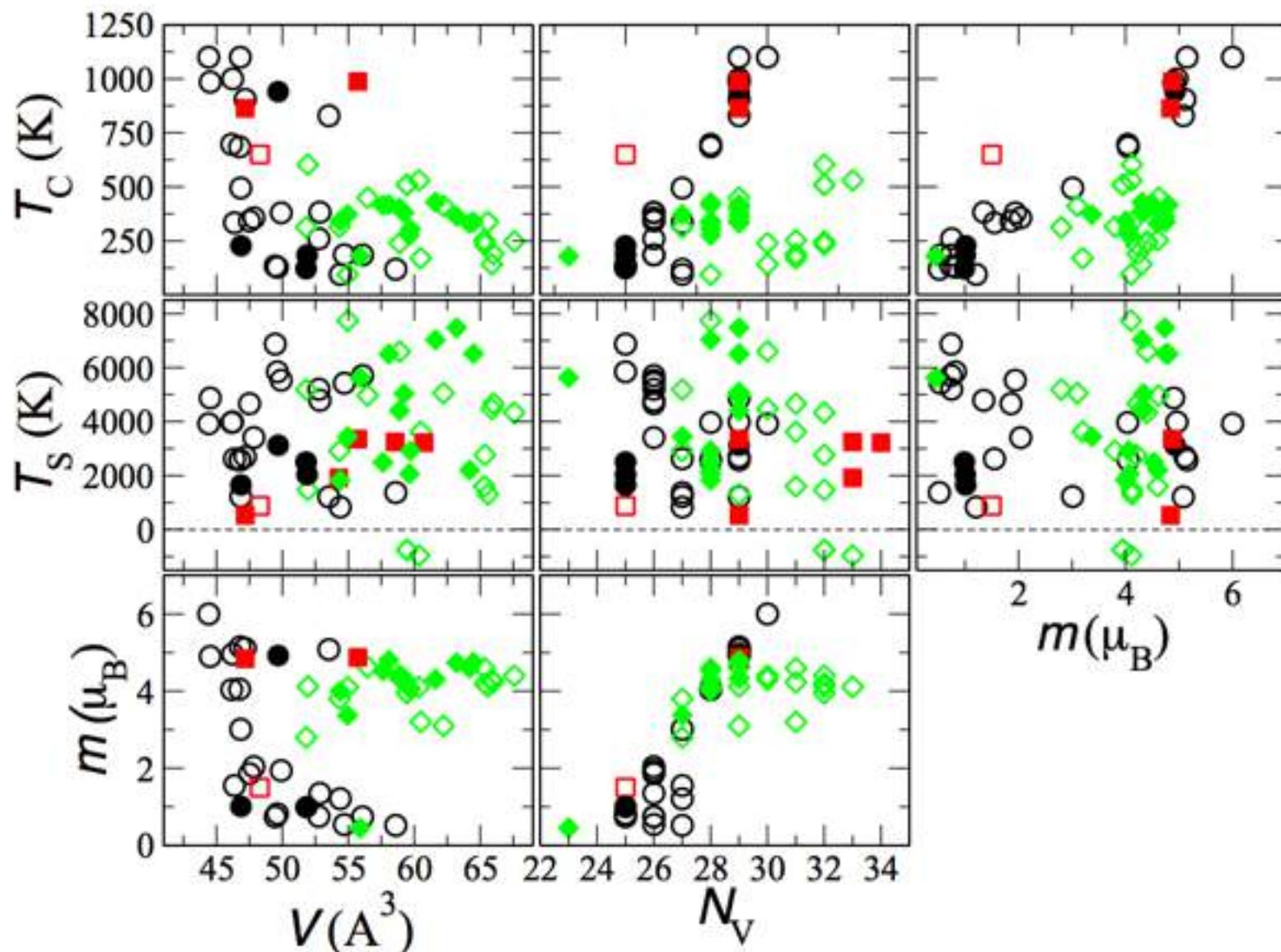
Material	V (Å)	μ	ΔE (eV)	T		T
Co	47.85	2.0	-0.30	3007		352
Mn	48.93	2.0	-0.32	3524		760
...	...	...	...	...		...
Mn	54.28	9.03	-0.17	1918		?

Analysis

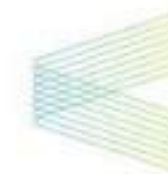
Co_2XY

Mn_2XY

$X_2\text{Mn}Y$

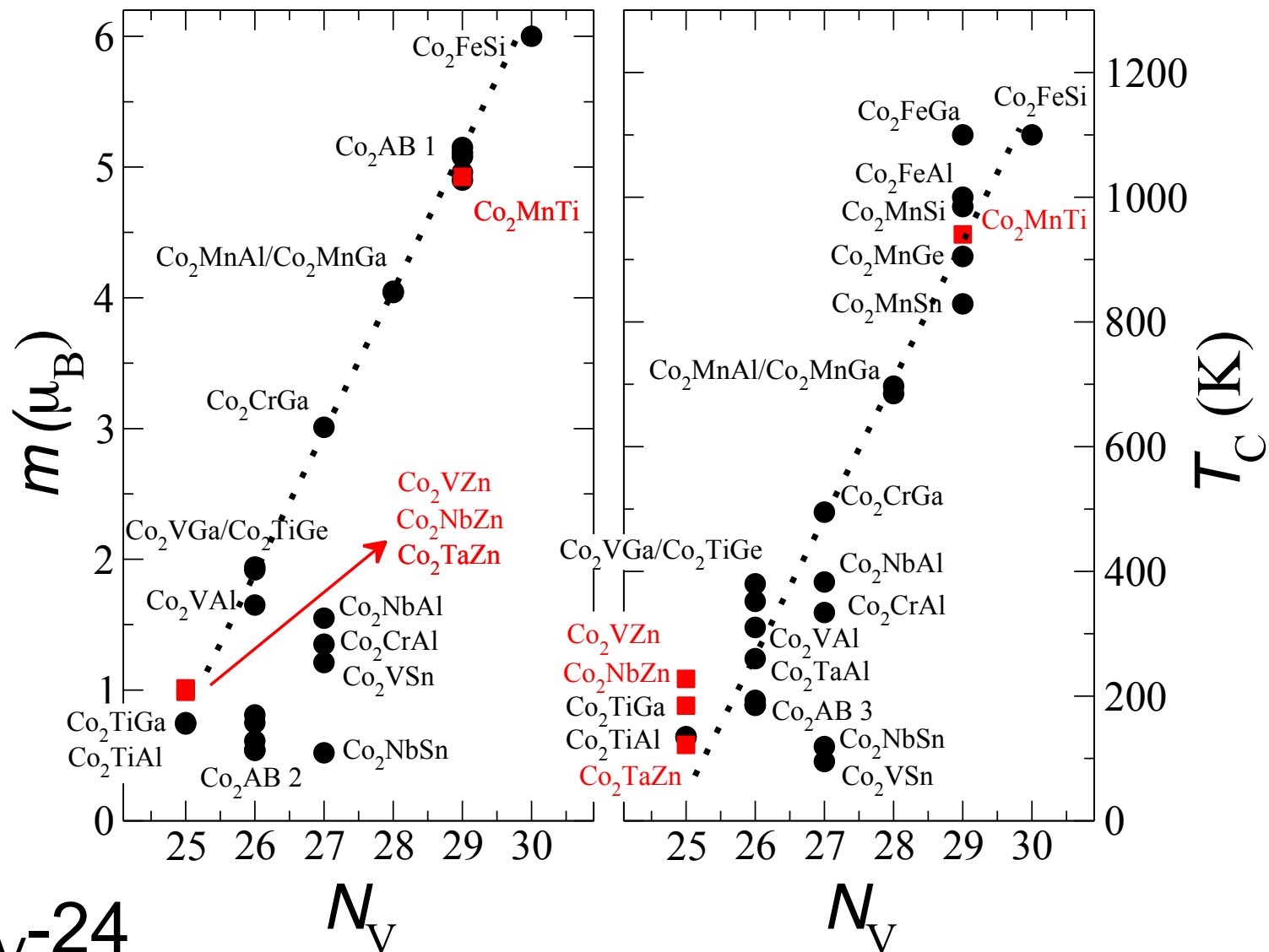


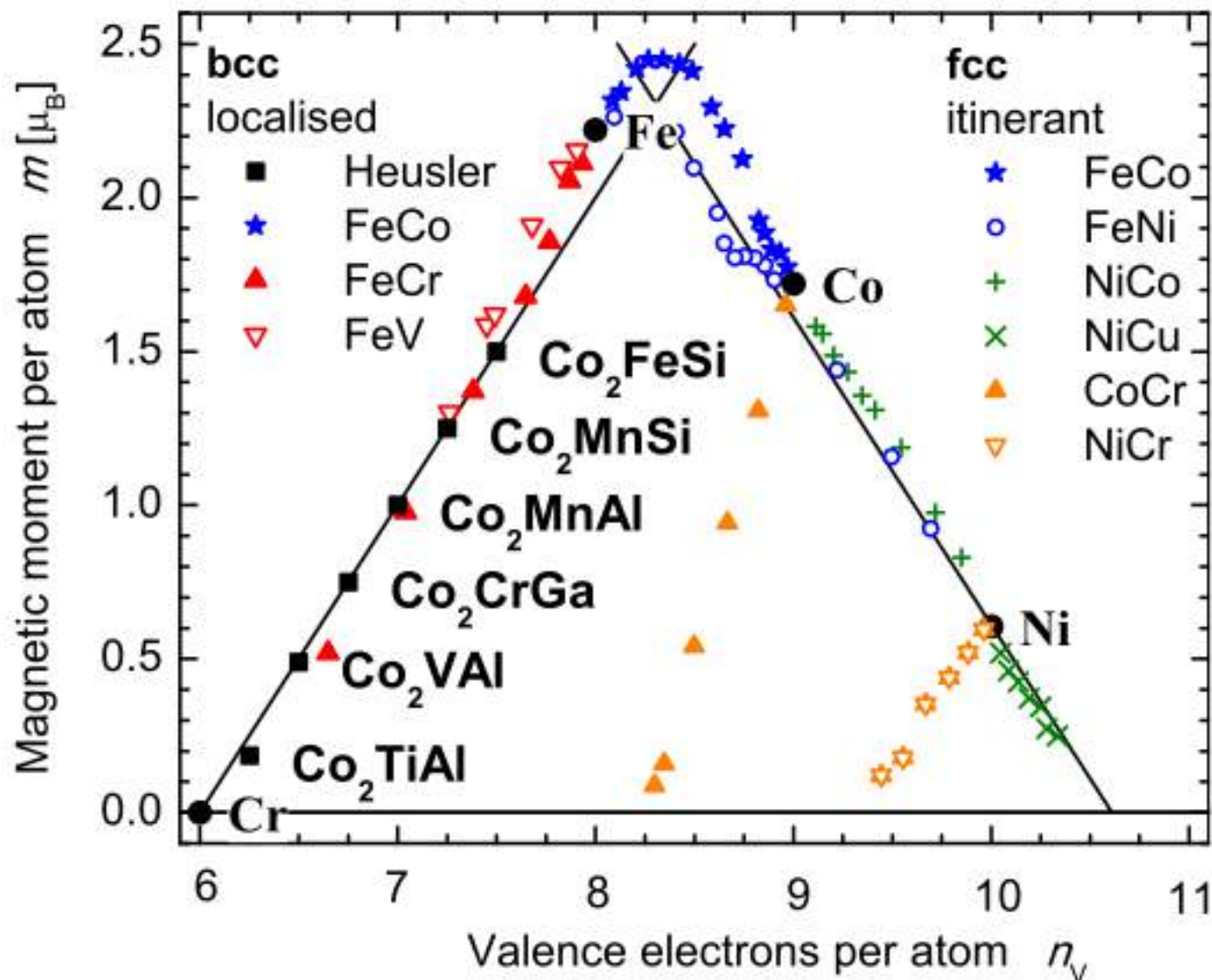
Co₂YZ

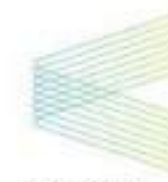


Co₂YZ

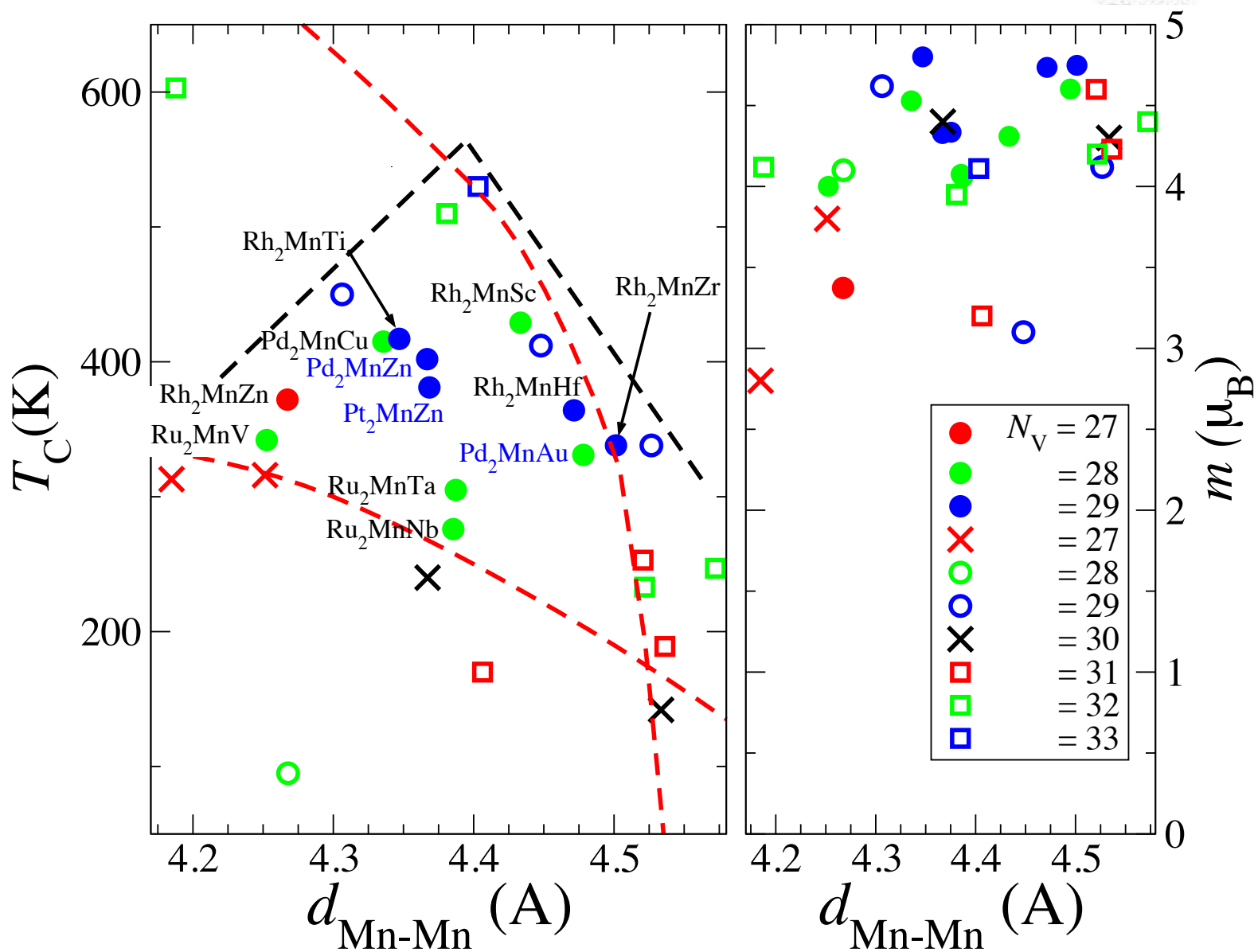
Slater-Pauling



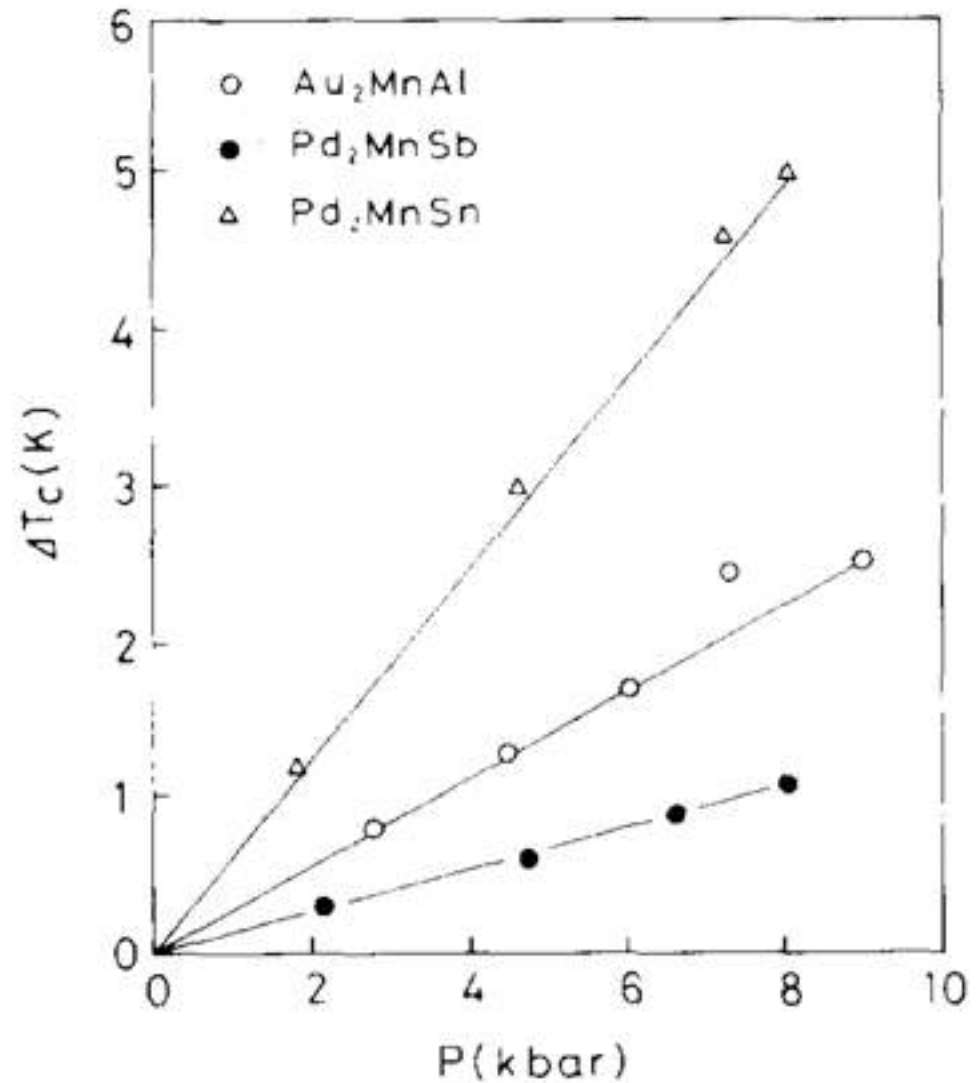




Castelliz-Kanomata curve

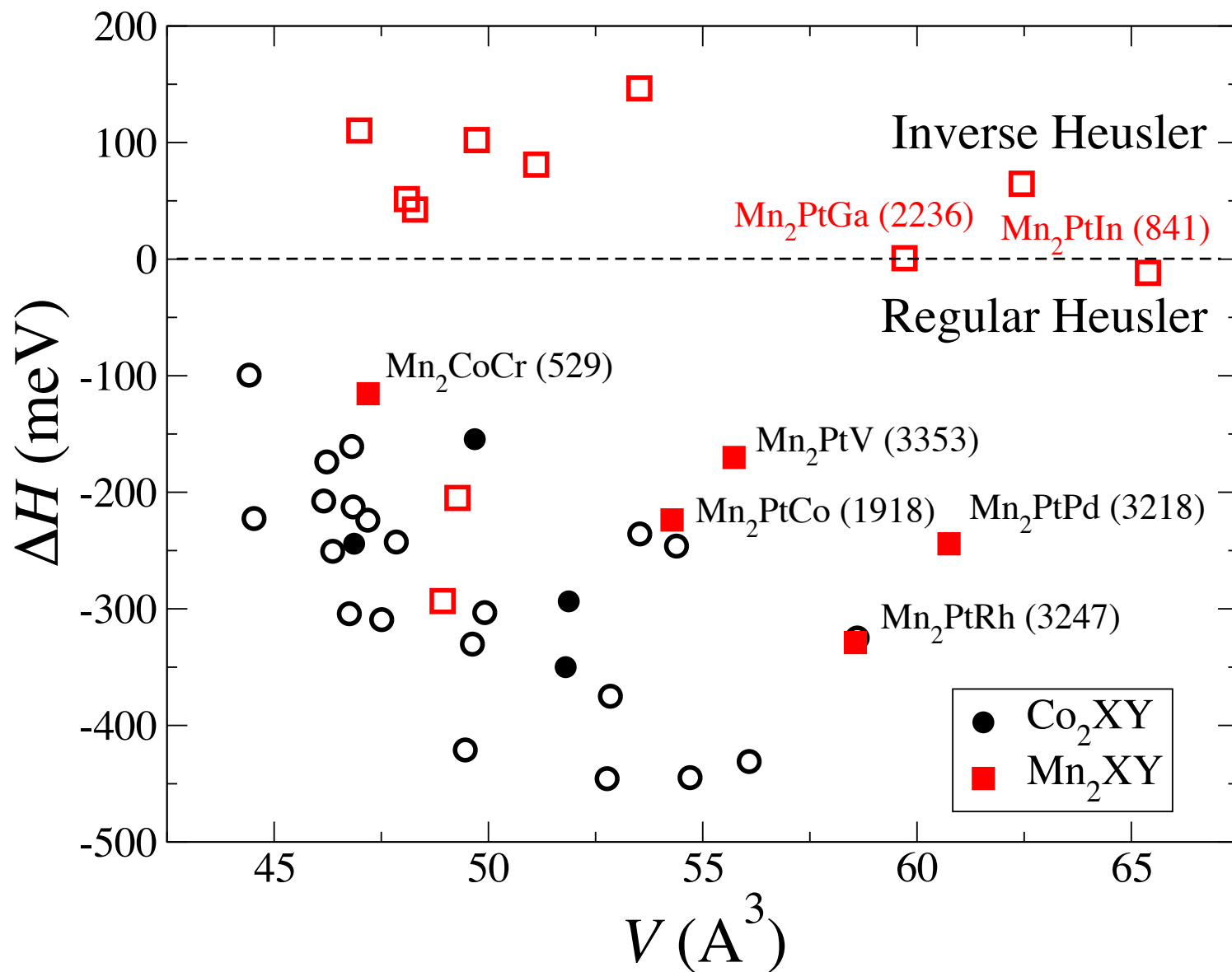


$X_2\text{MnZ}$

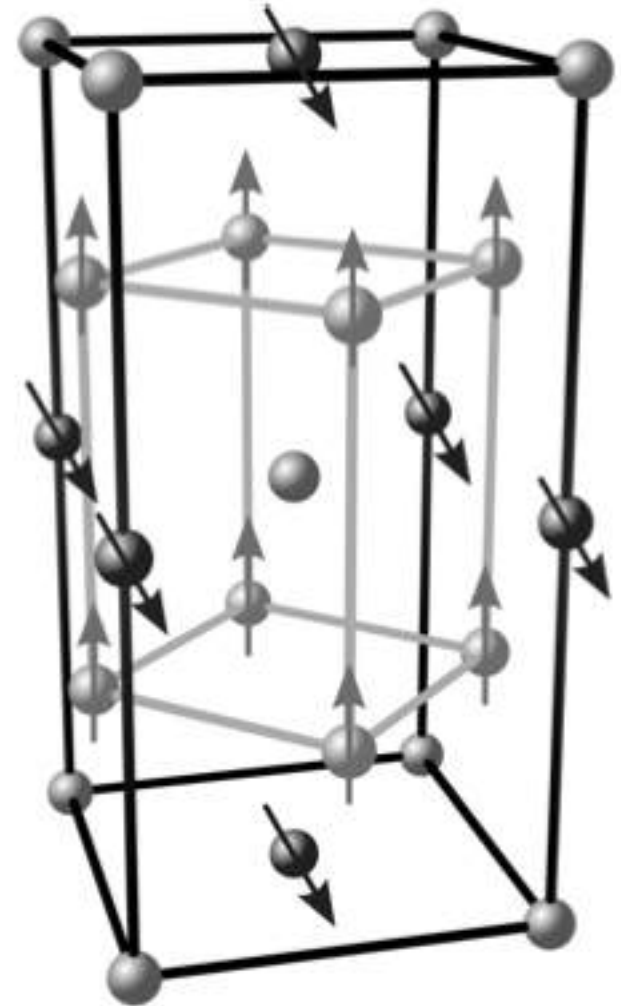
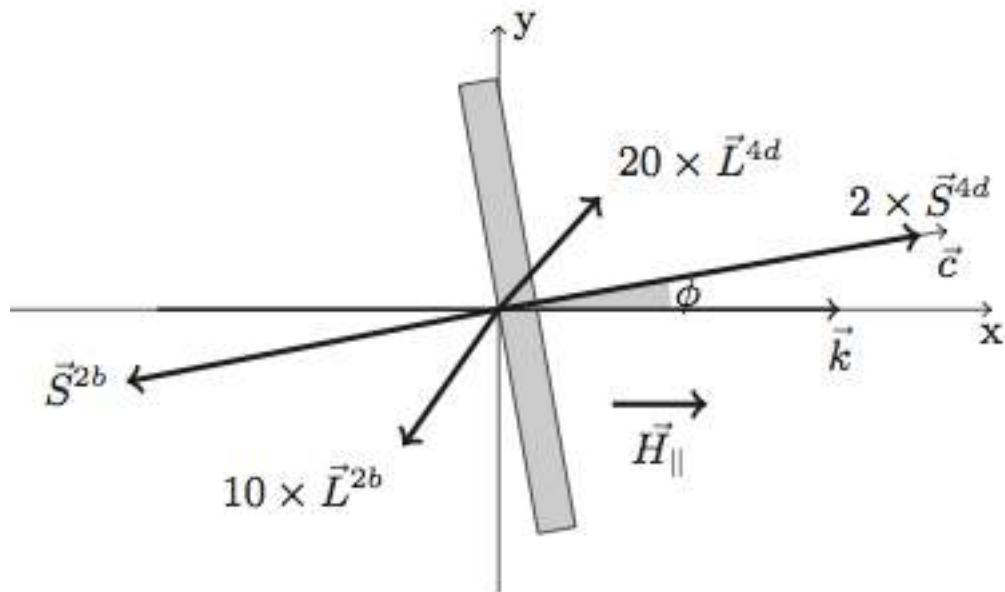


Mn_2YZ

Mn_2YZ



Mn₃Ga

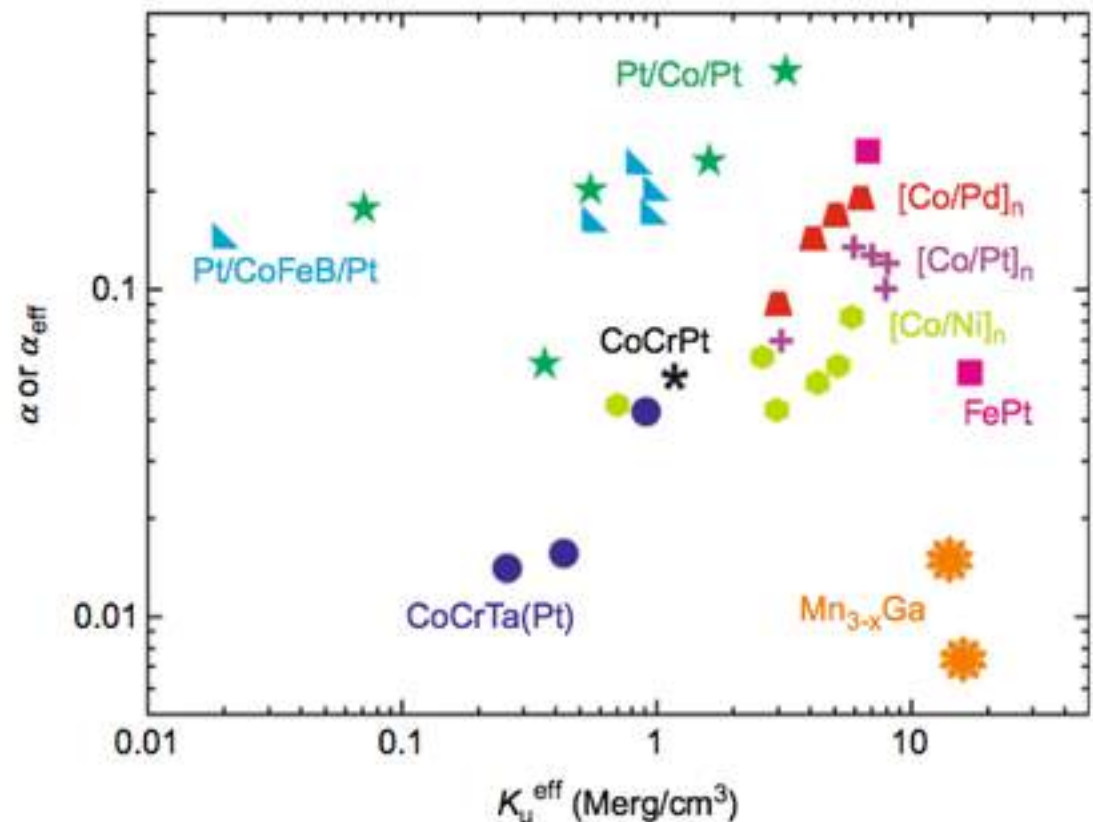


Tetragonal distortion



Descriptor 3: Magneto-crystalline anisotropy

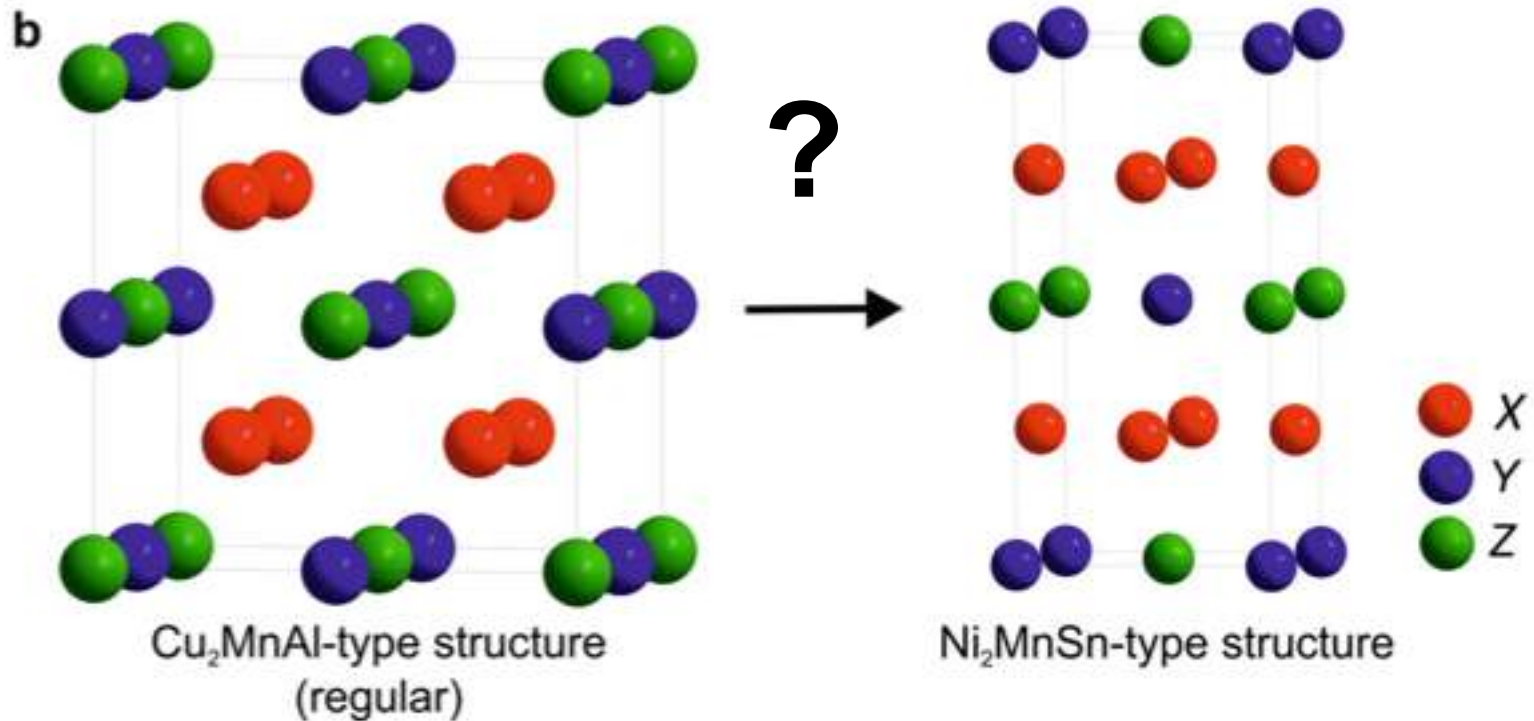
Little magnetic anisotropy in cubic symmetry.
Tetragonal distortion does not much better!



Tetragonal distortion

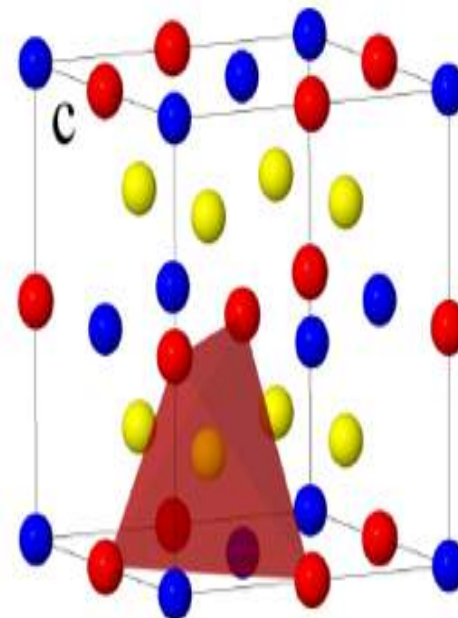
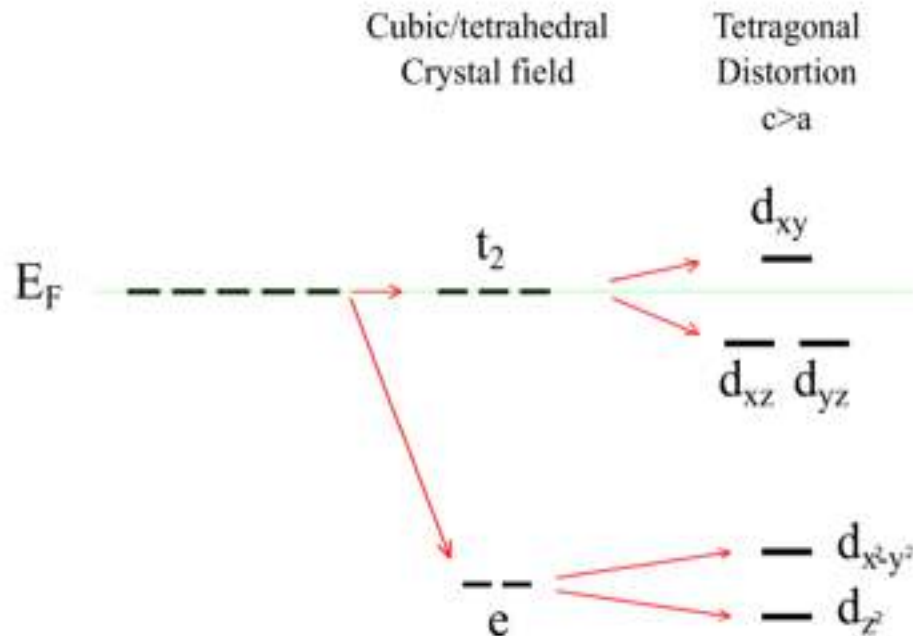


CRANN



Tetragonal distortion

CRANN



Mn_3Ga

Ni_2MnGa

Mn_2NiGa

Rh_2VSn

Pd_2NbSn

Mn_3Ge

Ni_2MnSn

Rh_2CrSn

Pd_2TbSn

Ni_2MnIn

Co_2NbSn

Rh_2FeSn

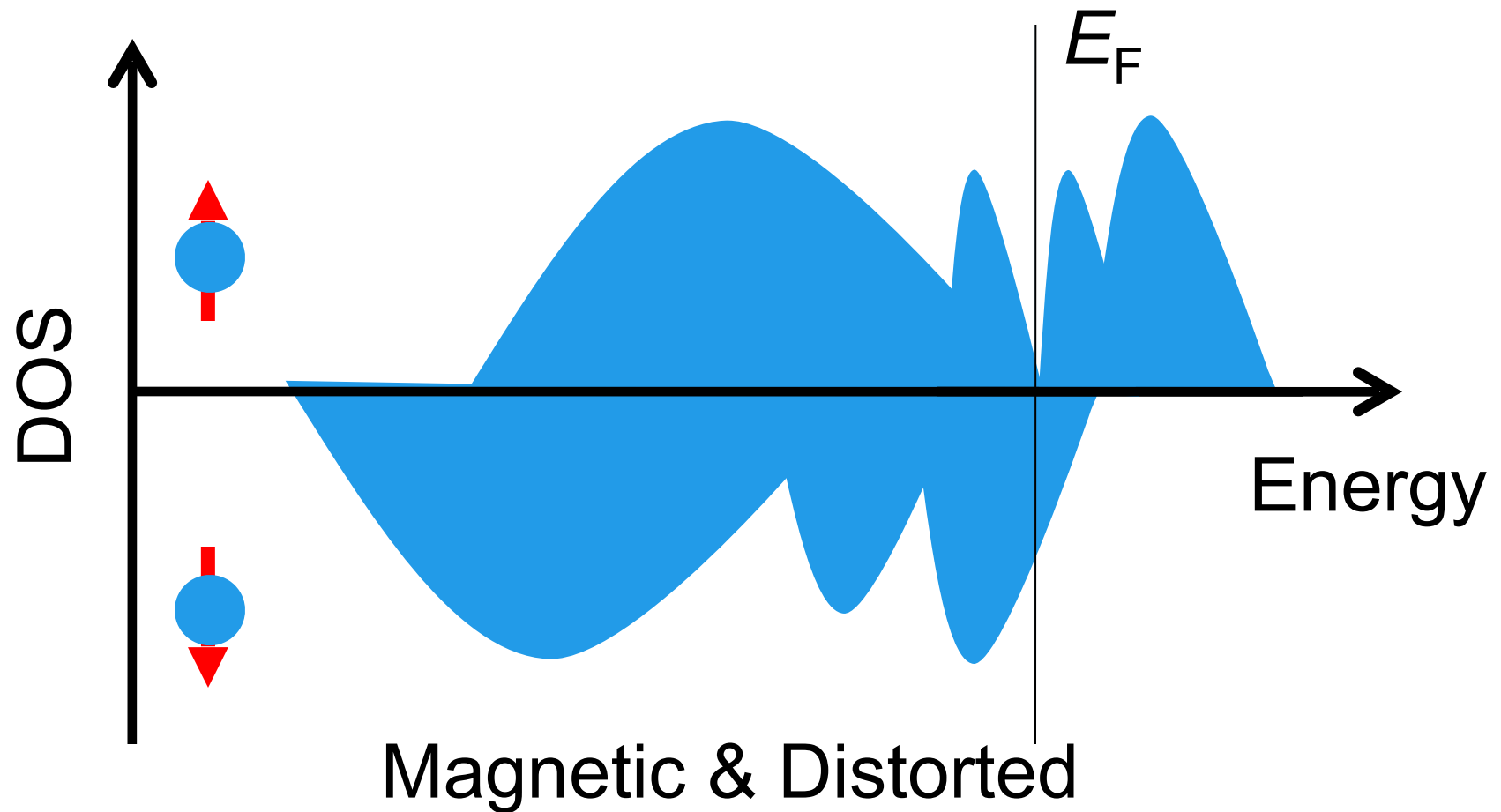
Pd_2DySn

Rh_2CoSn

Mechanism for tetragonal distortion



Stoner Criterion vs band Jahn-Teller distortion



Tetragonal distortion



Among our 22:

2 turn diamagnetic



3 remain magnetic

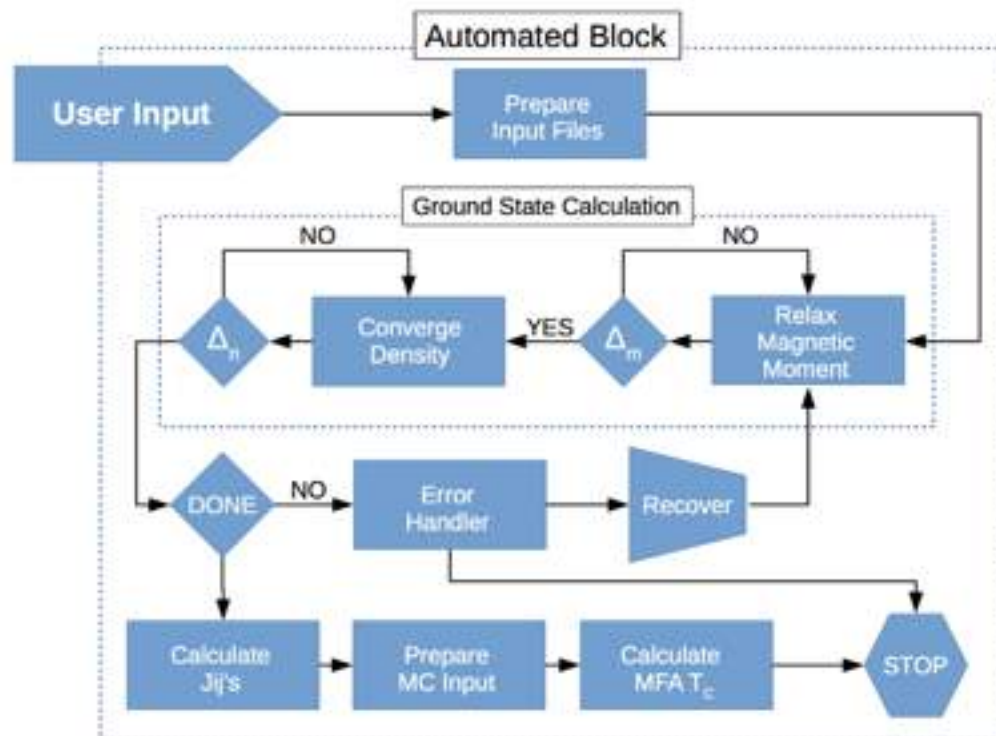


$$P_F \sim 0, \quad T_C \sim 300-400, \quad T_N \sim 2000-5000$$



CRANN

A different workflow



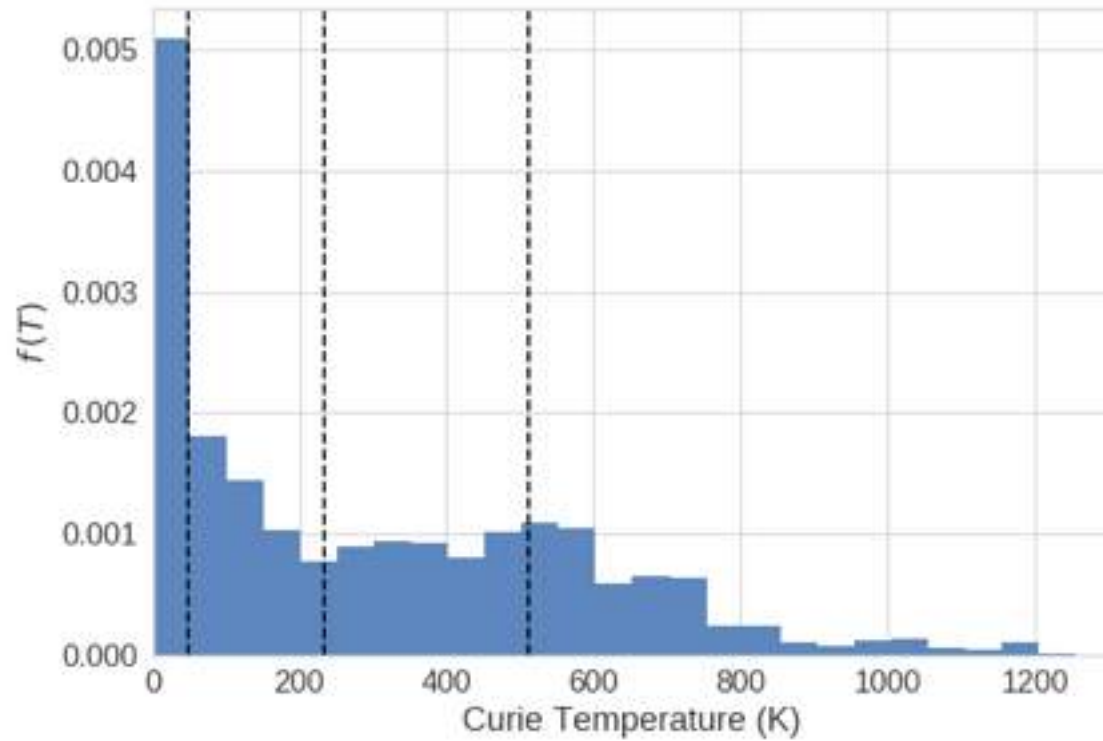
Machine Learning



This is all about processing data

$$(\{Z_i\}, \{N_i\}, \{\zeta_i\}, \{M_i\}, V) \xrightarrow{\text{ML}} y$$

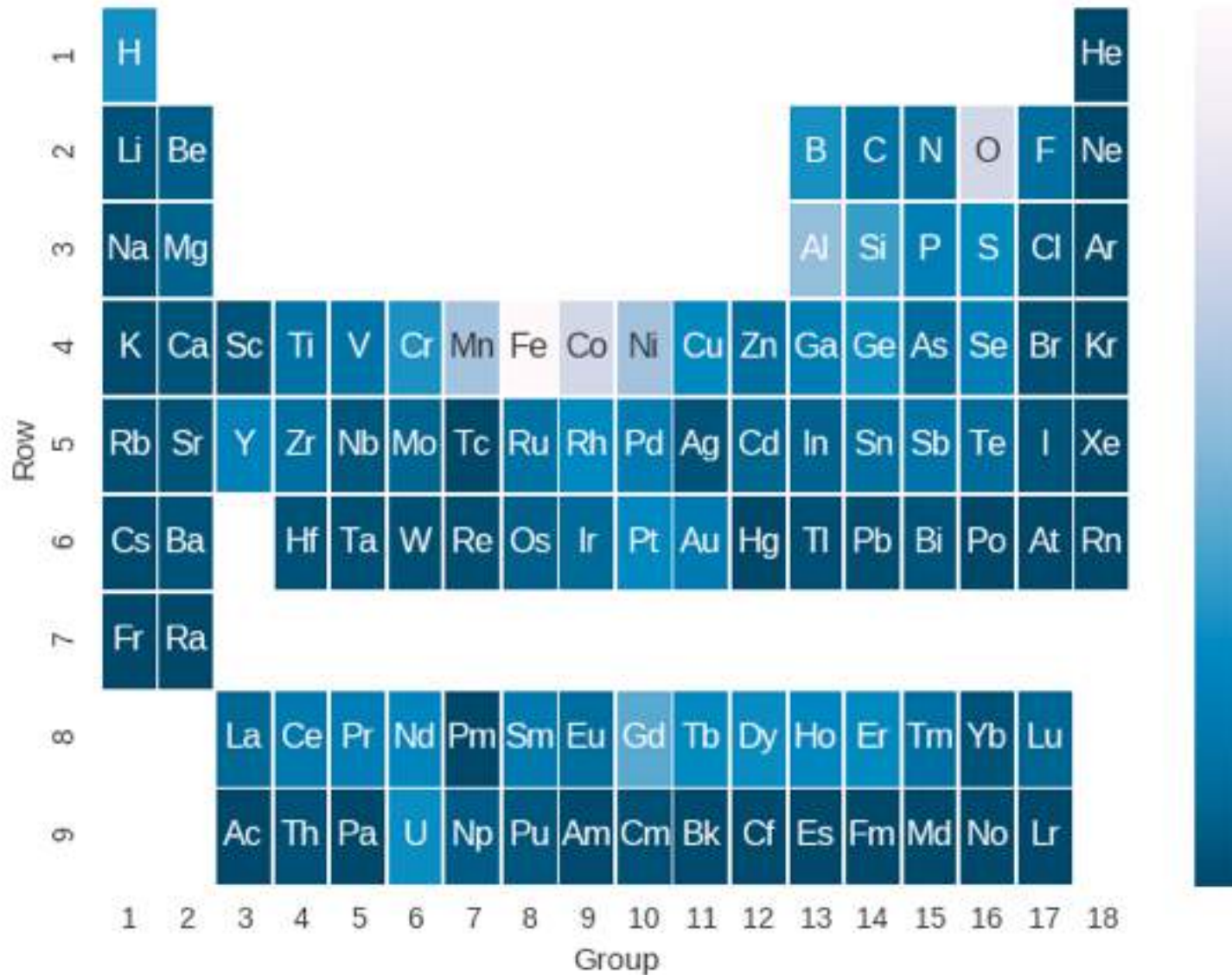
Example: T_C of magnets



Example: T_c of magnets



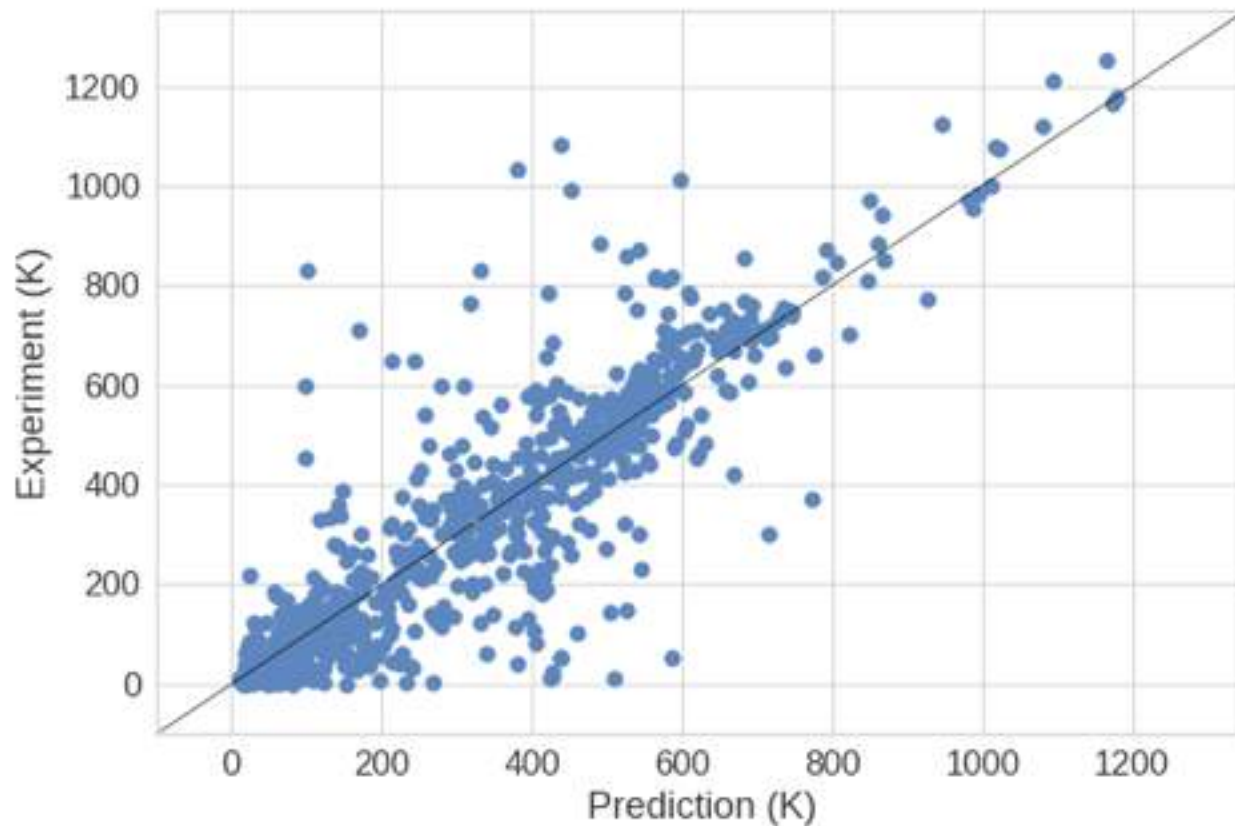
CRANN



Example: T_c of magnets

ML algorithm

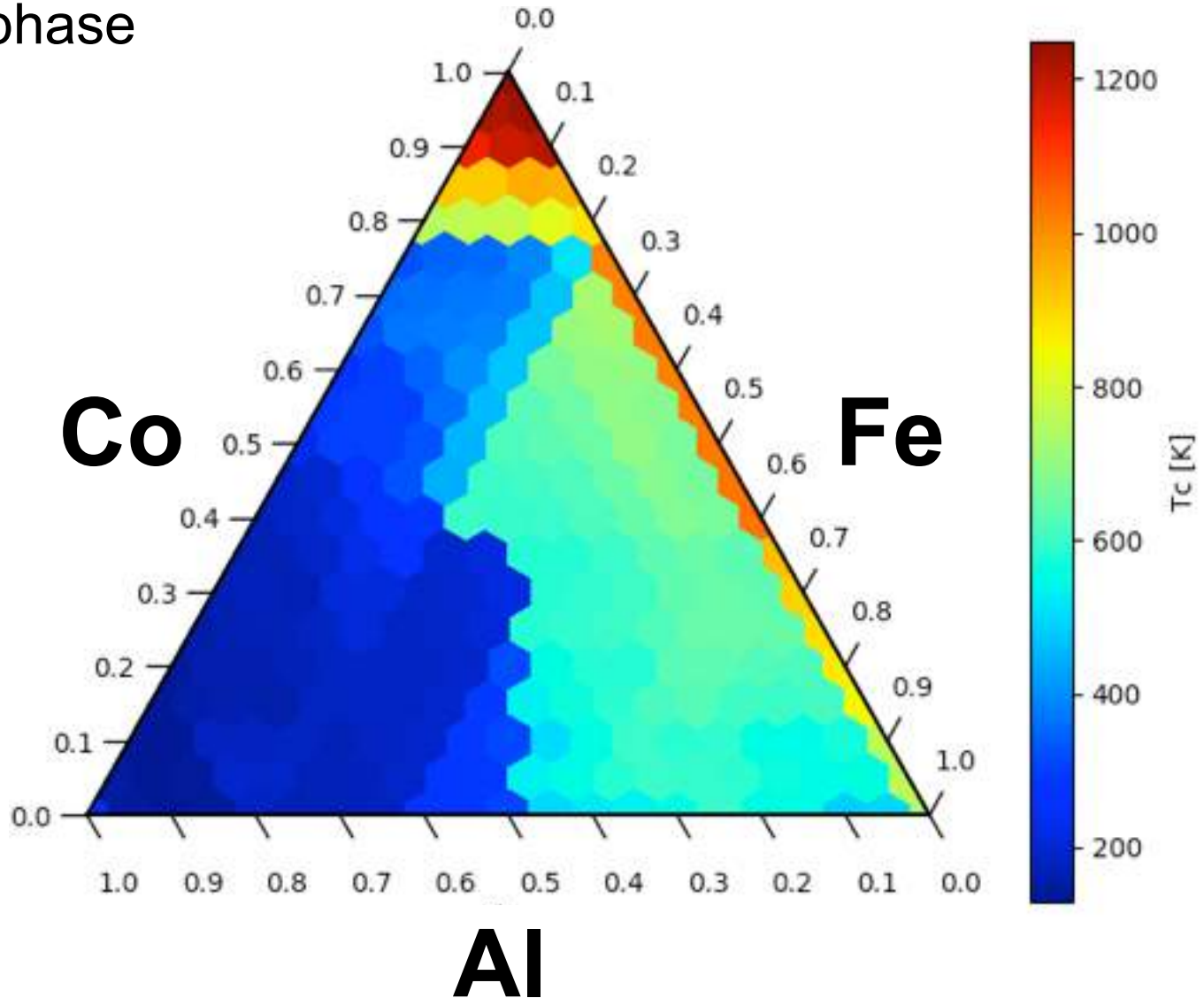
$$(\{Z_i\}, \{N_i\}, \{\zeta_i\}, \{M_i\}, V) \longrightarrow T_c$$



Example: T_C of magnets

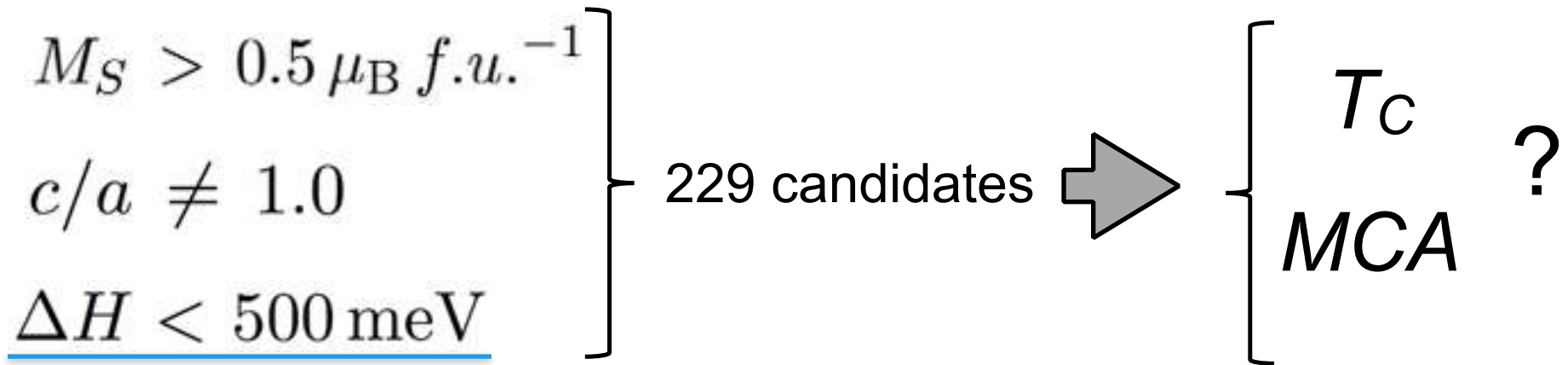


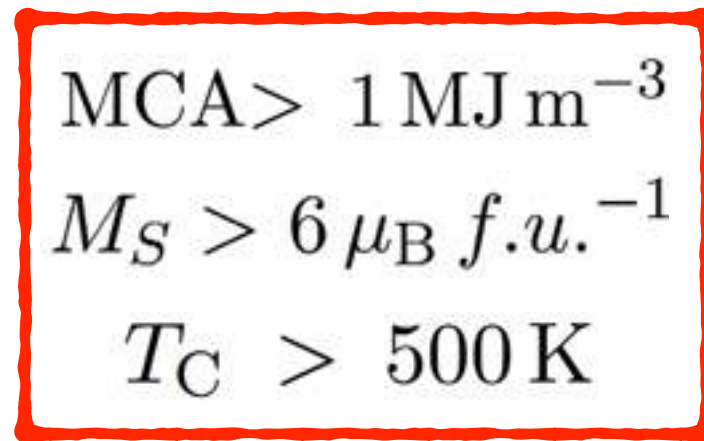
Al-Fe-Co phase
diagram



Targeted screening

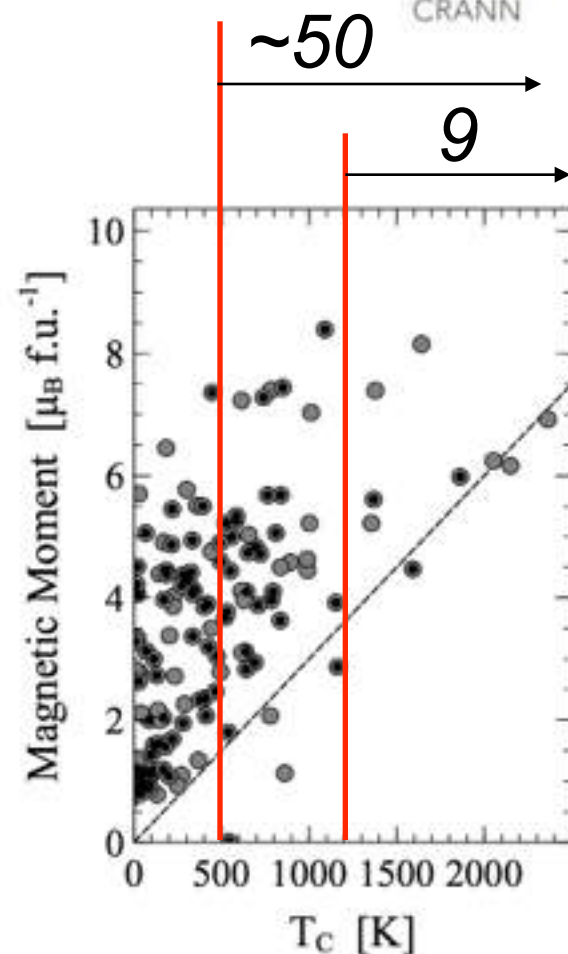
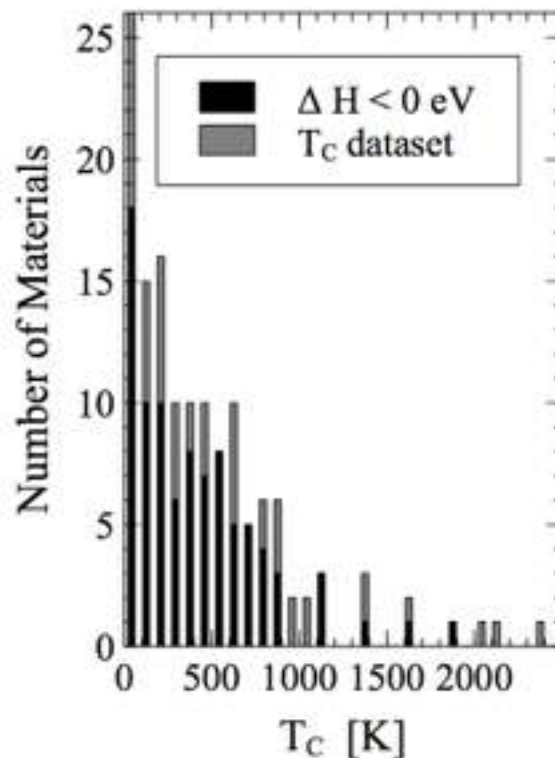
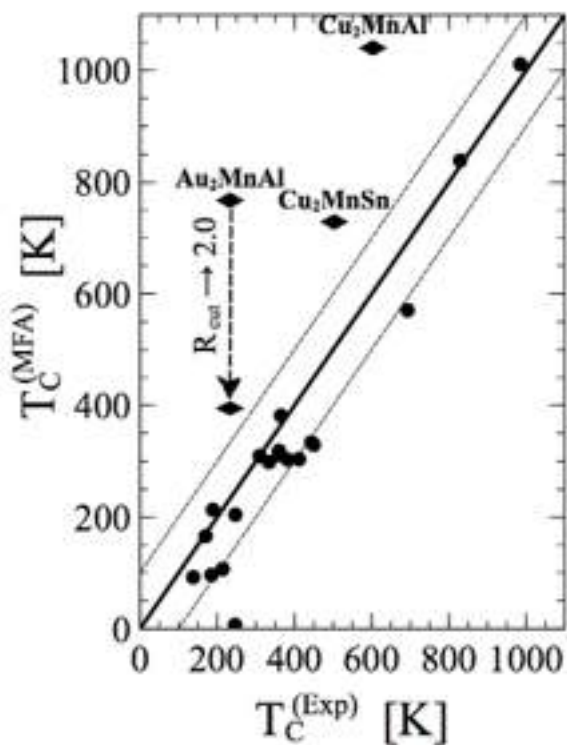
Looking for new permanent magnets:




$$\begin{array}{l} MCA > 1 \text{ MJ m}^{-3} \\ M_S > 6 \mu_B f.u.^{-1} \\ T_C > 500 \text{ K} \end{array}$$

Targeted screening

T_C



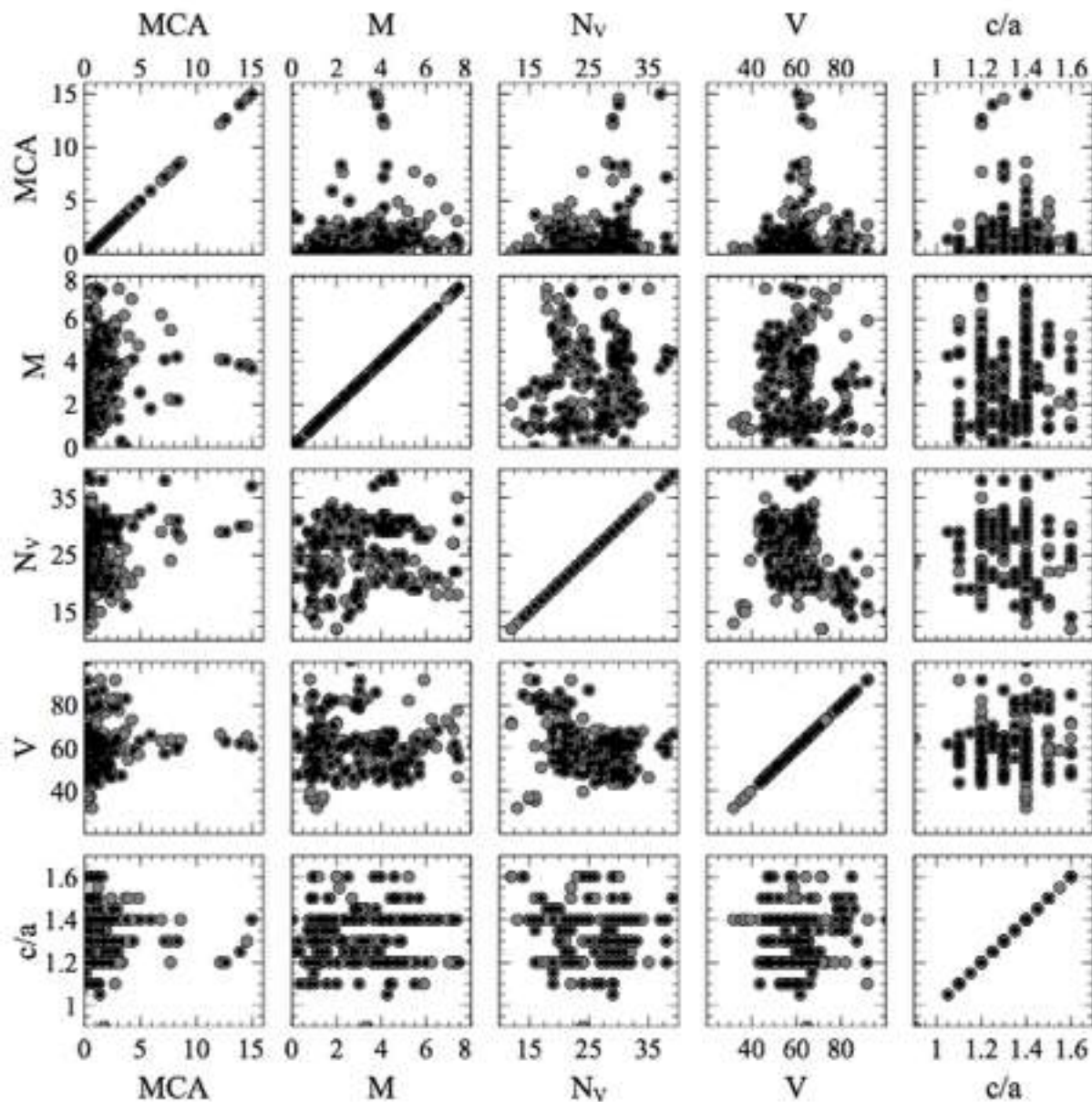
From DFT + MFA

Targeted screening

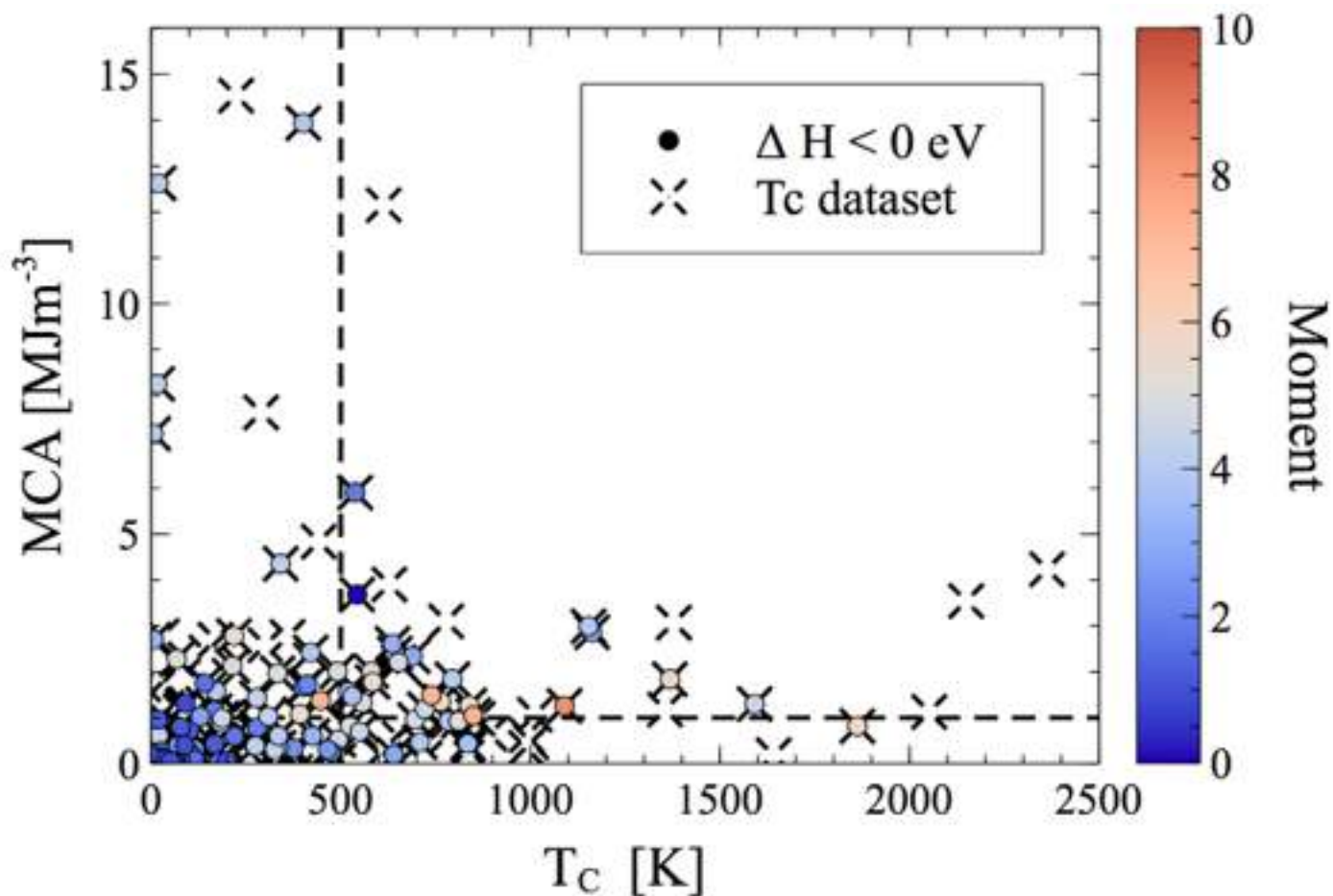


MCA

*From DFT-SO +
magnetic force
theorem*



Targeted screening



Fe₂MnS
Mn₂CuS
Mn₂MgS
Fe₂GeCo
Mn₂CuAl
Cr₂ZnSb
Mn₂ZnAl
Fe₂NiSb

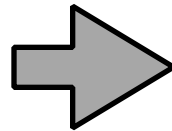
Lots of data: machine learning



ML algorithm

$(\{Z_i\}, \{N_i\}, \{\zeta_i\}, \{M_i\}, V) \longrightarrow \textit{Property (MCA)}$

Accurate = Selective



Useful materials
will be left out

The lottery example

Who won the last National lottery ?

NO

Lots of data: machine learning

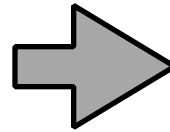


Strategy: use machine learning to screen the **NOT** hard magnets

ML algorithm

$(\{Z_i\}, \{N_i\}, \{\zeta_i\}, \{M_i\}, V) \longrightarrow \text{Property (MCA)}$

Accurate = Selective



Useful materials
will be left out

Selecting hard magnets

Hard

Soft +
Hard

Selecting soft magnets

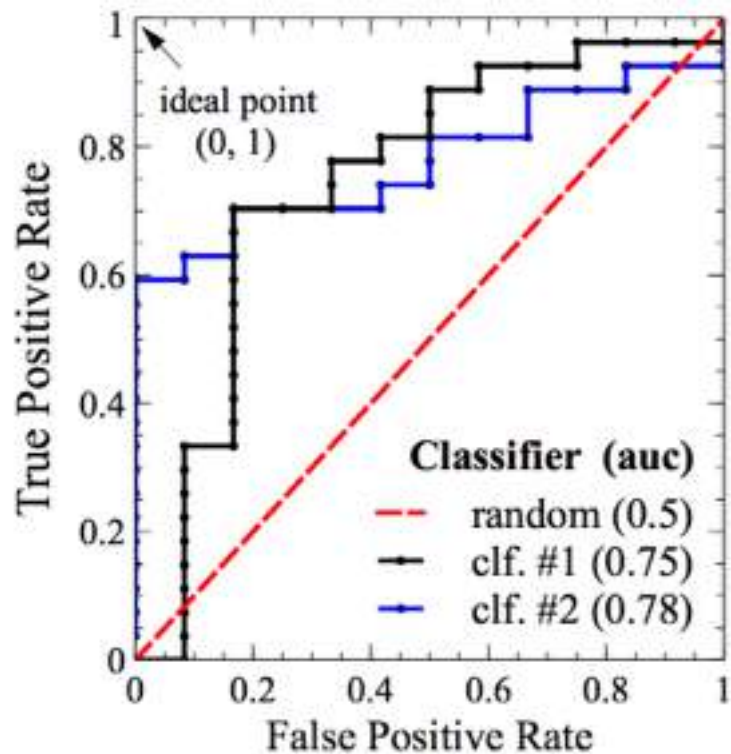
Soft

Hard +
Soft

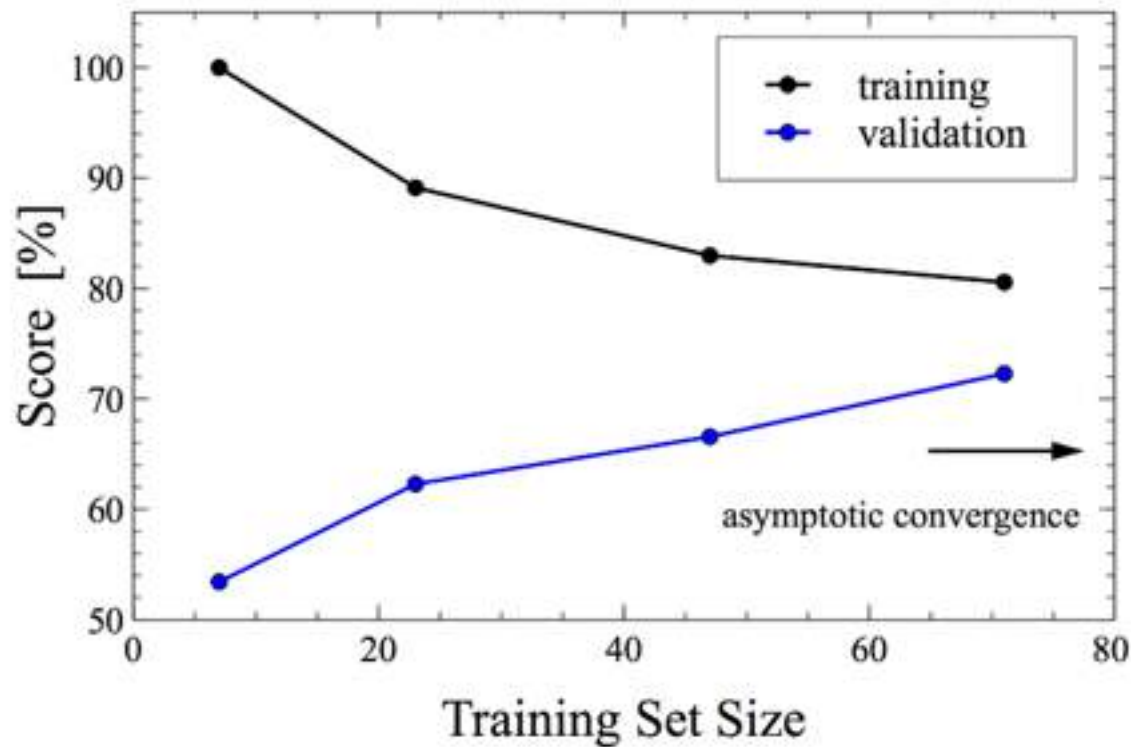
Lots of data: machine learning



Receiver operating curve (ROC)



60% TPR with 0 FPR



Need ~80 data for learning

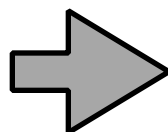
Machine learning *workflow*



250,000 candidates

2000 candidates

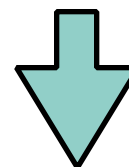
229 candidates



1000 used for DFT + ML

80 used for DFT + ML

80 used for DFT + ML



249,000 remaining

1920 remaining

149 remaining



ML TPR 60% (50:50 population)

Don't calculate 30% = 50

Don't calculate 30% = ~650

Don't calculate 30% = ~80,000

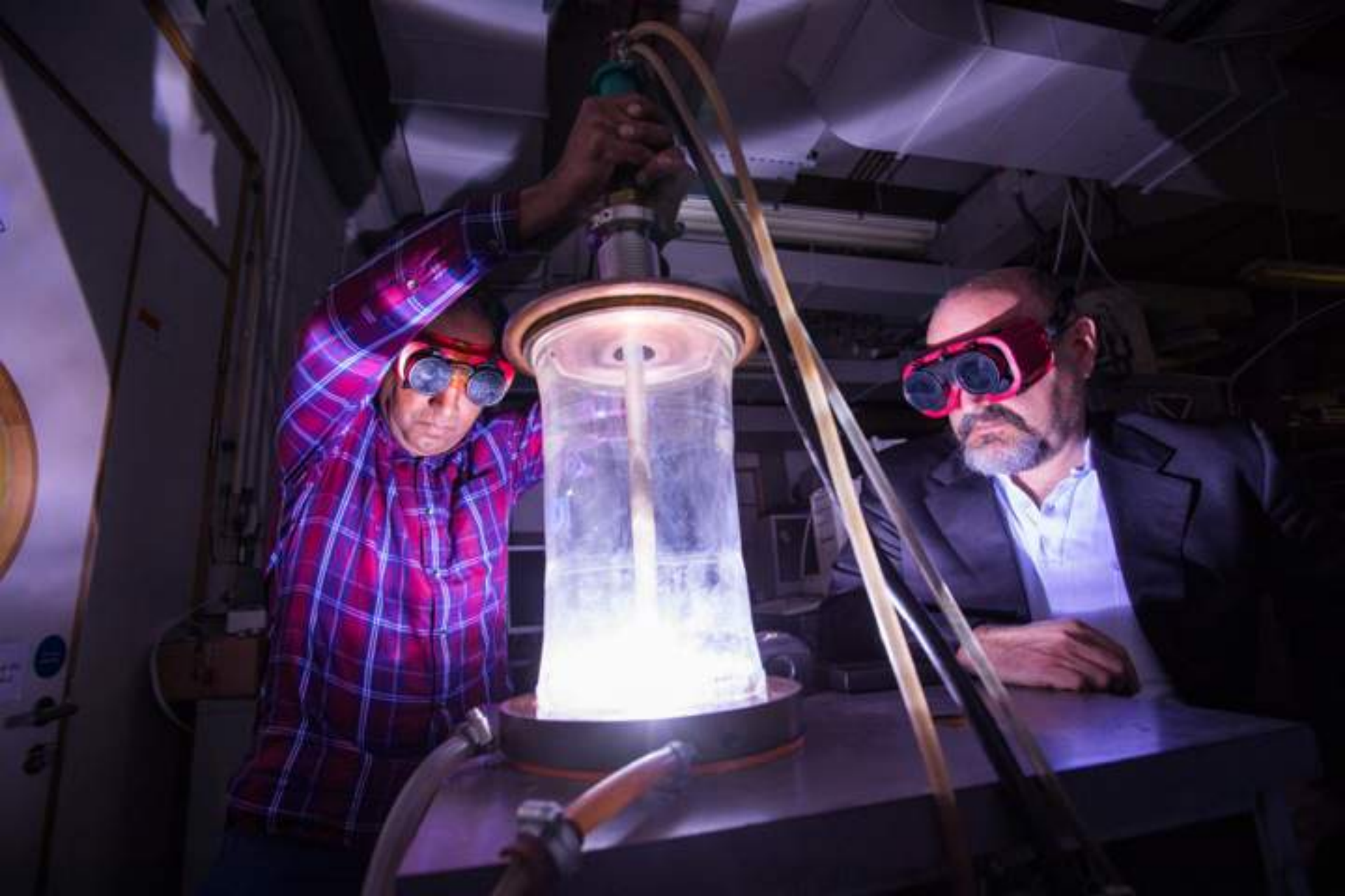
Limitations



Two issues in materials science

$$\underbrace{(\{Z_i\}, \{N_i\}, \{\zeta_i\}, \{M_i\}, V)}_N \quad \text{curse of dimensionality} \quad \rho \longrightarrow m^N$$

Our “big data” are not big yet



S. Sanvito et al., *Accelerated discovery of new magnets in the Heusler alloy family*, Science Advances **3**, e1602241 (2017)

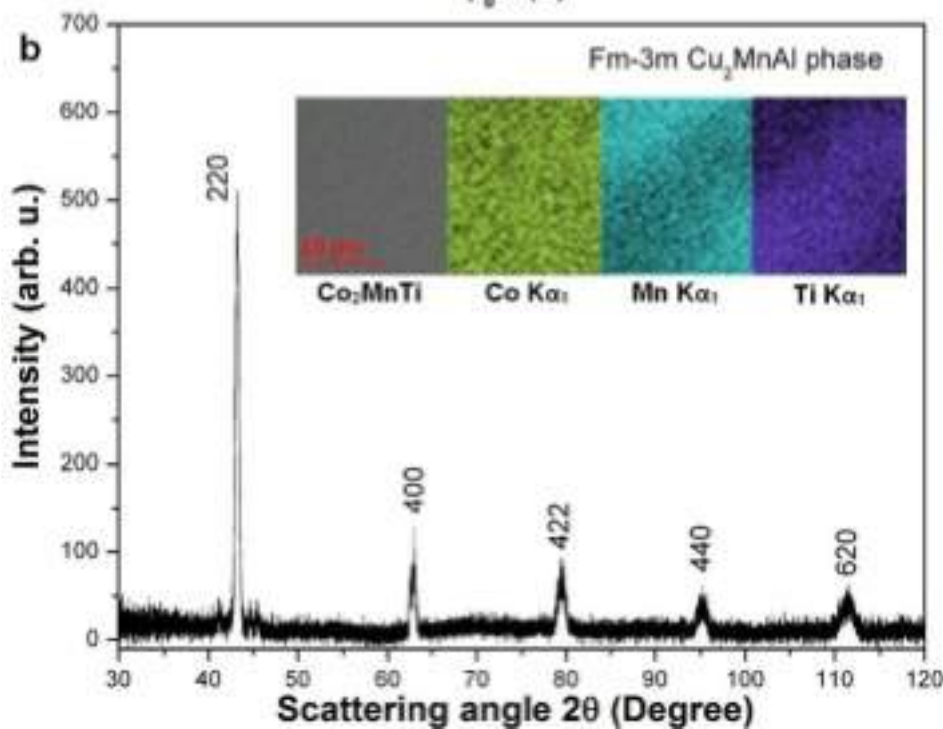
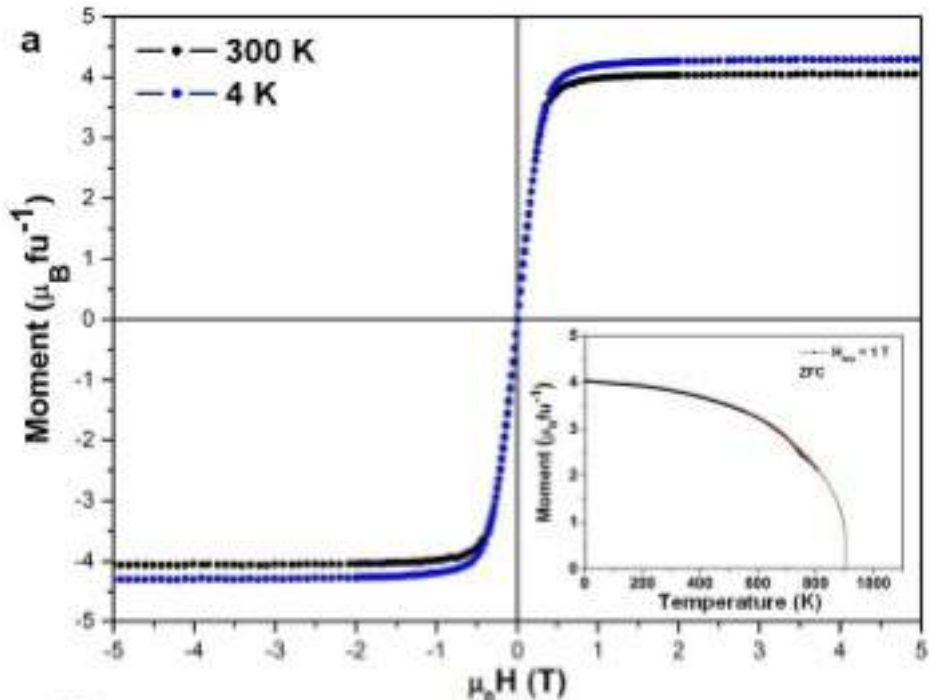
Co₂MnTi

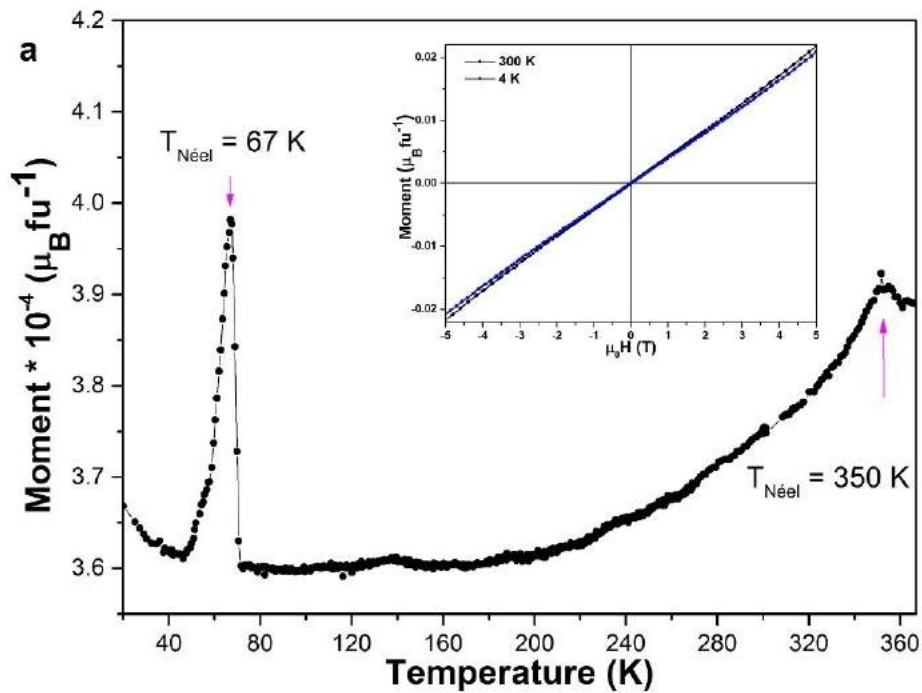
$$T_C^{\text{measured}} = 940\text{K}$$

$$T_C^{\text{predicted}} = 938\text{K}$$

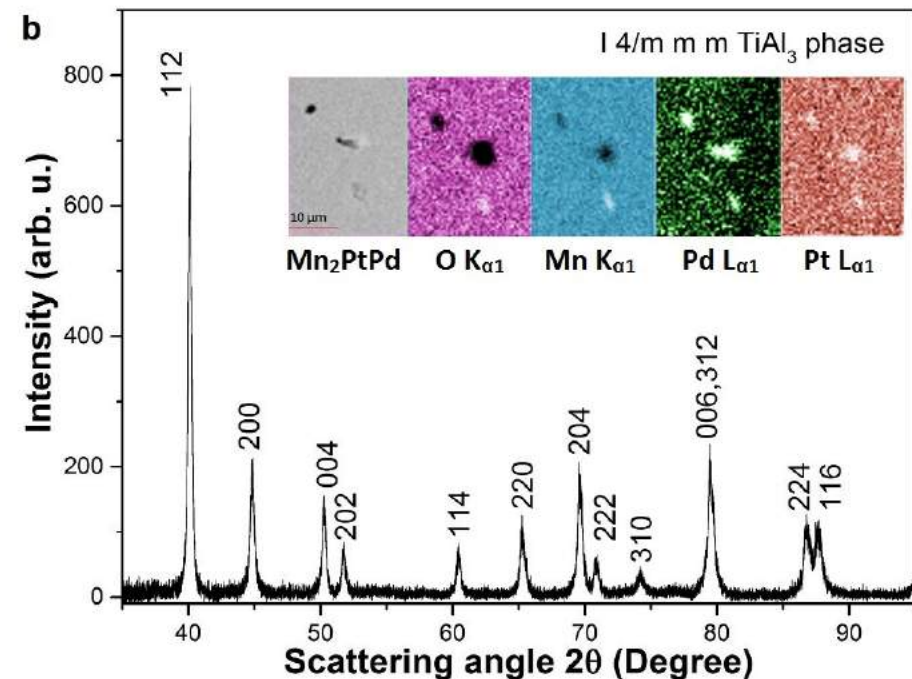
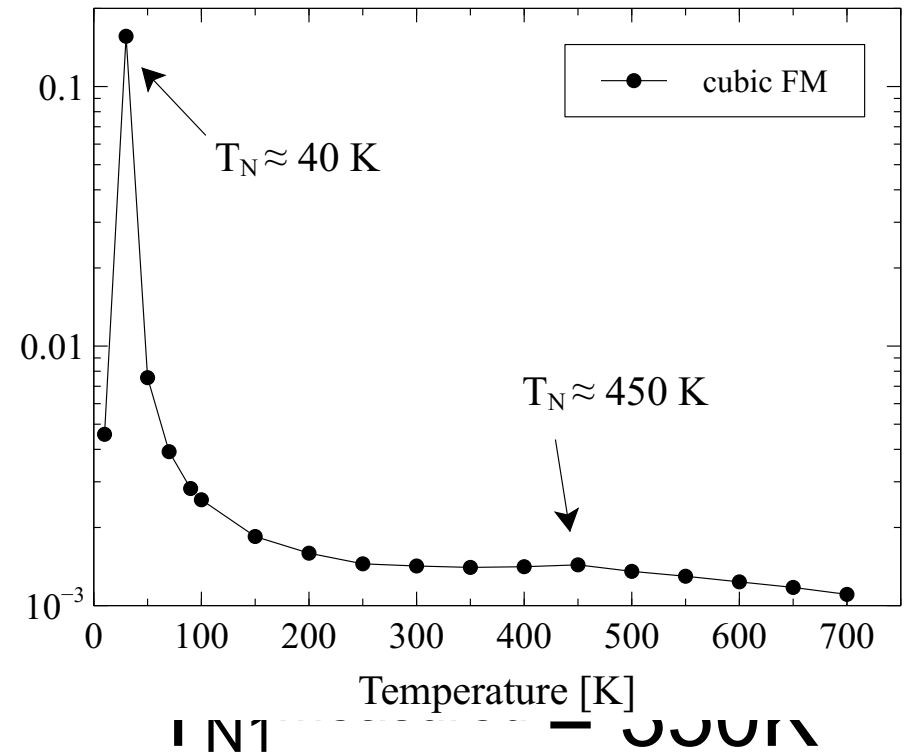
Prepared by arc melting in
an Ar atmosphere

Courtesy J.M.D. Coey's Lab
(P. Tozman, M. Venkatesan)





Magnetic Susceptibility [a.u.]



Complex antiferromagnetic order

Courtesy J.M.D. Coey's Lab
(P. Tozman, M. Venkatesan)

Bottom line

Did we find one ?





COMPUTATIONAL SPINTRONICS

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Duke Team:

Stefano Curtarolo, Junkai Xue, Kevin Rasch, Corey Oses

