

innovating nanoscience



CRANN

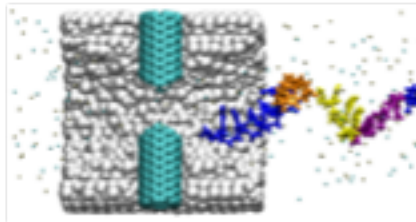
The long way to the discovery of new materials made it short

Stefano Sanvito (sanvitos@tcd.ie)

School of Physics and CRANN, Trinity College Dublin, IRELAND

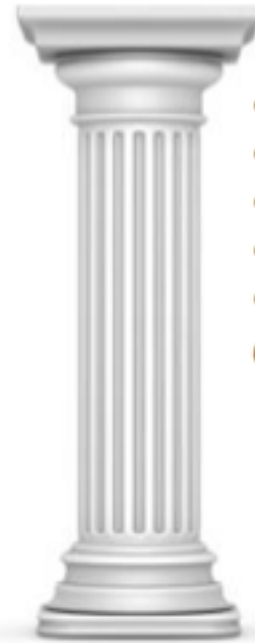
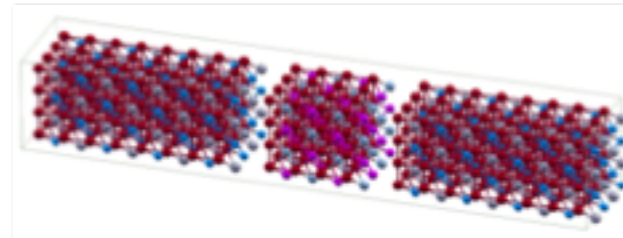
Two main pillars

Large-scale electronic structure simulations



- Algorithm development
- Capability computing
- Access to large infrastructures
- Software distribution

Materials Genomics



- Database construction
- Strong data-mining element
- Capacity computing
- On-line infrastructures
- Large international collaboration

Sustaining CRANN
experimental activity

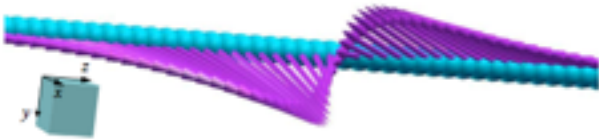


Theory activity

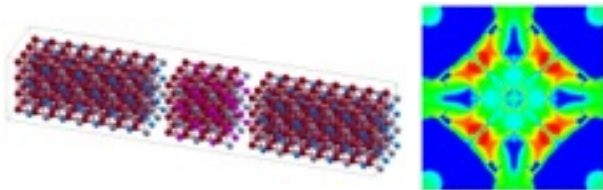


Spin electronics

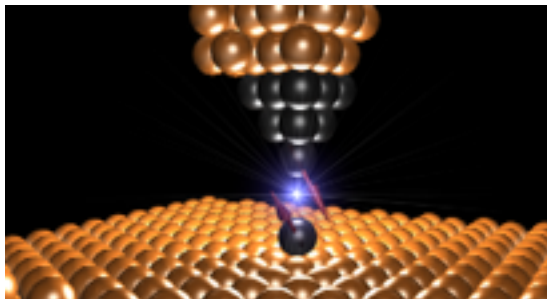
Spin-dynamics



Spin-transport

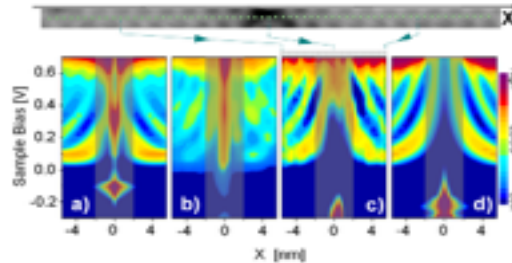


Spin excitation/torque

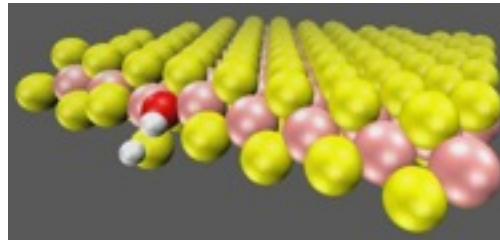


Materials

Transport and STM



2D/topological

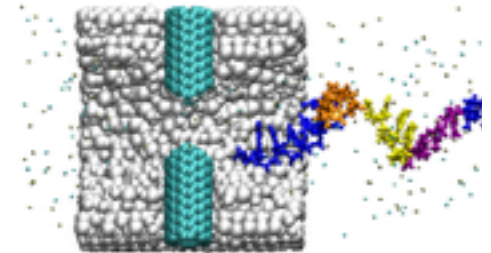


Magnetic Genoma

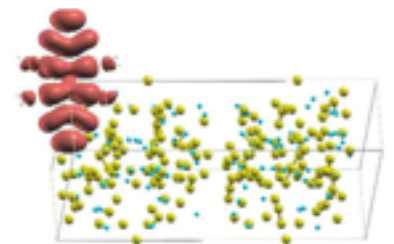


Organics

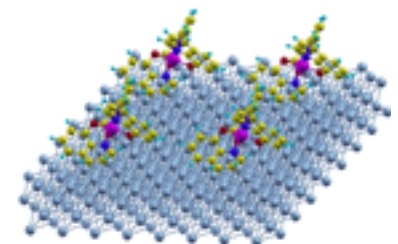
DNA sequencing



Diffusive Transport



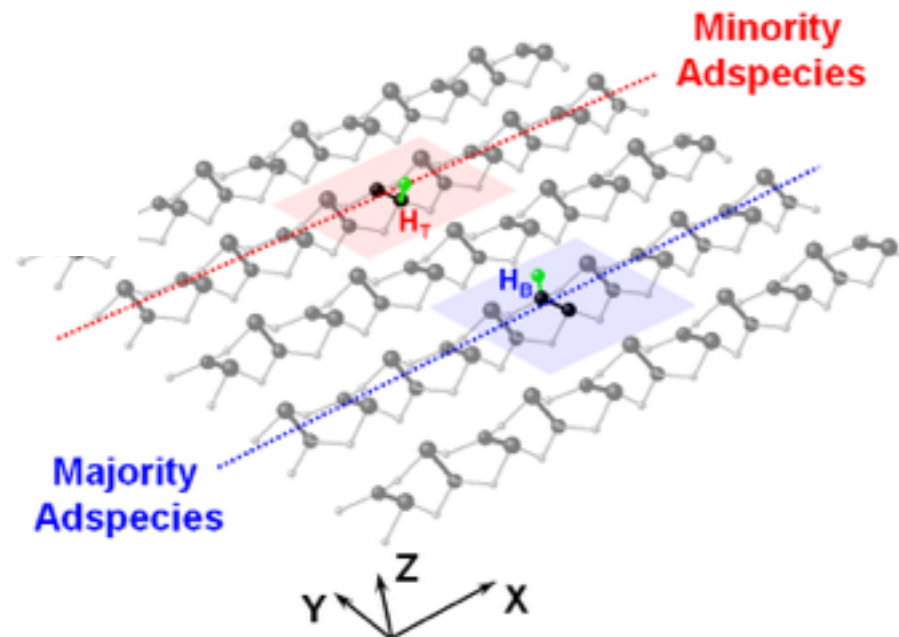
Organic spintronics





Quantum playground 1

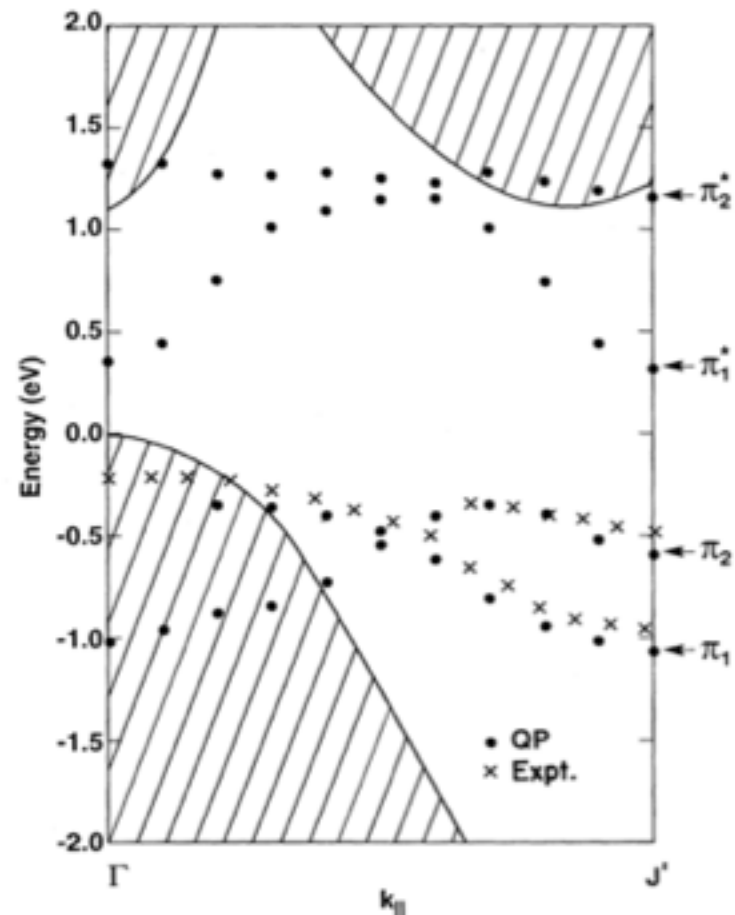
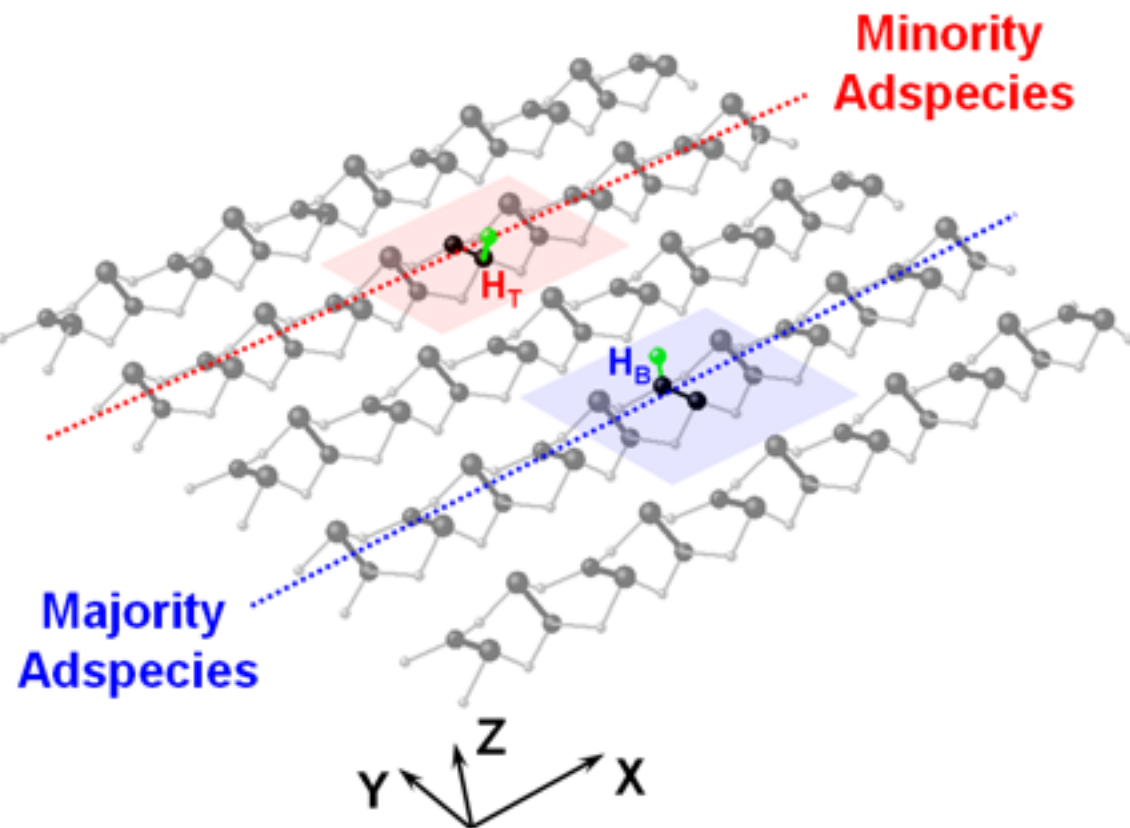
H on Si (100)



H on Si (100)

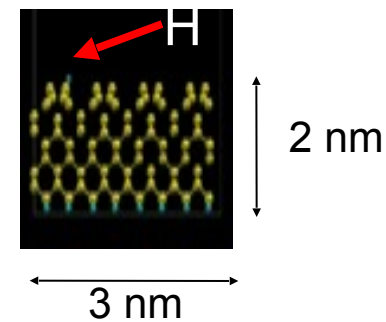
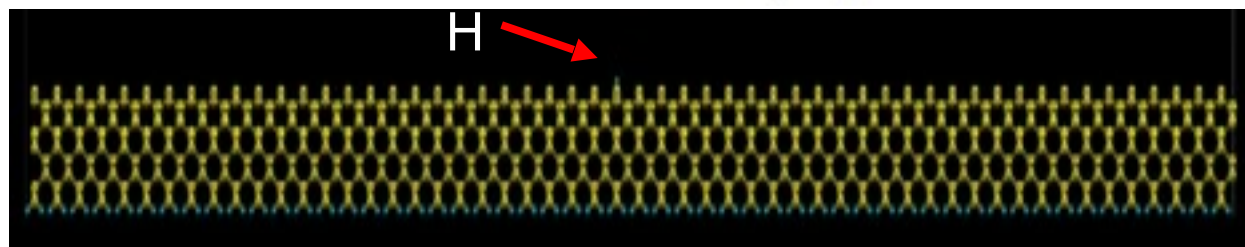
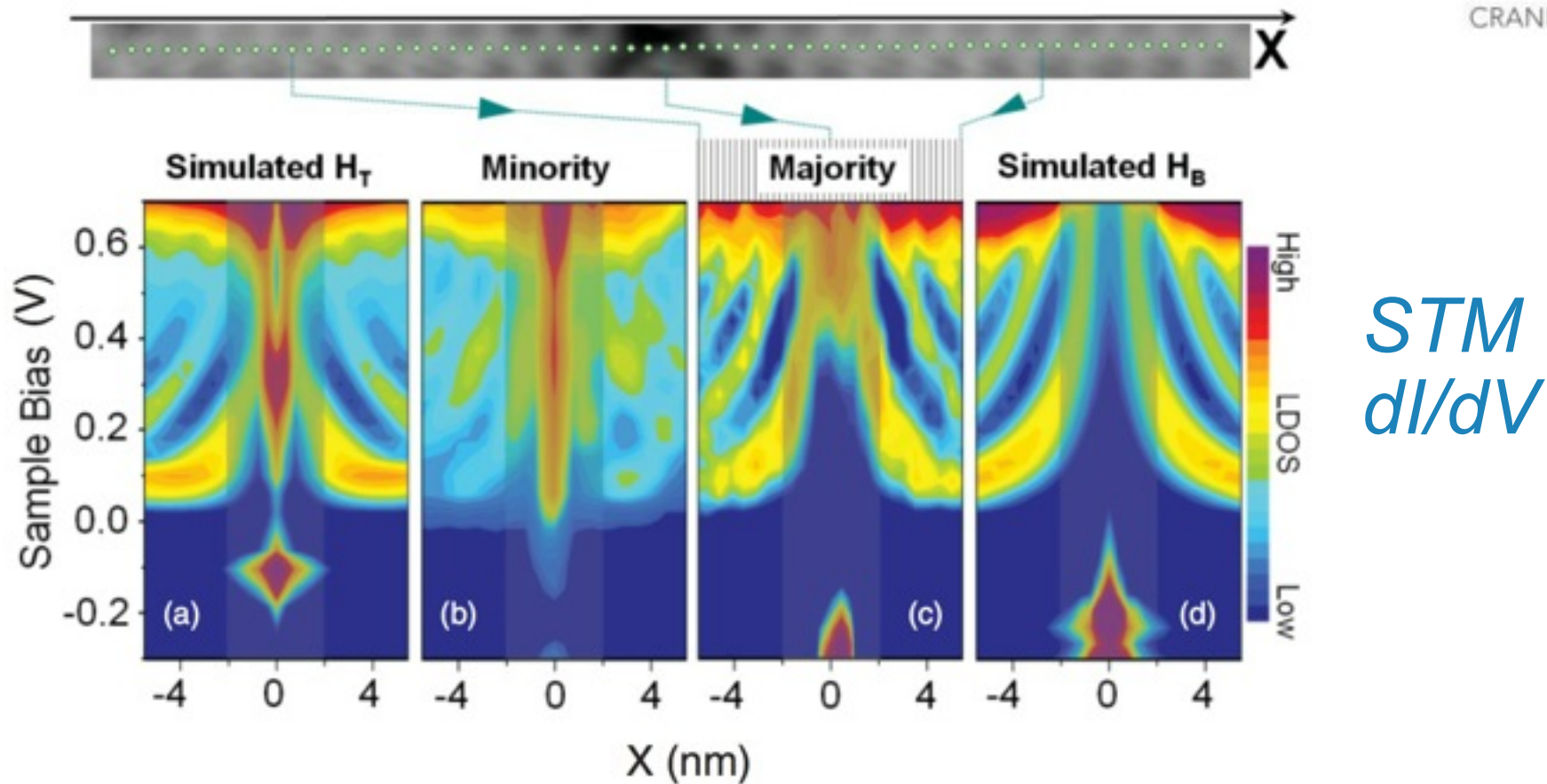


GW Band



H on Si (100): single centre

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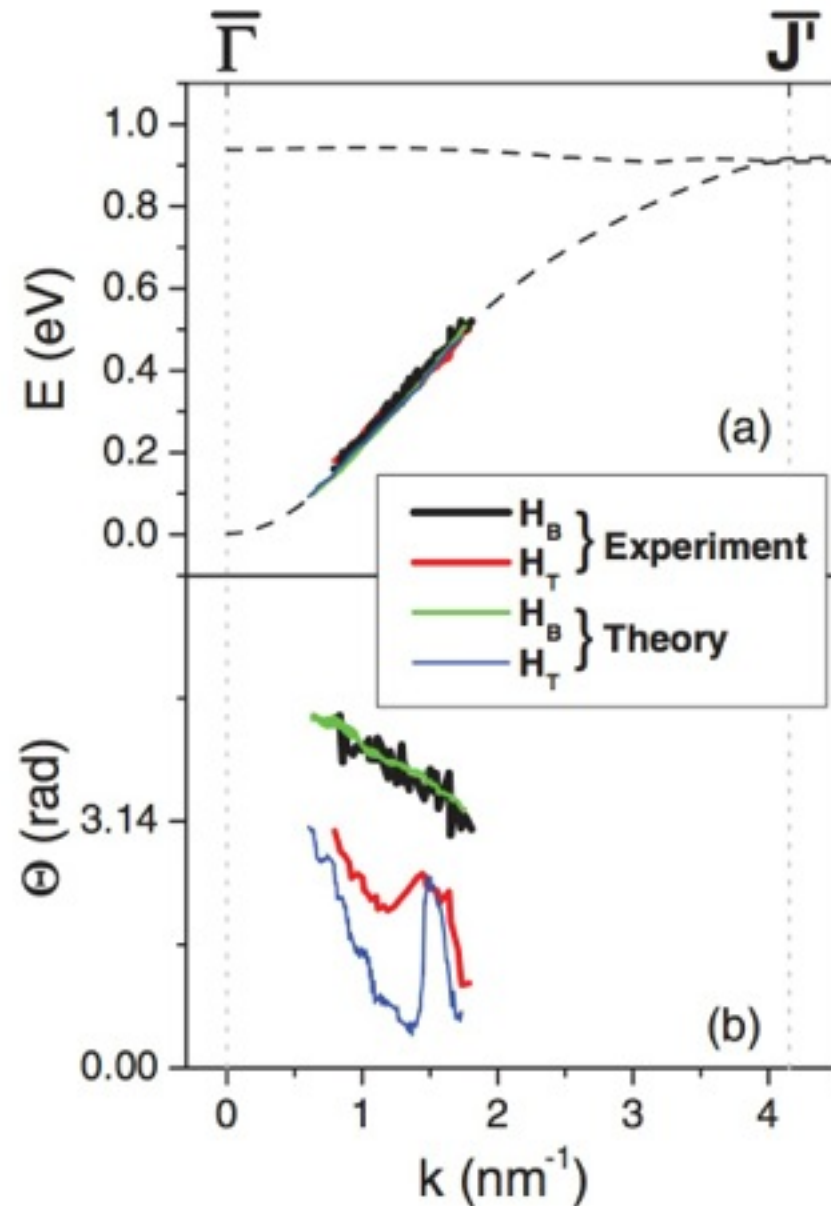


H on Si (100): single centre



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Scattering analysis

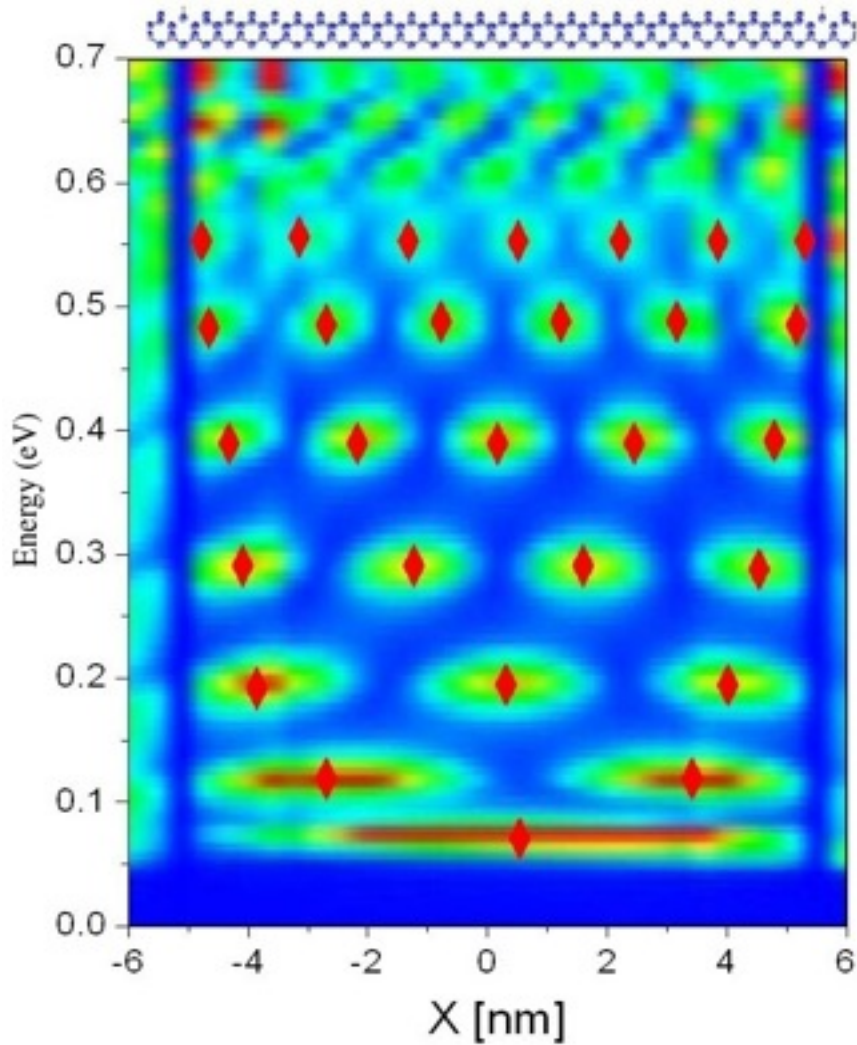


H on Si (100): heterostructures

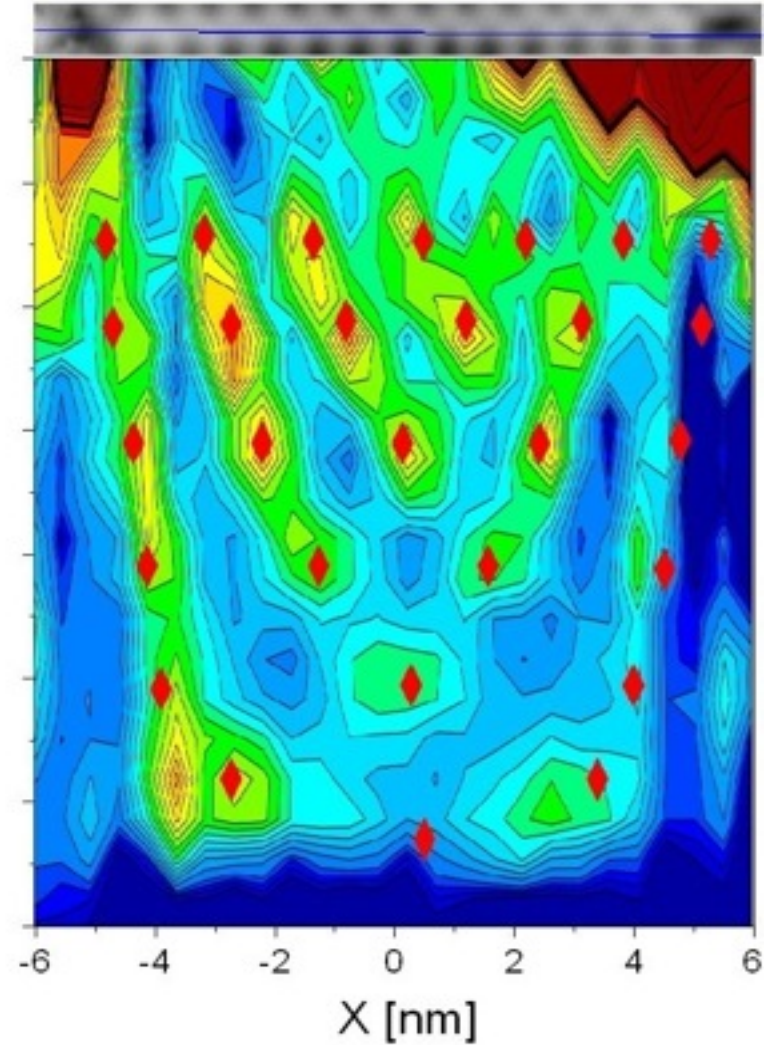


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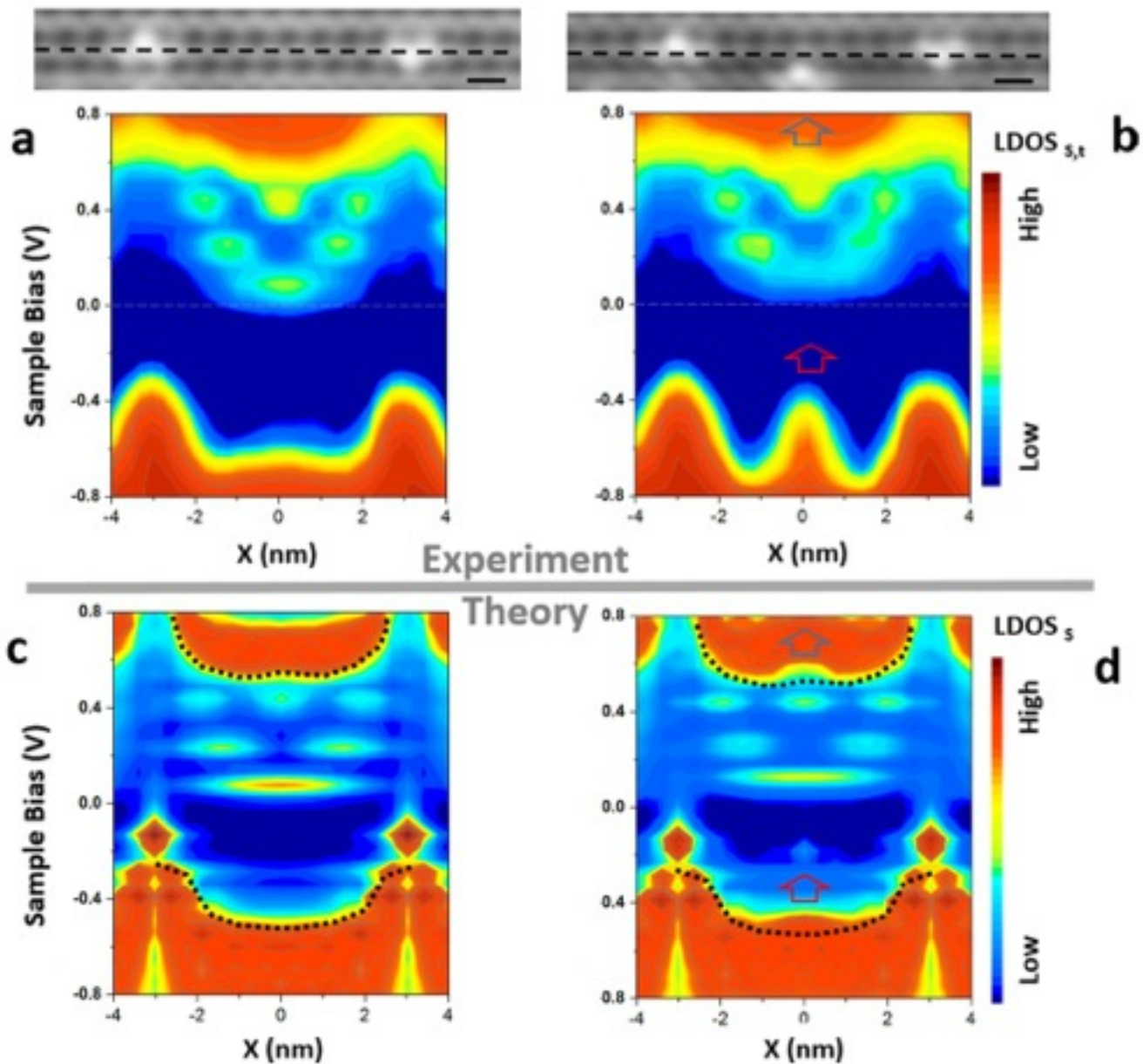
Theory



Experiment



H on Si (100): heterostructures



PRB **84**, 195321 (2011)

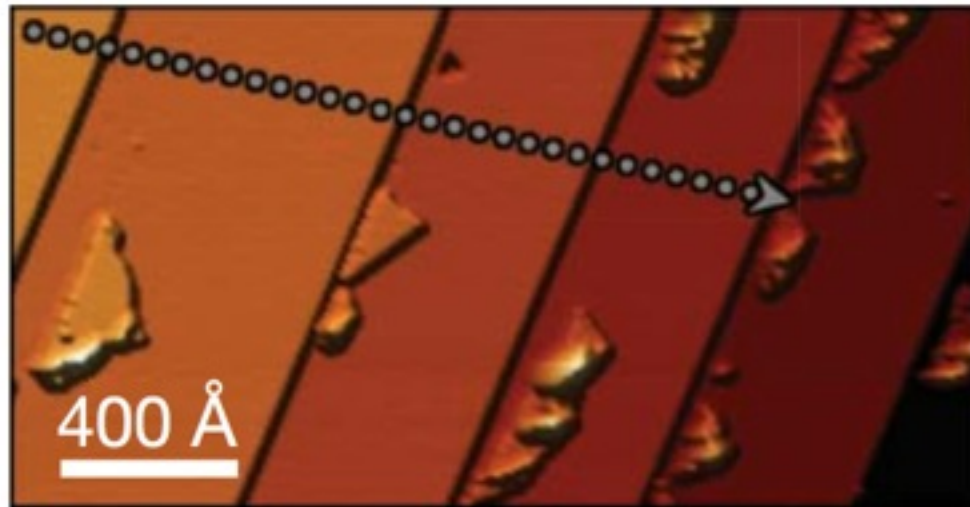
Nano Lett. **15**, 2881
(2015)



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Quantum playground 2

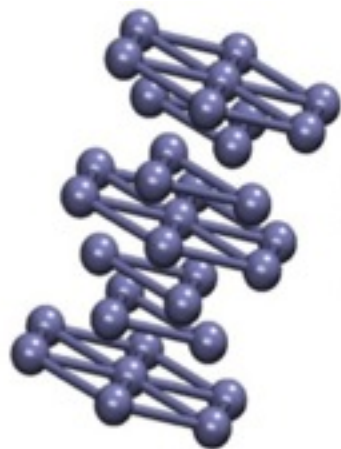
Topological surfaces



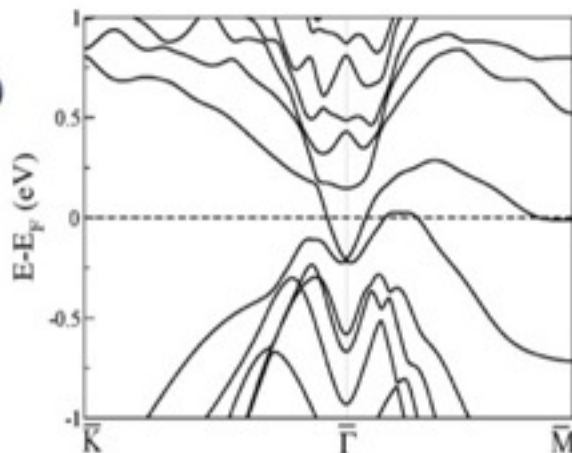
Scattering at topological surfaces



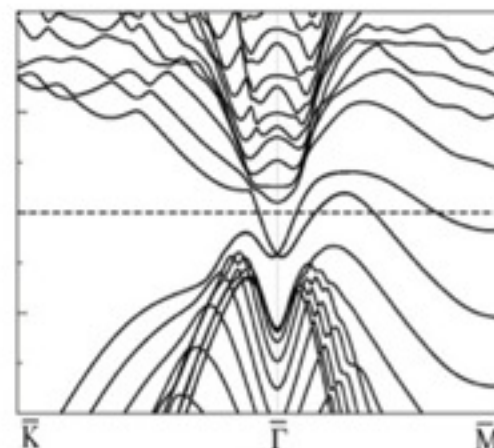
Sb (111)



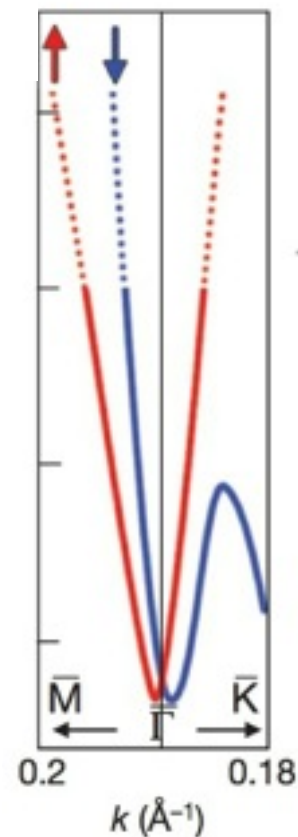
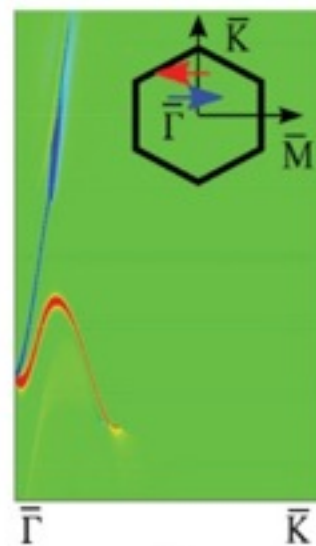
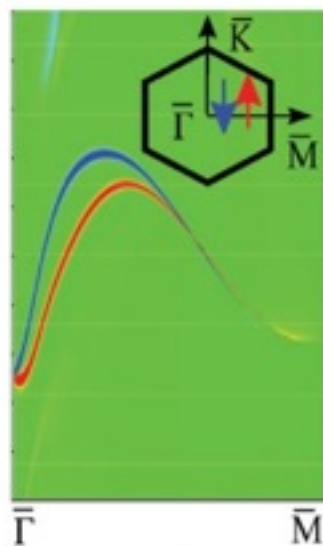
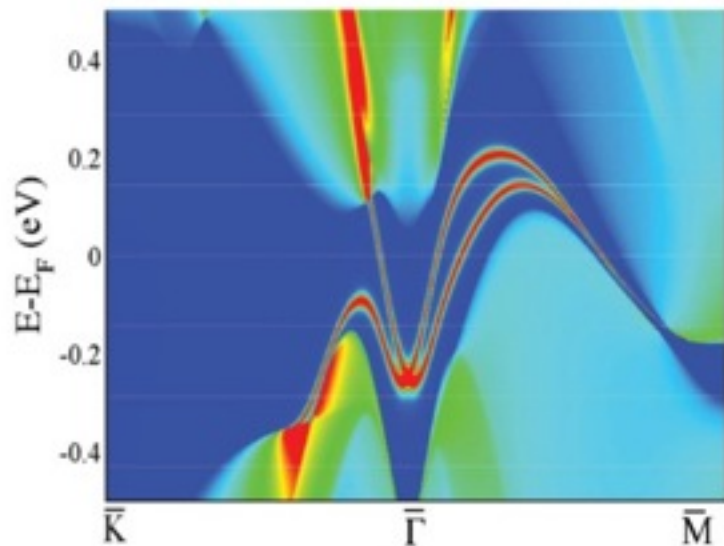
(a)



(b)



(c)



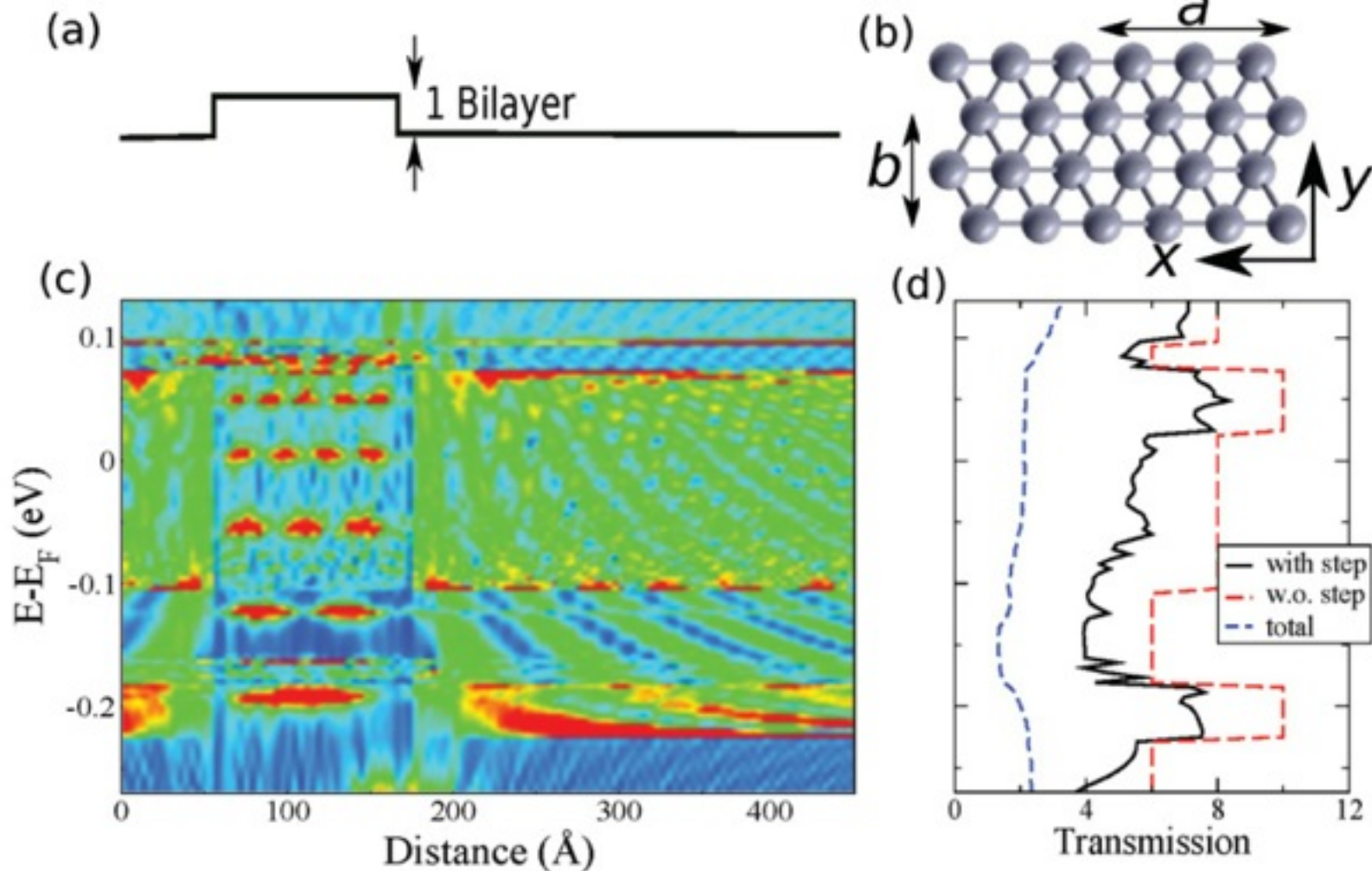
Nature **466**,
343 (2012)

Simulated ARPES

Scattering at topological surfaces



Sb (111): scattering at step edge

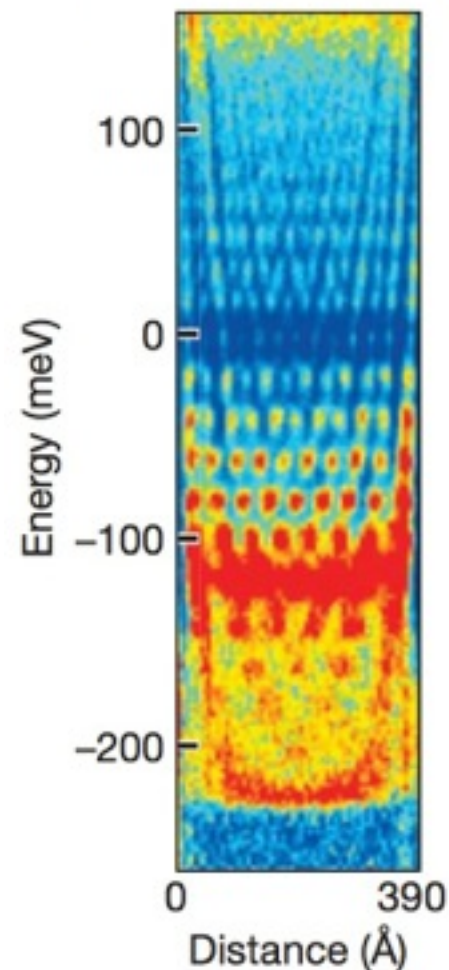
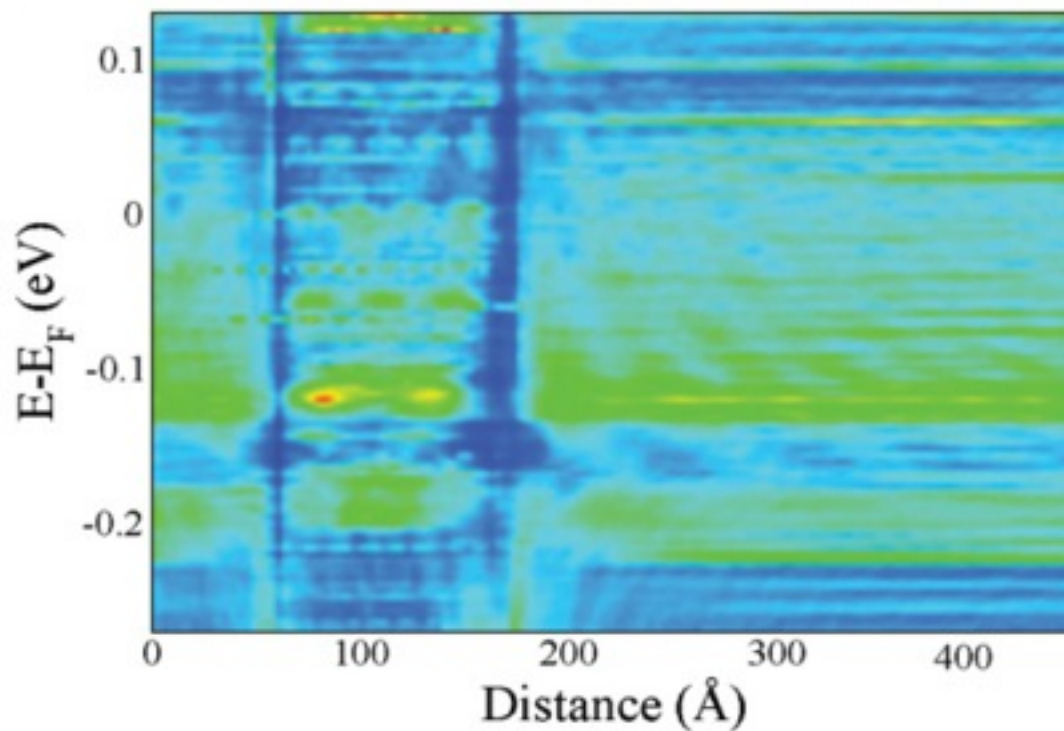


Transport along $\bar{\Gamma} - \bar{M}$

Scattering at topological surfaces

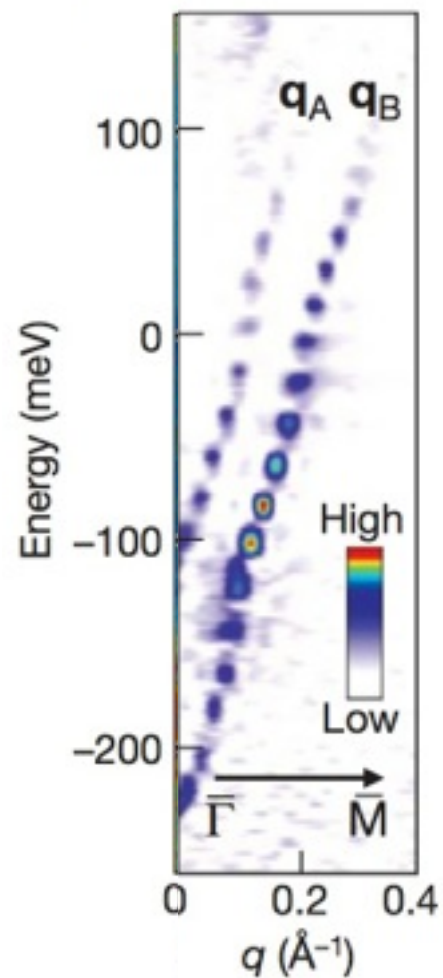
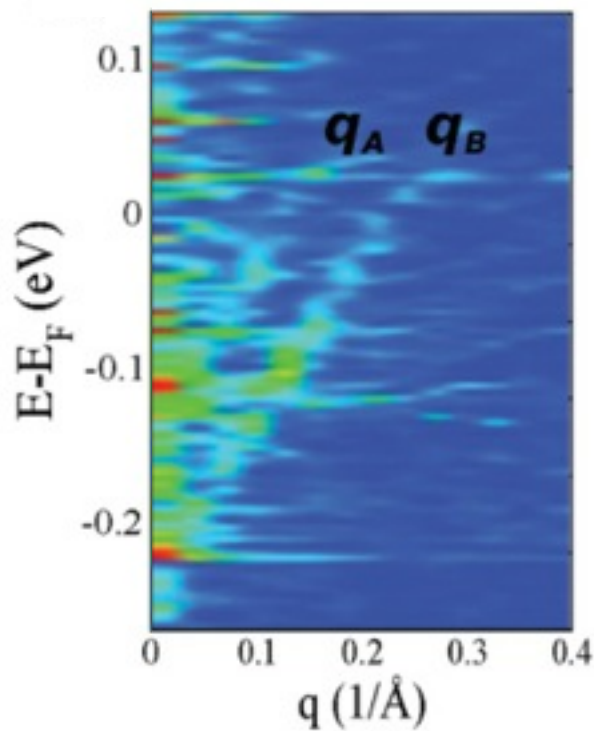


Sb (111): scattering at step edge



Scattering at topological surfaces

Sb (111): scattering at step edge



Can we find new quantum playgrounds ?



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

Take the example of magnetism

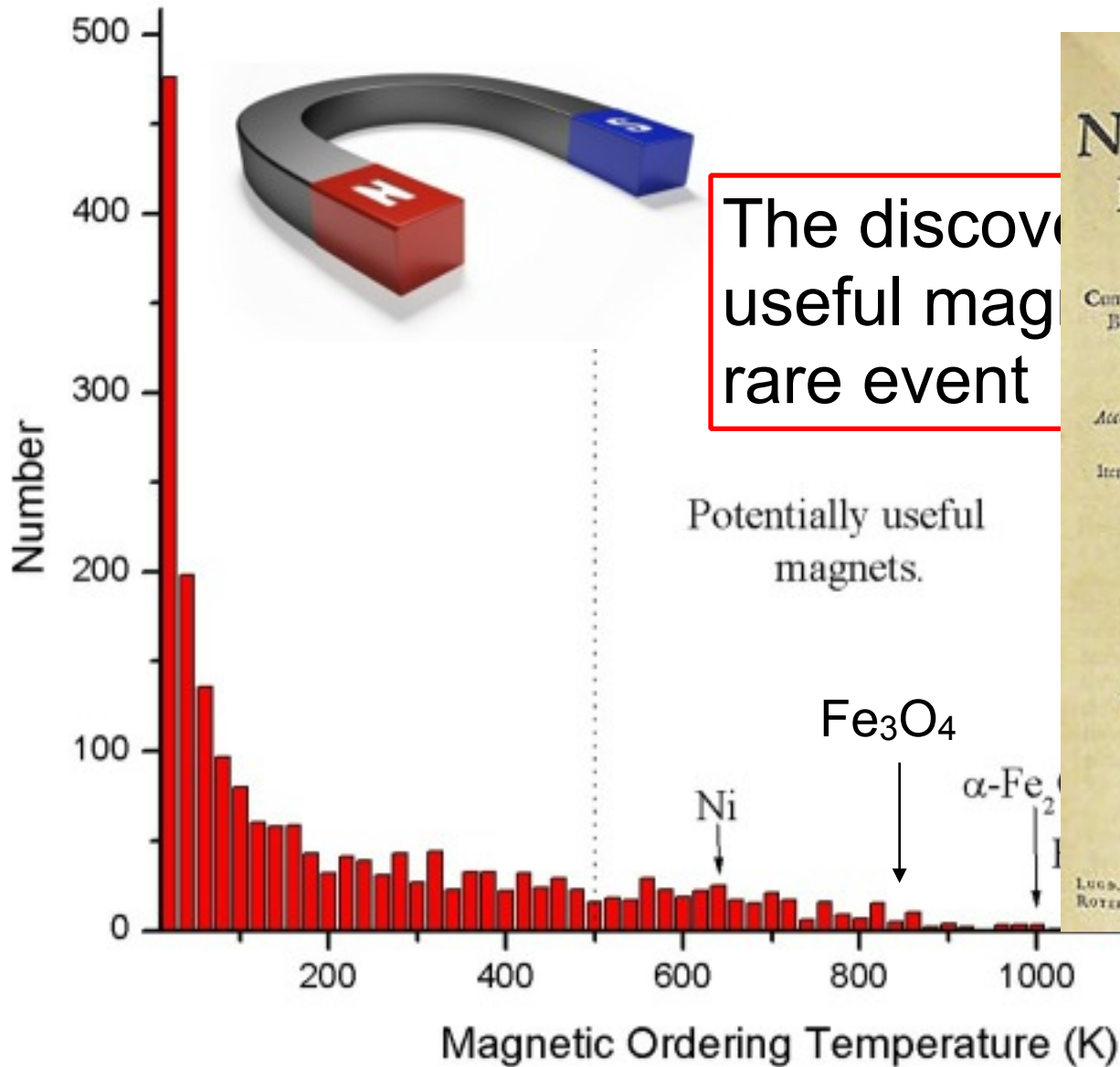
Fe, Co, Ni, $\text{Nd}_2\text{Fe}_{14}\text{B}$, LaMnO_3 , Fe_3O_4

~2,000

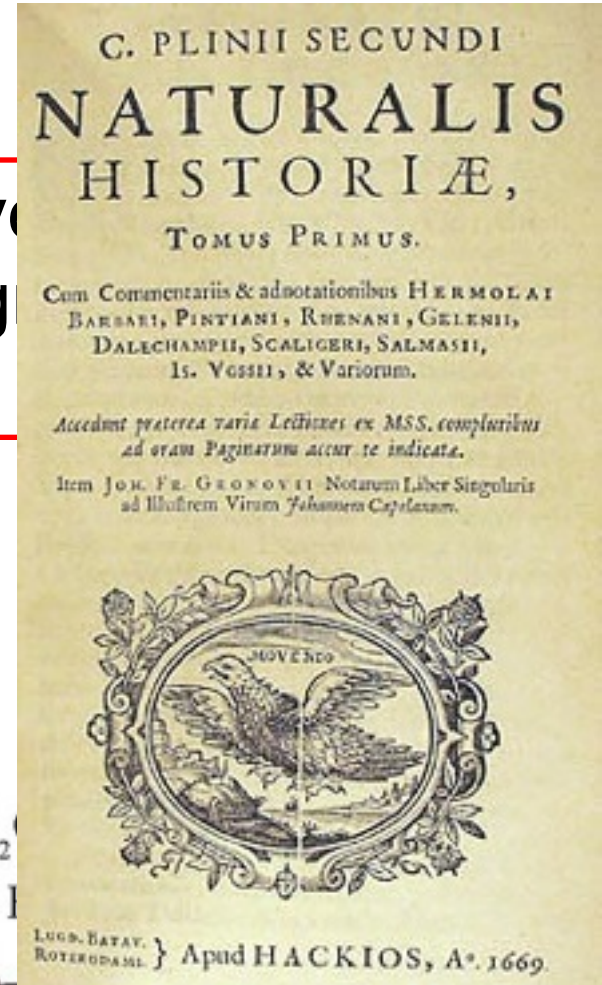
Magnetism is rare



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The discovery of useful magnets is a rare event



Magnetism is complicated



PERIODIC TABLE OF THE ELEMENTS

PERIODIC TABLE OF THE ELEMENTS

GROUP I A, II A, III A, IV A, V A, VI A, VII A, VIII B, IX B, X B, I B, II B

RELATIVE ATOMIC MASS (A_r)

GROUP IUPAC, GROUP CAS

ATOMIC NUMBER (Z), SYMBOL, ELEMENT NAME

STANDARD STATE (25 °C; 101 kPa): Ne - gas, Fe - solid, Ga - liquid, Tl - synthetic

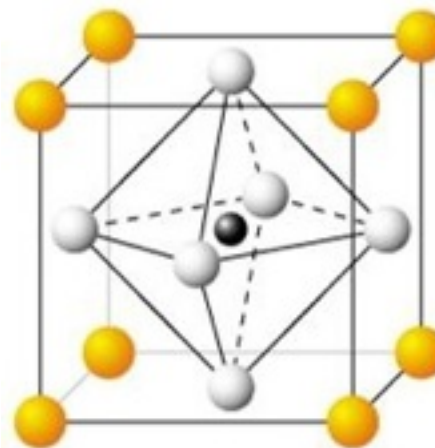
Legend: Metal, Semimetal, Nonmetal, Alkali metal, Alkaline earth metal, Transition metals, Lanthanide, Actinide, Chalcogens element, Halogens element, Noble gas

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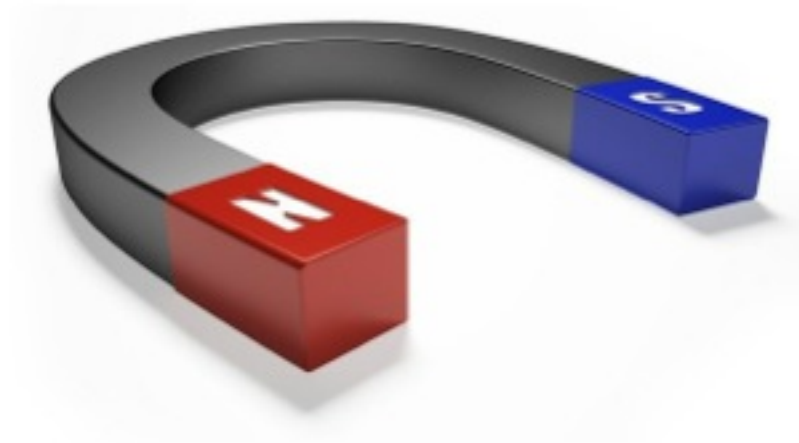
(1) Pure Appl. Chem., 73, No. 4, 667-683 (2001)
Relative atomic mass is shown with five significant figures. For elements with no stable nuclides, the value enclosed in brackets indicates the mass number of the longest-lived isotope of the element.
However three such elements (Tl, Pa, and U) do have a characteristic terrestrial isotopic composition, and for these an atomic weight is tabulated.
Editor: Aditya Vaidya (adiva@rediffmail.com)

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

SrMoO_3	SrTcO_3 $T_N = 500\text{C}$	SrRuO_3 $T_C = -100\text{C}$
------------------	---	--



The magnetic genome project



with Stefano Curtarolo, Duke

The magnetic genome project



CRANN

nature
materials

REVIEW ARTICLE

PUBLISHED ONLINE: 20 FEBRUARY 2013 | DOI: 10.1038/NMAT3568

The high-throughput highway to computational materials design

Stefano Curtarolo^{1,2*}, Gus L. W. Hart^{2,3}, 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



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The AFLOW consortium



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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)

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 quinary
- About 113,000 entries (75.6%) have been assigned a structure type.
- There are currently 6,336 structure prototypes.
- **Lots of redundancy**

Virtual Materials Growth (existing materials)

Duke calculated single elements, binary, ternary and some quaternary (about 50,000)

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



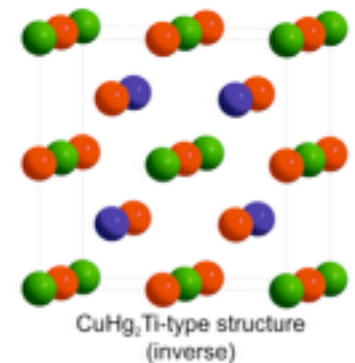
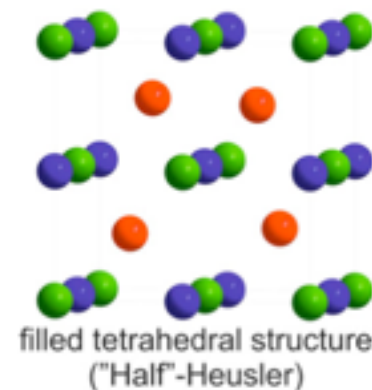
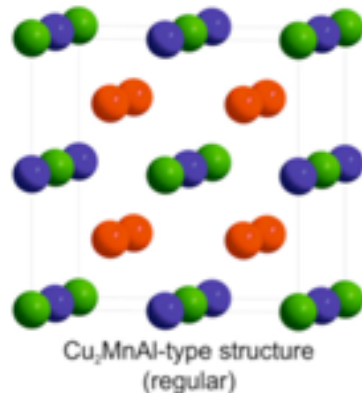
~250
known ...

~1000
claimed ...

~90
magnetic ...

X_2YZ Heusler compounds

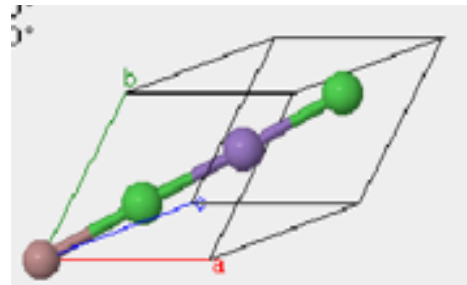
H 2.20																	He	
Li 0.98	Be 1.57											B 2.04	C 2.55	N 3.04	O 3.44	F 3.98	Ne	
Na 0.93	Mg 1.31											Al 1.61	Si 1.90	P 2.19	S 2.58	Cl 3.16	Ar	
K 0.82	Ca 1.00	Sc 1.36	Ti 1.54	V 1.63	Cr 1.66	Mn 1.55	Fe 1.83	Co 1.88	Ni 1.91	Cu 1.90	Zn 1.65	Ga 1.81	Ge 2.01	As 2.18	Se 2.55	Br 2.96	Kr 3.00	
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



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~236,000 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	57-70 *	71 Lu 174.97	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]	89-102 **	103 Lr [262]	rutherfordium 104 Rf [261]	dubnium 105 Db [262]	seaborgium 106 Sg [266]	bohrium 107 Bh [264]	hassium 108 Hs [269]	meitnerium 109 Mt [268]	unnilennium 110 Uun [279]	ununennium 111 Uuu [273]	unbinilium 112 Uub [277]	unquadium 114 Uuq [289]										

* 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]	einsteinium 99 Es [252]	fermium 100 Fm [257]	mendelevium 101 Md [258]	nobelium 102 No [259]

The magnetic genome project



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Rational materials storage

www.aflowlib.org

The screenshot displays the Aflowlib search interface. At the top, there is a search bar with the text "Search Aflowlib" and a "Search" button labeled "(50522 Compounds)". Below the search bar are tabs for "icsd", "elements", "binaries", and "Heuslers". The main area features a periodic table of elements. A tooltip for element 'X' is visible, showing its atomic number, mass, and various physical properties like electron count, density, lattice, and crystal structure. To the right of the periodic table are search operators: "and", "not", "or", "xor", and parentheses. Below the periodic table, there are filters for "Show 40 results per table. Limit to 1000 total results." and "# of Species:". At the bottom, there are several filter buttons categorized by material type (All Metals, Alkali Metals, Alkaline Earths, Transition Metals, Lanthanides, Other Metals, Nonmetals, Group 3A, Group 4A, Group 5A, Chalcogens, Halogens) and by property (Chemistry, Crystal, Electronics, Thermodynamics, Magnetics, Scintillation, Mechanical, 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)

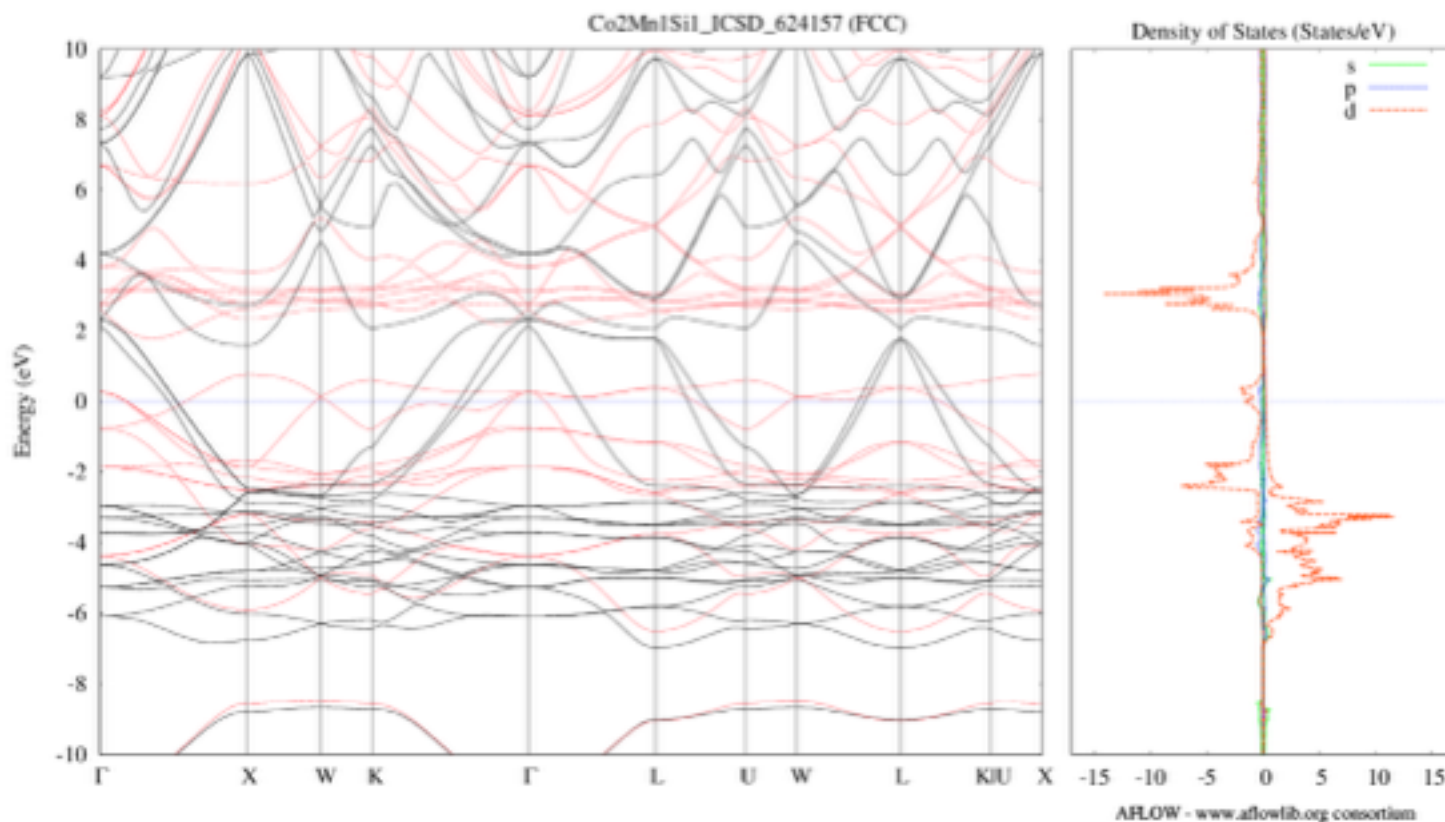
... and one theory for find them all



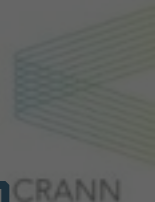
ELECTRONIC PROPERTIES

Band Gap:	0.000 eV (metal)	Fit Band Gap:	0.000 eV
Magnetic Moment:	7.382 μ_B	Magnetic Moment/atom:	1.845 μ_B /atom
Electron Mass(FIX):	XXX (m_0)	Hole Mass(FIX):	XXX (m_0)
Spin Polarization (E_F):	0.666	Spin Decomposition per atoms:	{1.758,1.758,4.019,-0.054} μ_B

Band Structure:



The magnetic genome project



nature materials

REVIEW ARTICLE

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

Finding *descriptors*

The high-throughput highway to computational materials design

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- 2) Simulating new materials

Robust electronic structure method: density functional theory (VASP)

A look at the full database

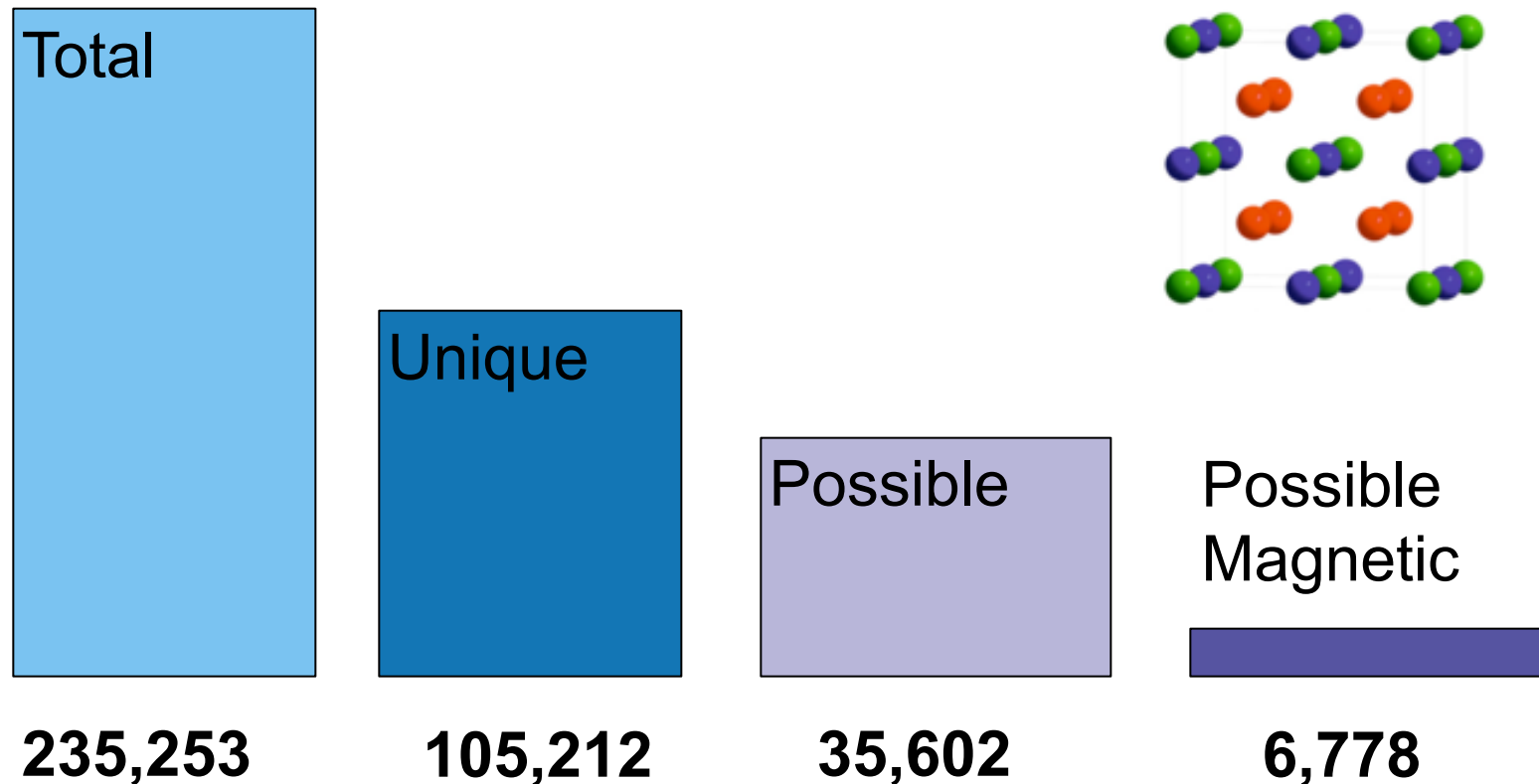


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Property: Can be made ?

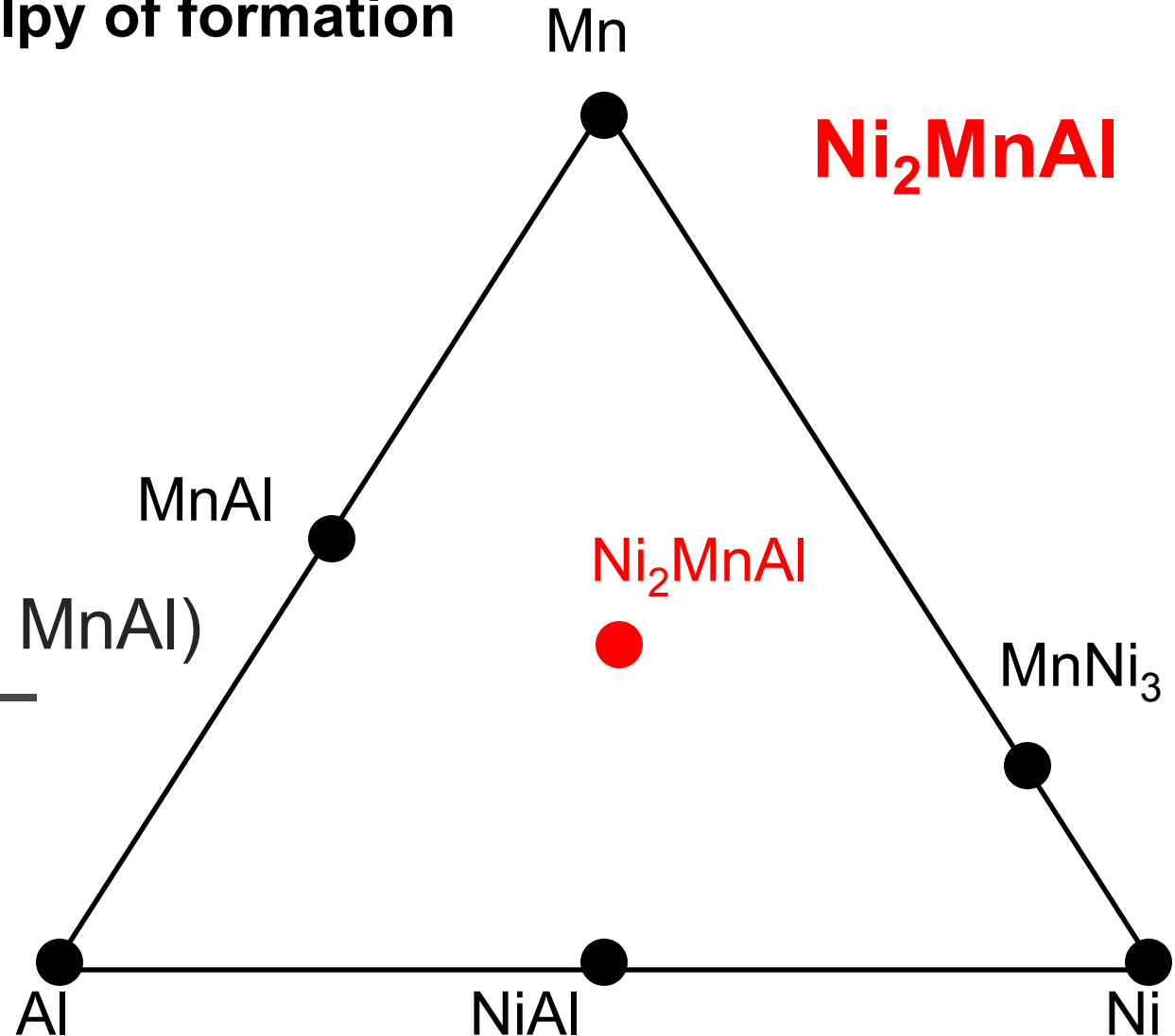
Descriptor 0:
Enthalpy of formation

$$\text{Energy (Ni}_2\text{MnAl)} < \text{Energy (2Ni + Mn + Al)}$$





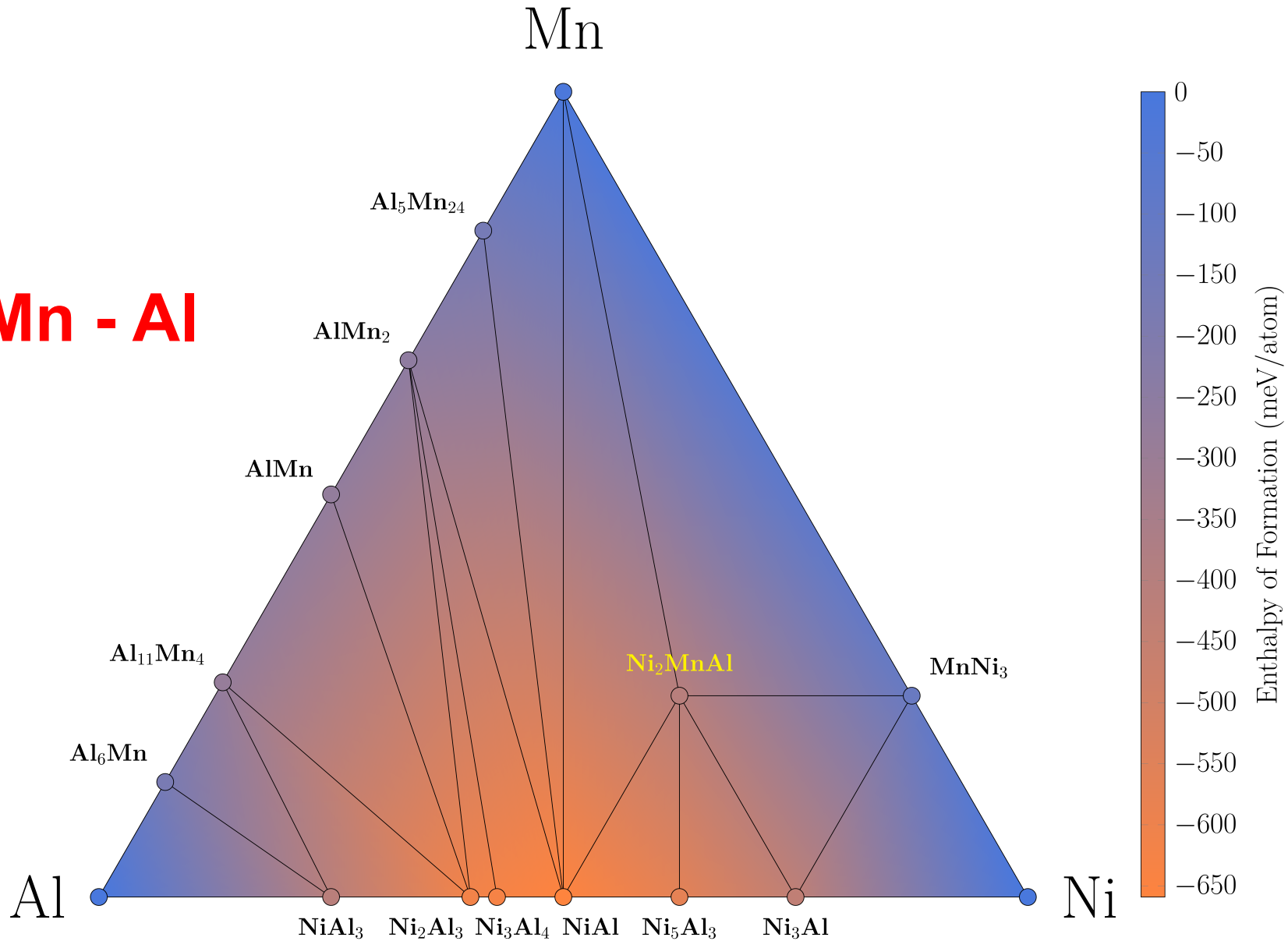
Descriptor 1: Enthalpy of formation



Stability analysis



Ni - Mn - Al



Look at the transition metal intermetallics

36,540

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	57-70 *	71 Lu 174.97	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	81 Tl 204.38	82 Pb 207.2	83 Bi 208.98	84 Po [209]	85 At [210]	86 Rn [222]					
francium 87 Fr [223]	radium 88 Ra [226]	89-102 **	103 Lr [262]	rutherfordium 104 Rf [261]	duobium 105 Db [262]	seaborgium 106 Sg [266]	bohrium 107 Bh [264]	hassium 108 Hs [265]	meitnerium 109 Mt [268]	unnilium 110 Uun [270]	ununium 111 Uuu [272]	unbibium 112 Uub [277]	114 Uuq [285]										

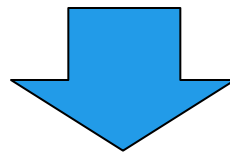
* Lanthanide series

** Actinide series

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36,540 possible → 248 stable

22 magnetic → 8 Robust



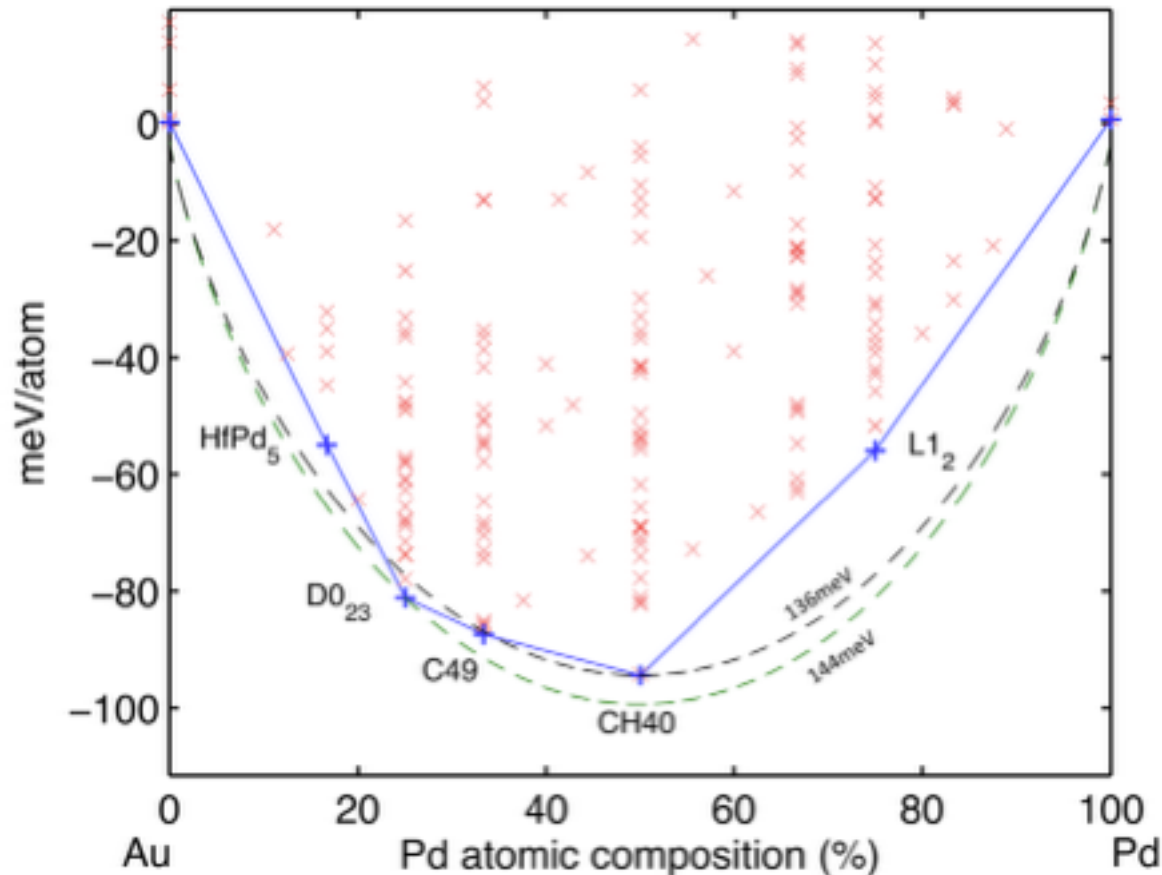
Extrapolating

236,000 possible → 1550 stable

138 magnetic → 50 Robust



Descriptor 2: Entropic temperature

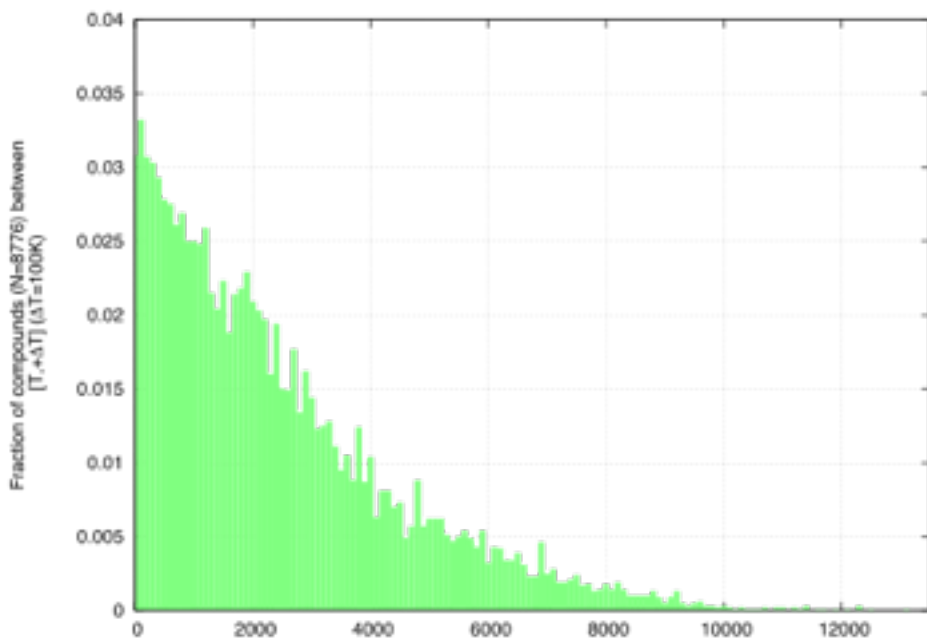


$$T_S = \max_i \frac{\Delta H(A_{x_i} B_{1-x_i})}{k_B [\log(x_i) + (1-x_i)\log(1-x_i)]}$$

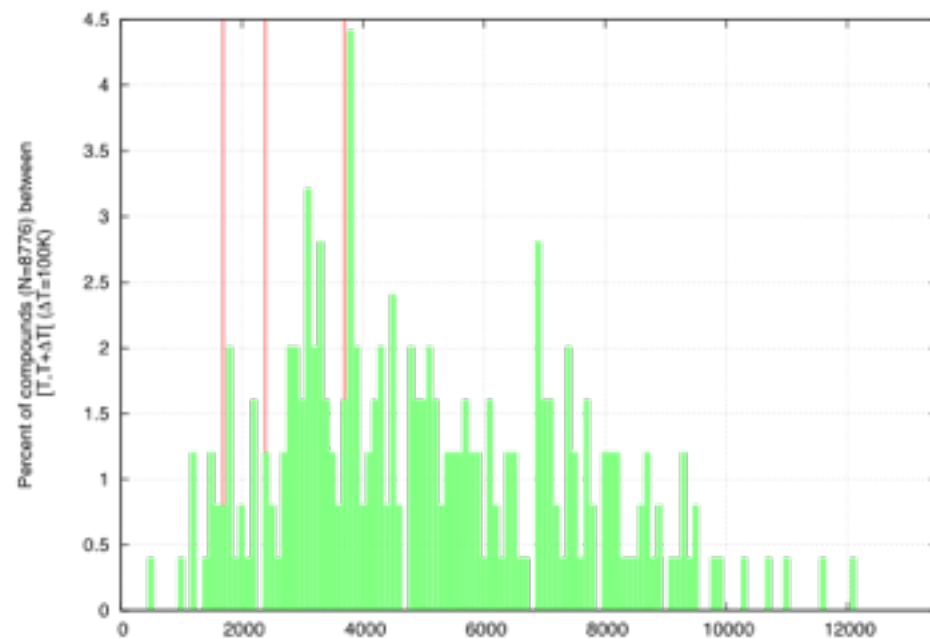
Descriptor 2: Entropic temperature

$N=8776$

$N=248$



T_s



T_s

Weibull distribution

Descriptor 3: Critical temperature

Known Heusler
ferromagnets

Co_2XY

Fe_2MnY

Ni_2MnY

Mn_2XY

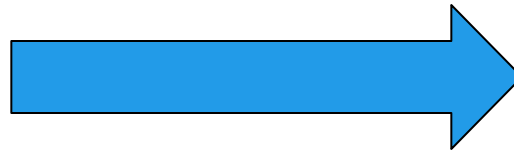
Rh_2MnY

Cu_2MnY

Pd_2MnY

Au_2MnY

Generalized regression model based on
valence, volume, spin decomposition



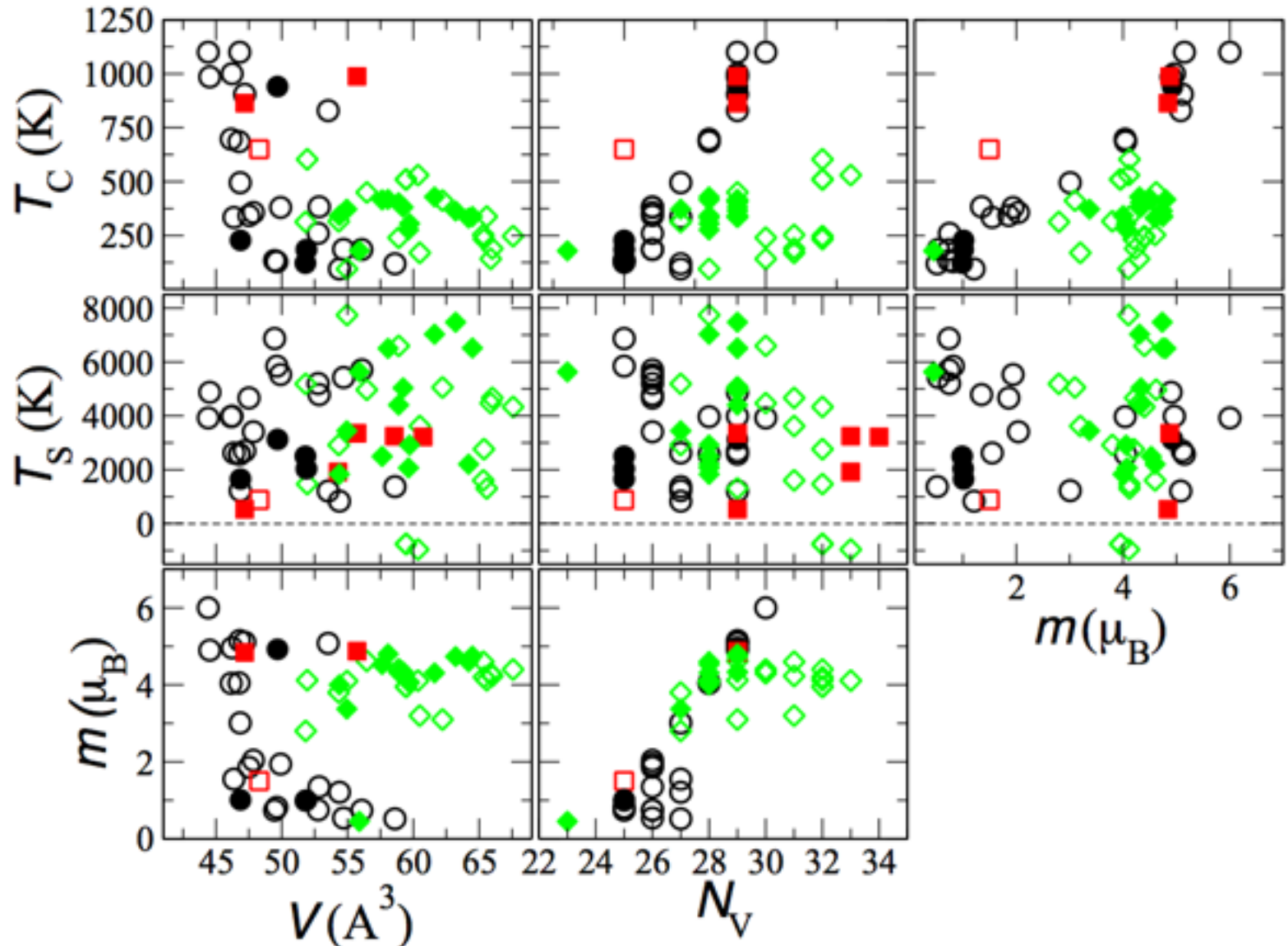
Prediction of T_C

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



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Co_2XY

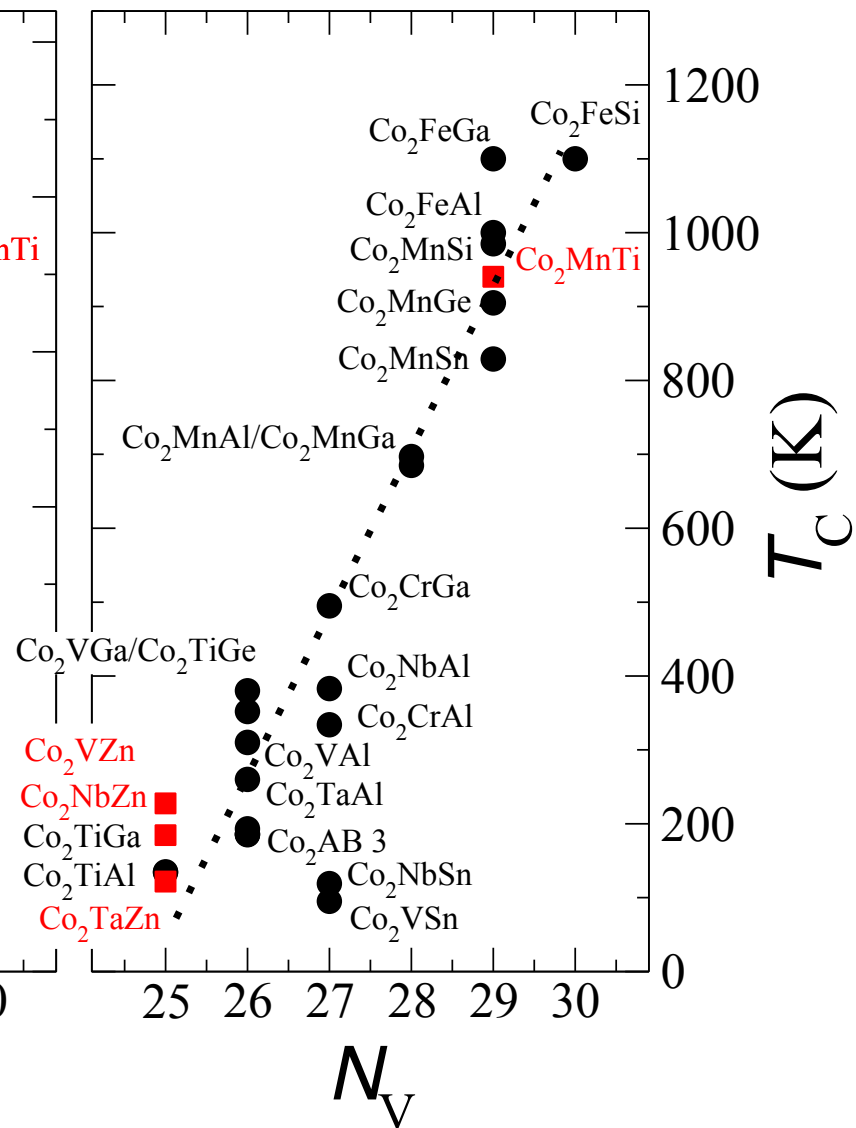
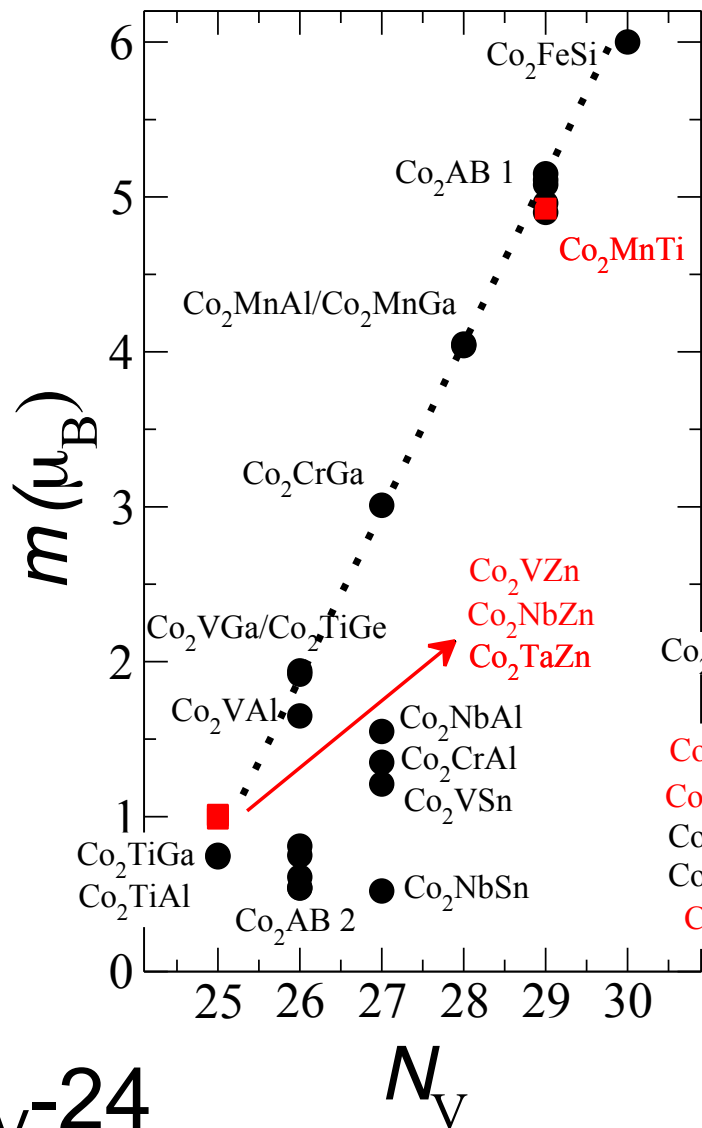
Mn_2XY

X_2MnY

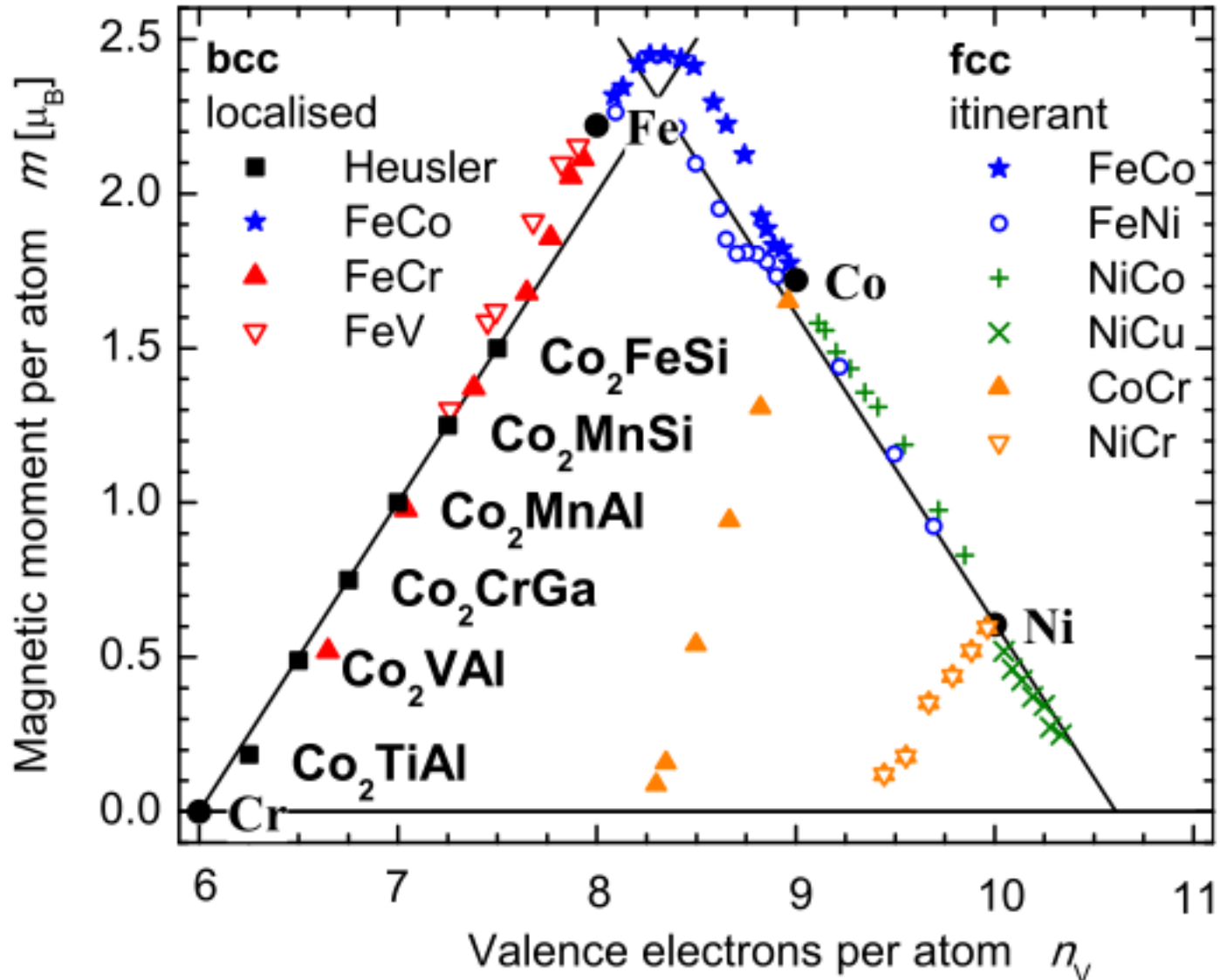


Co₂YZ

Slater-Pauling



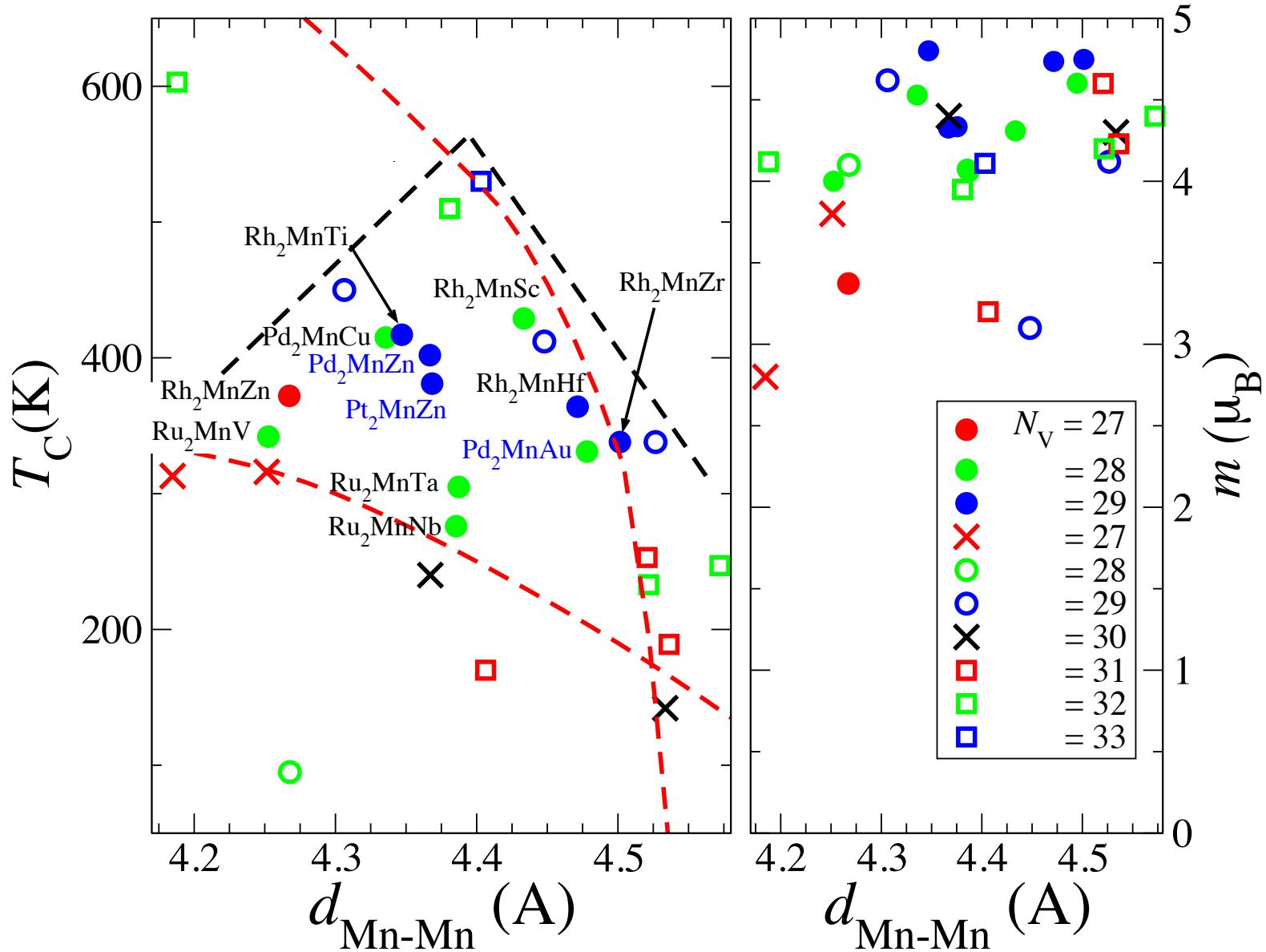
$$m_{X_2YZ} = N_V - 24$$

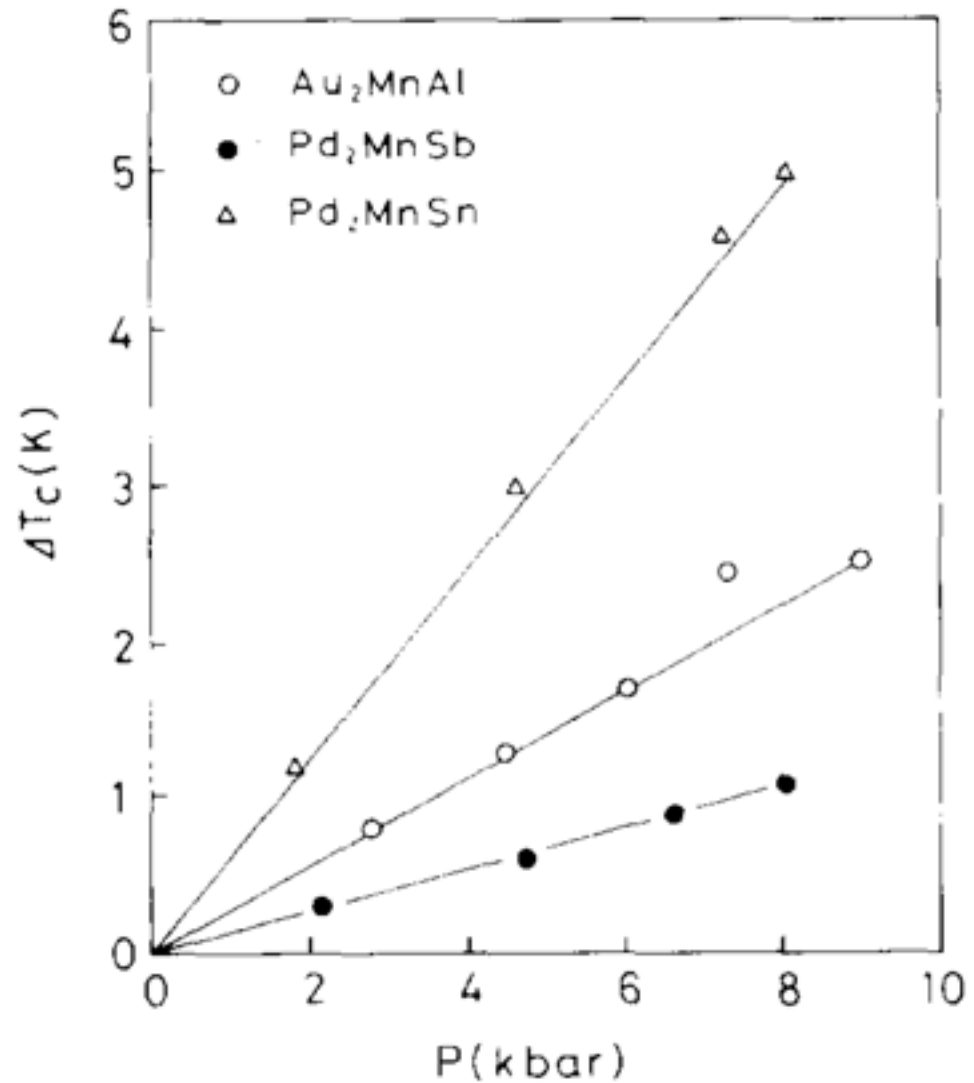


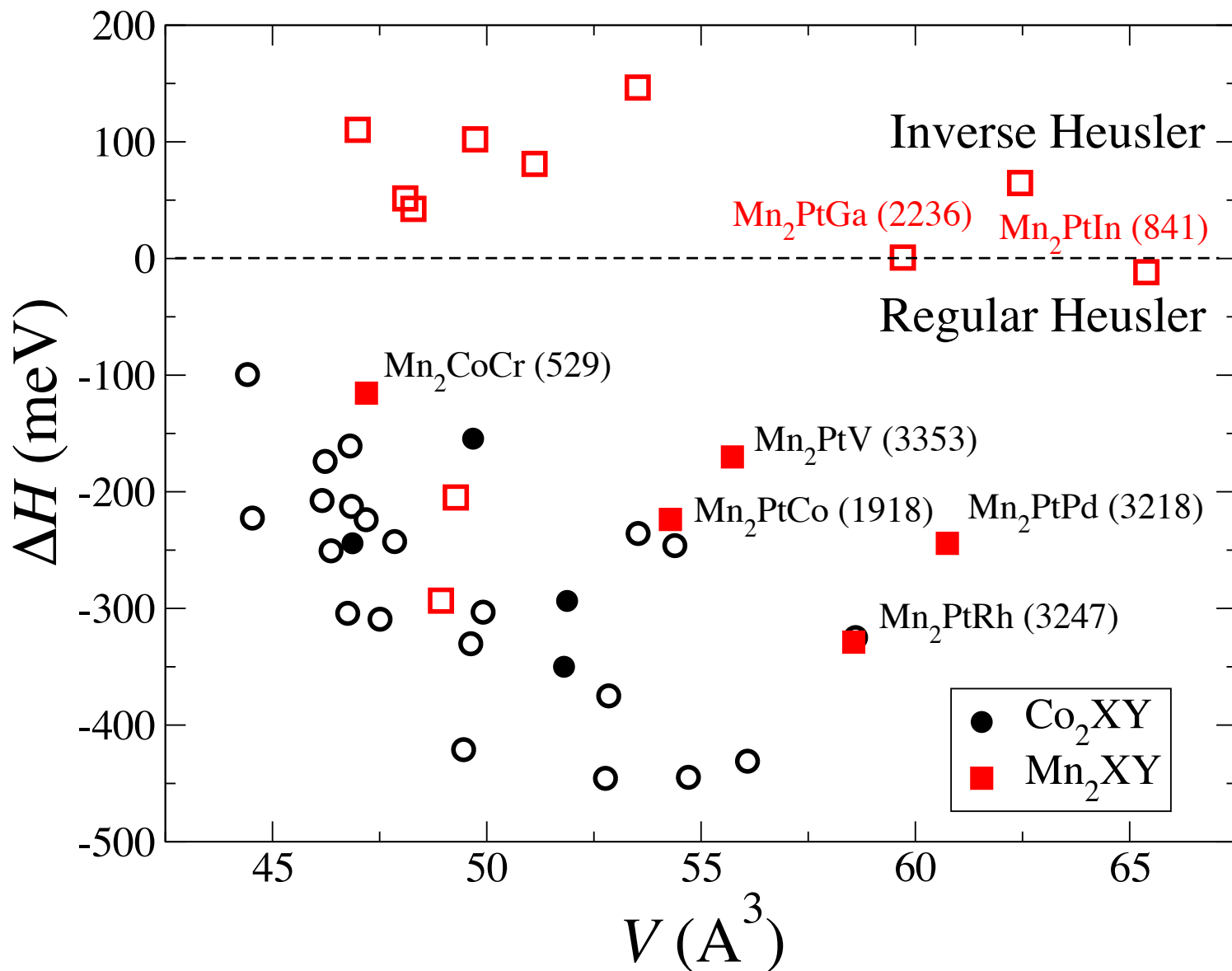


X_2MnZ

Castelliz-Kanomata curve



 X_2MnZ 

Mn₂YZ

OK, but does all that work?

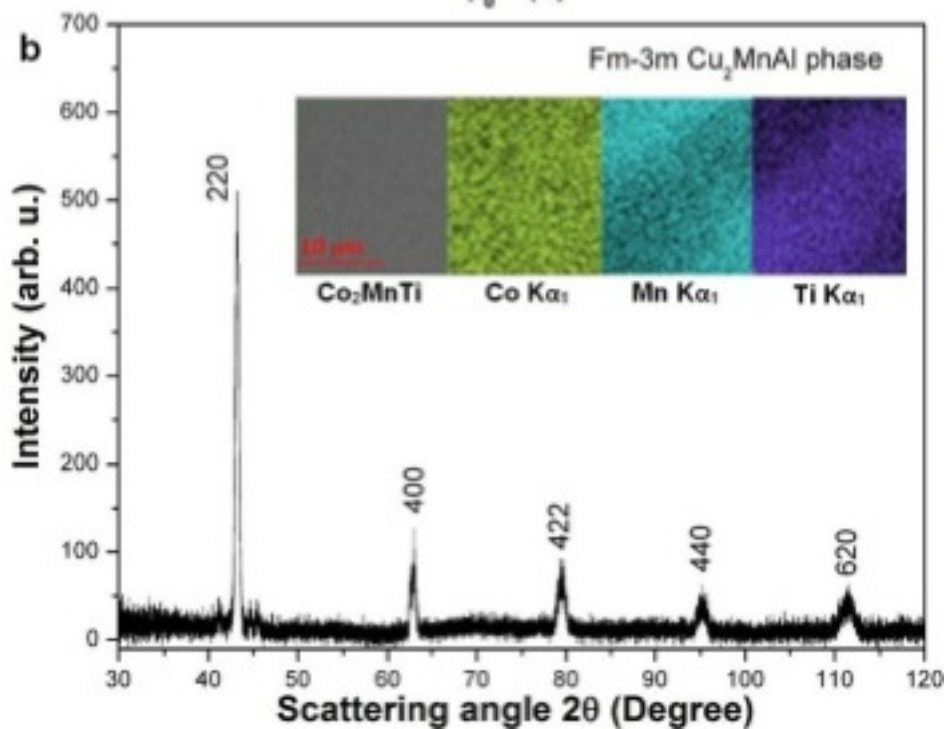
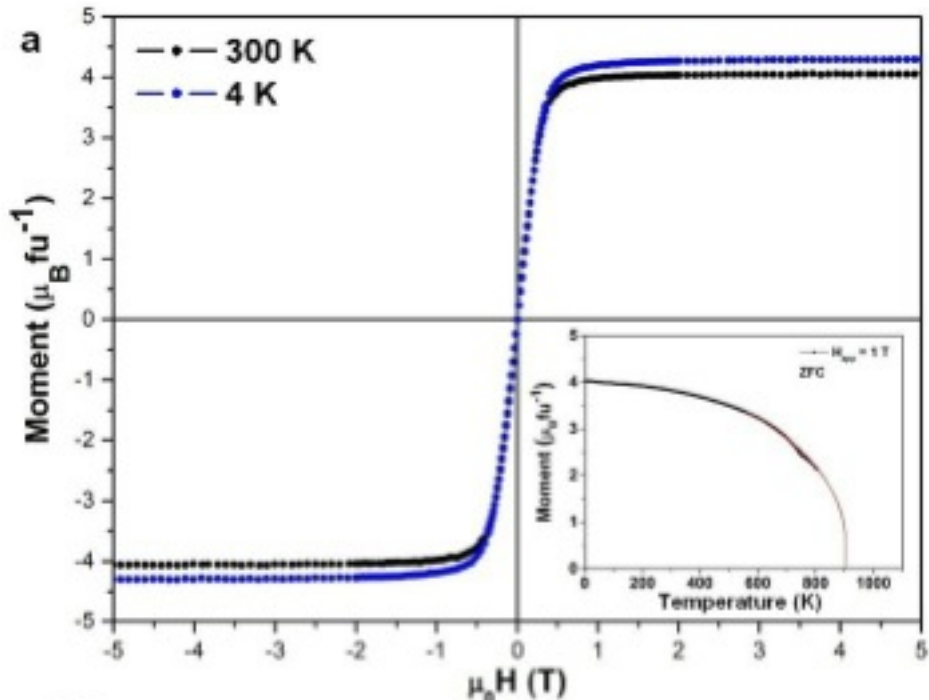
Co₂MnTi

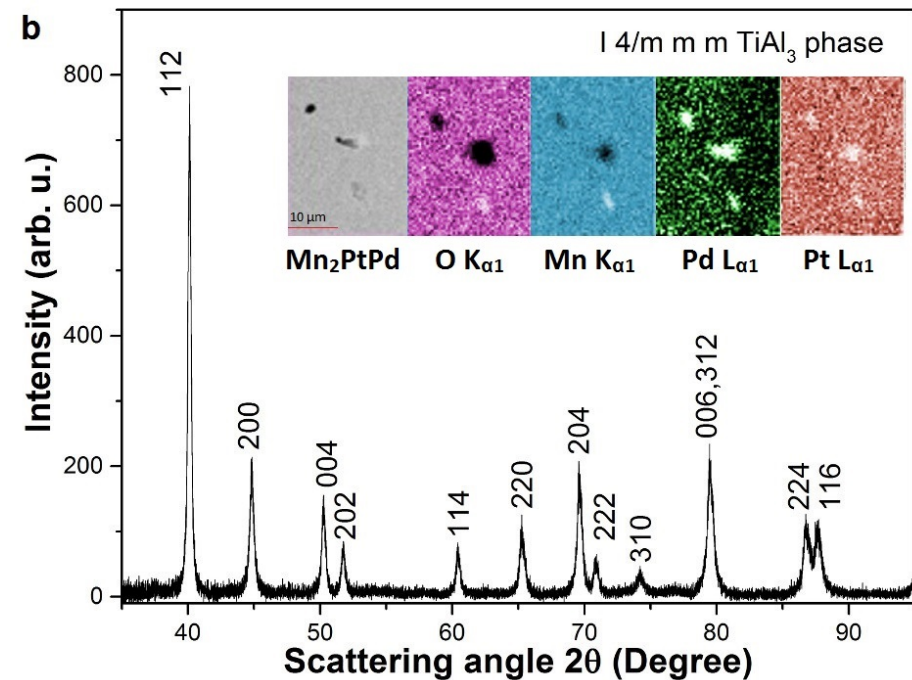
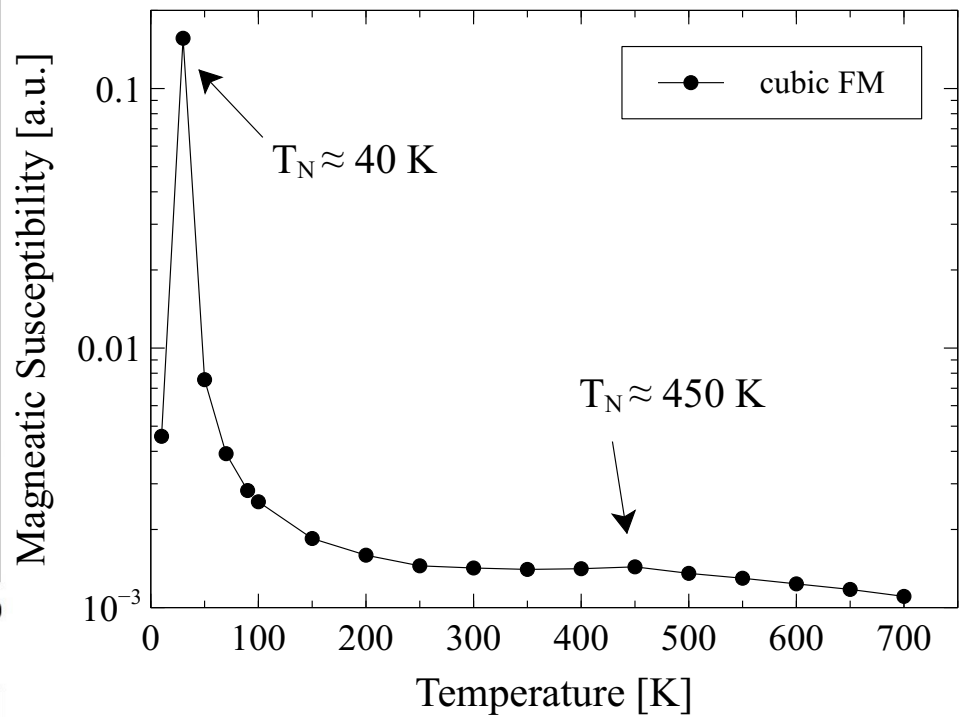
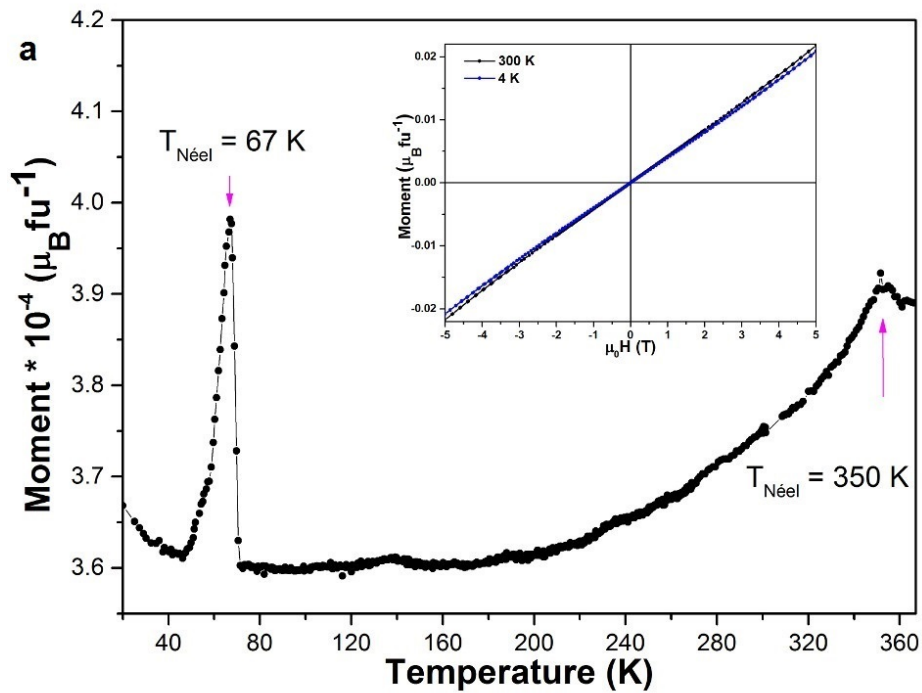
$T_C^{\text{measured}} = 940\text{K}$

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

Prepared by arc melting in an Ar atmosphere

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





Complex antiferromagnetic order

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

Bottom line



CRANN

Did we find one ?





COMPUTATIONAL SPINTRONICS

SANVITO RESEARCH GROUP
TRINITY COLLEGE, DUBLIN



TCD Team:

Tom Archer, Anurag Tiwari, Mario Zic, Awadhesh Narayan, Ivan Rungger, Mauro Mantega

Duke Team:

Stefano Curtarolo, Junkai Xue, Kevin Rasch, Corey Oses



TCHPC



innovating nanoscience



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The long way to the discovery of new materials made it short

Stefano Sanvito (sanvitos@tcd.ie)

School of Physics and CRANN, Trinity College Dublin, IRELAND