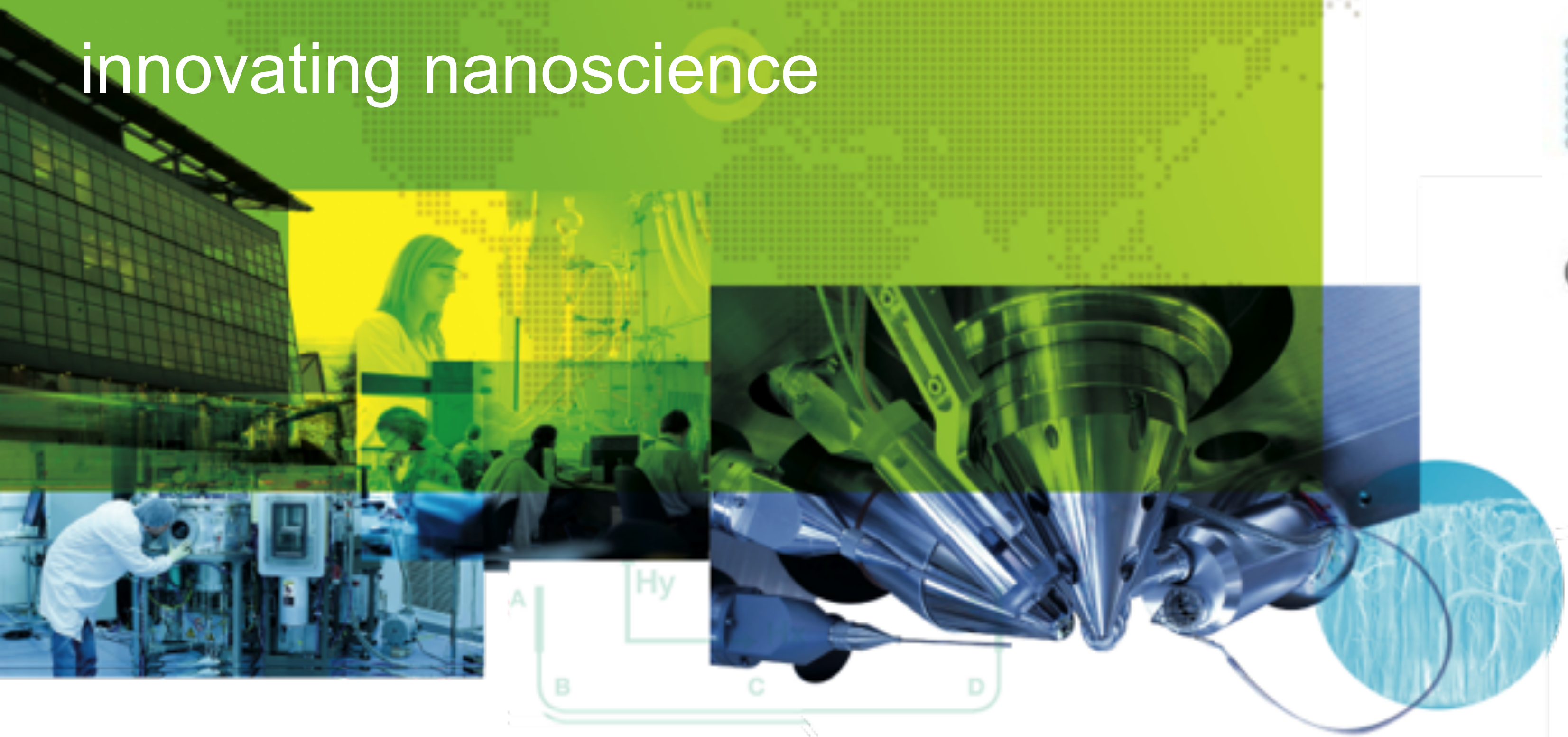
innovating nanoscience



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

Trinity College
The University of Dublin

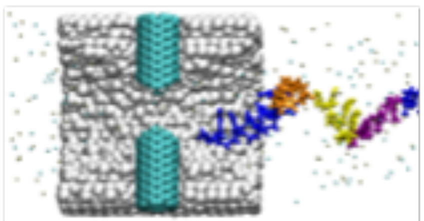
sfi
science foundation ireland
fondúireacht eolaíochta éireann

Theory activity

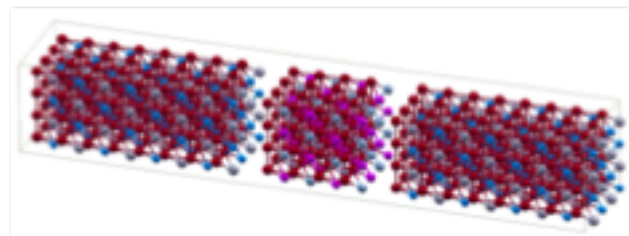
CRANN

Two main pillars

Large-scale electronic structure simulations



Materials Genomics



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

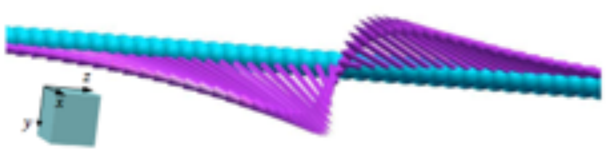
Sustaining CRANN experimental activity

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

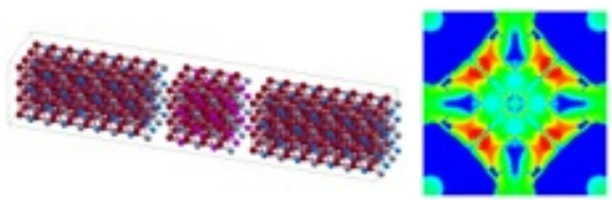
Theory activity

Spin electronics

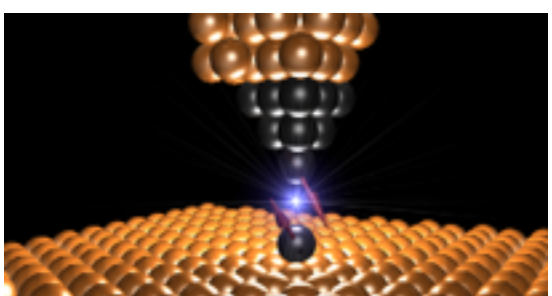
Spin-dynamics



Spin-transport

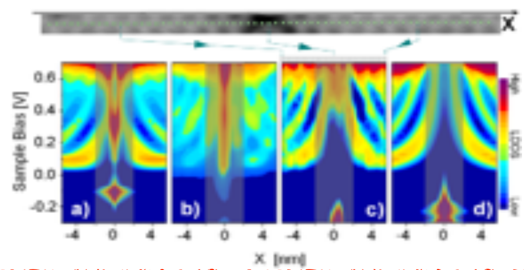


Spin excitation/torque

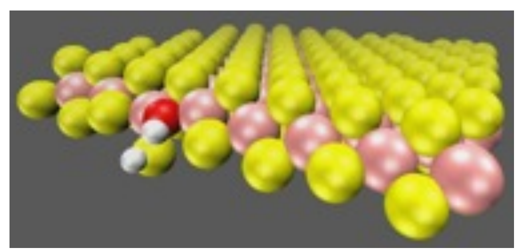


Materials

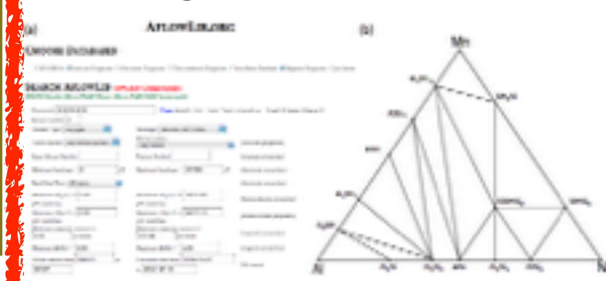
Transport and STM



2D/topological

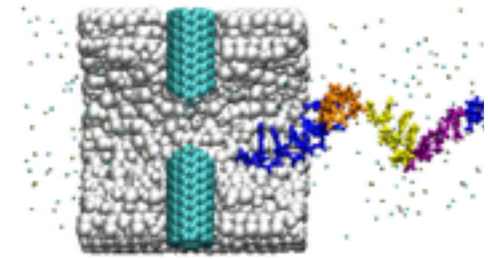


Magnetic Genoma

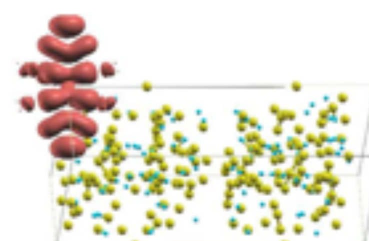


Organics

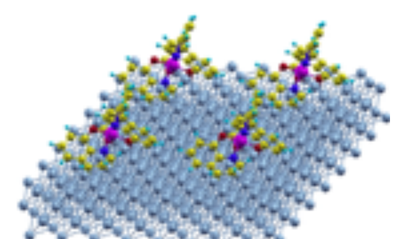
DNA sequencing



Diffusive Transport

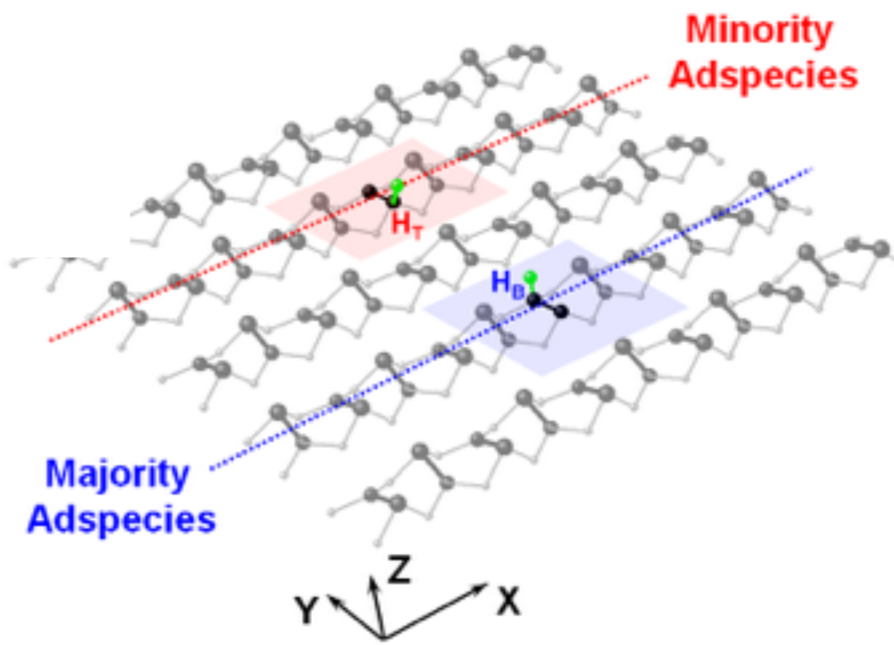


Organic spintronics



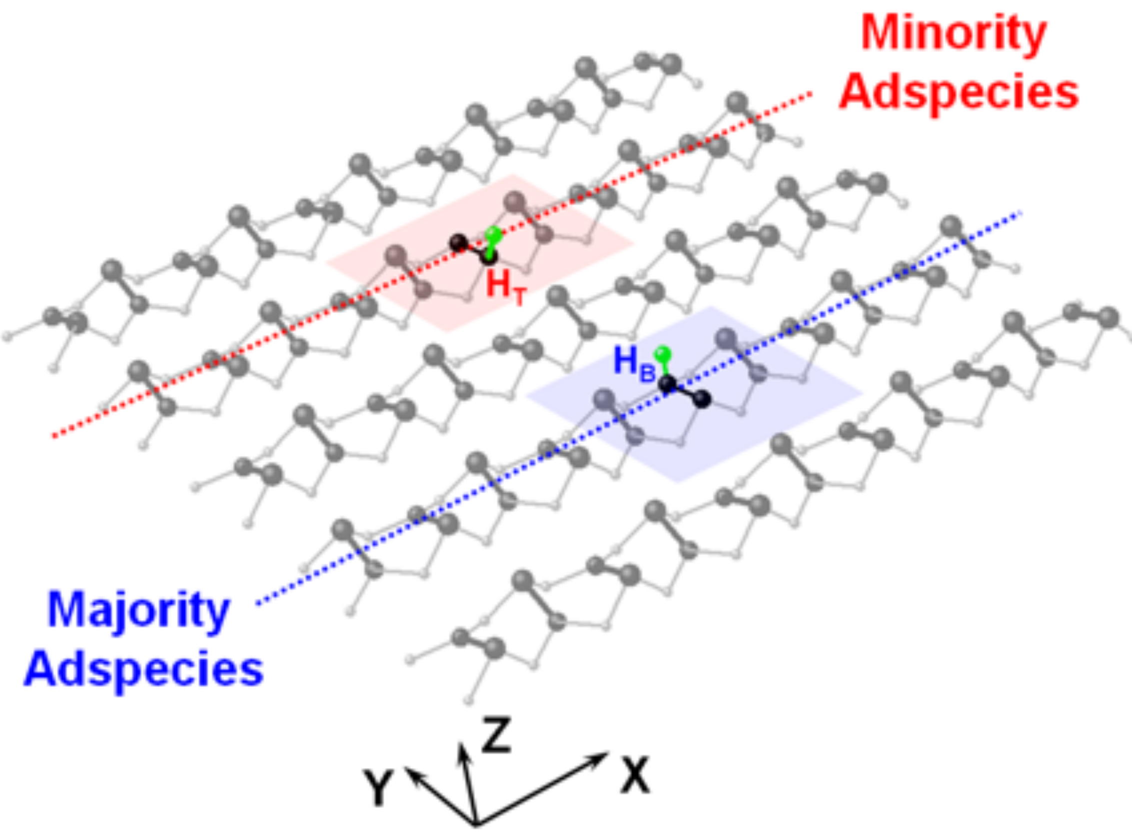
Quantum playground 1

H on Si (100)

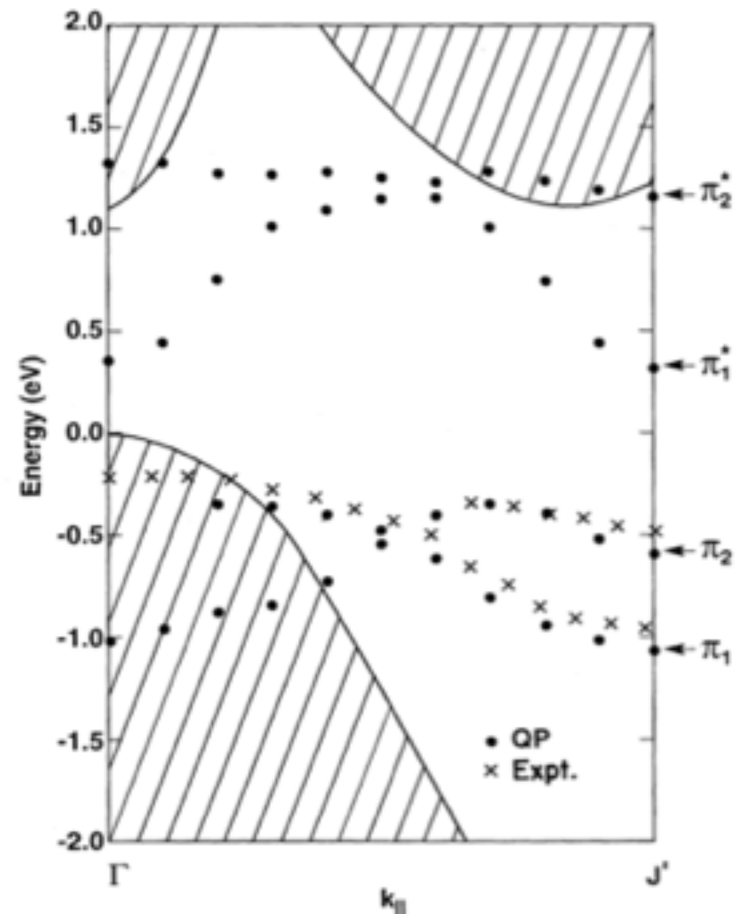


B. Naydenov, M. Mantega, I. Rungger, SS and J.J. Boland, Phys. Rev. B **84**, 195321 (2011)

H on Si (100)

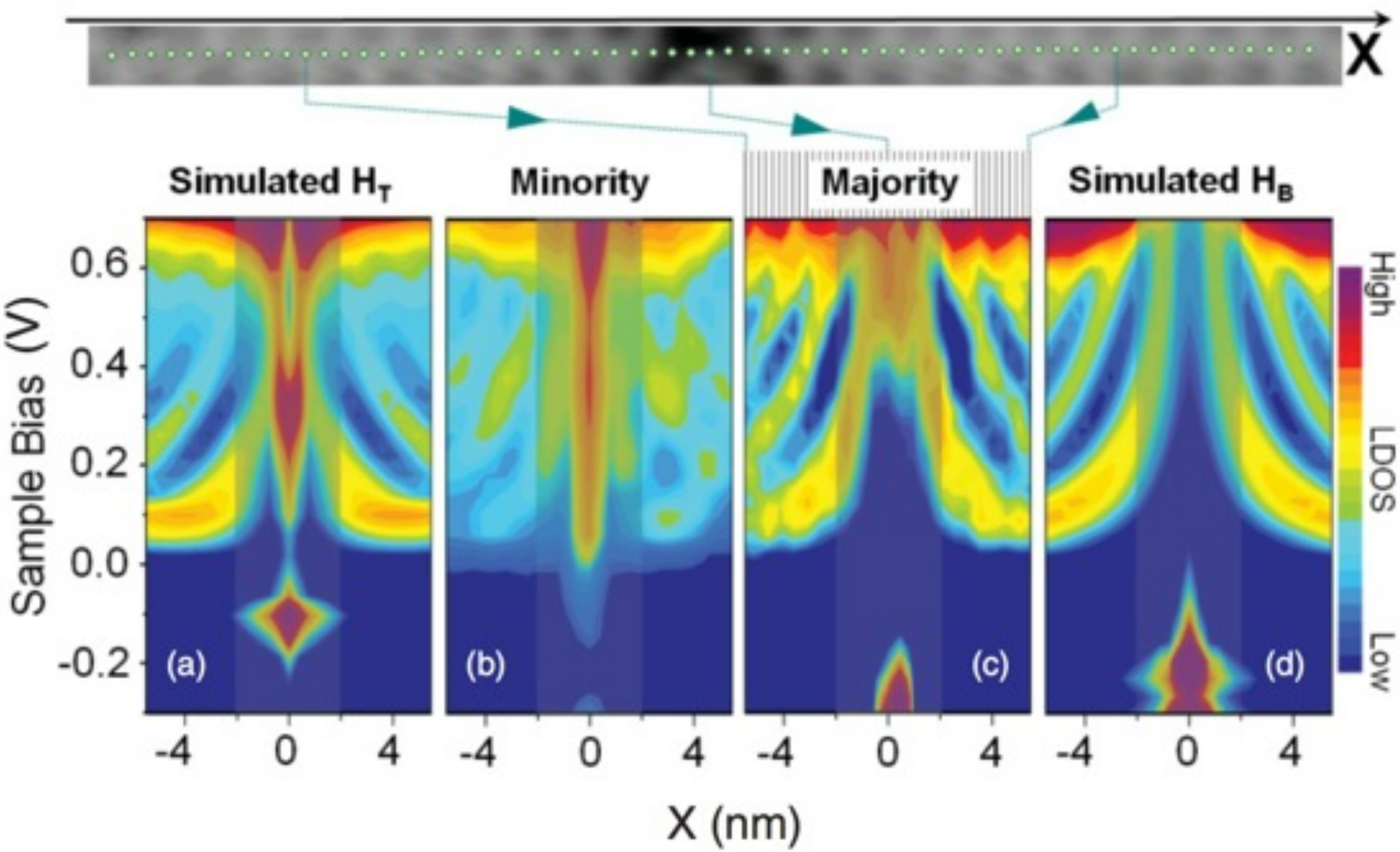


GW Band

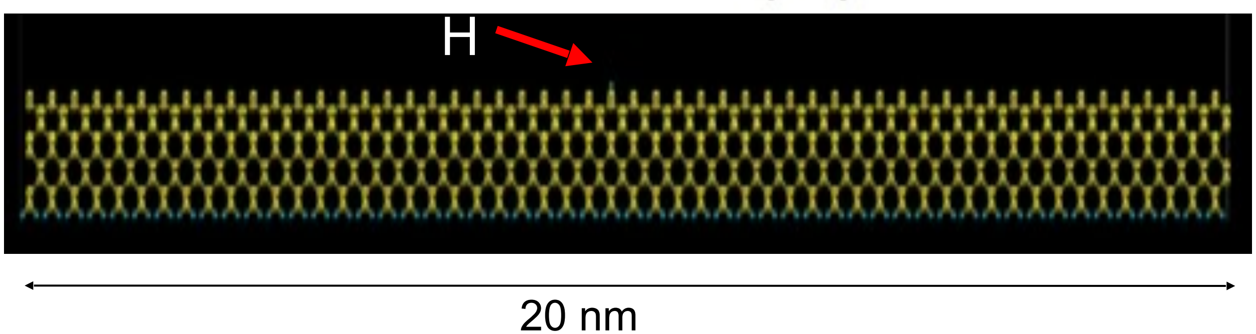


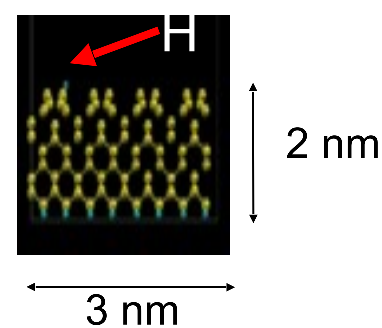
J.E. Northrup, Phys. Rev. B **47**, 10032 (1993)

H on Si (100): single centre



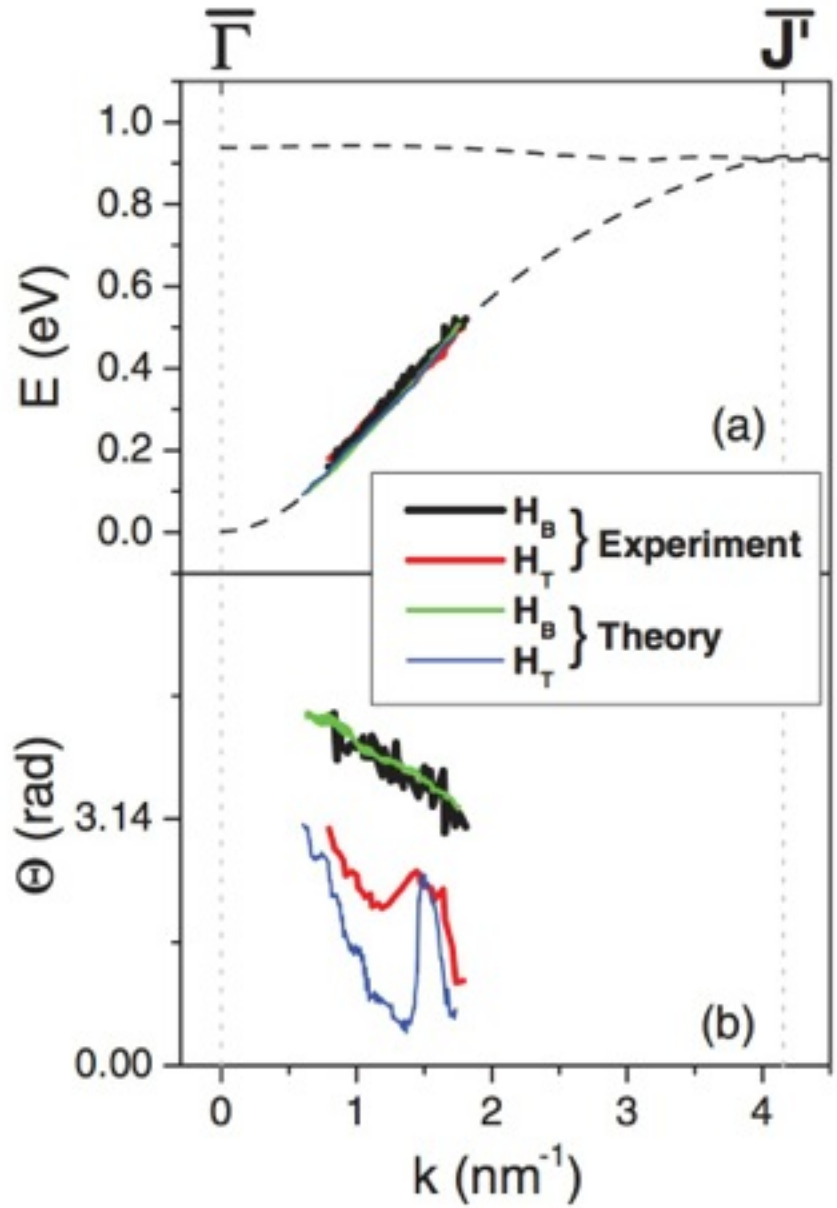
STM dI/dV





H on Si (100): single centre

Scattering analysis



H on Si (100): heterostructures

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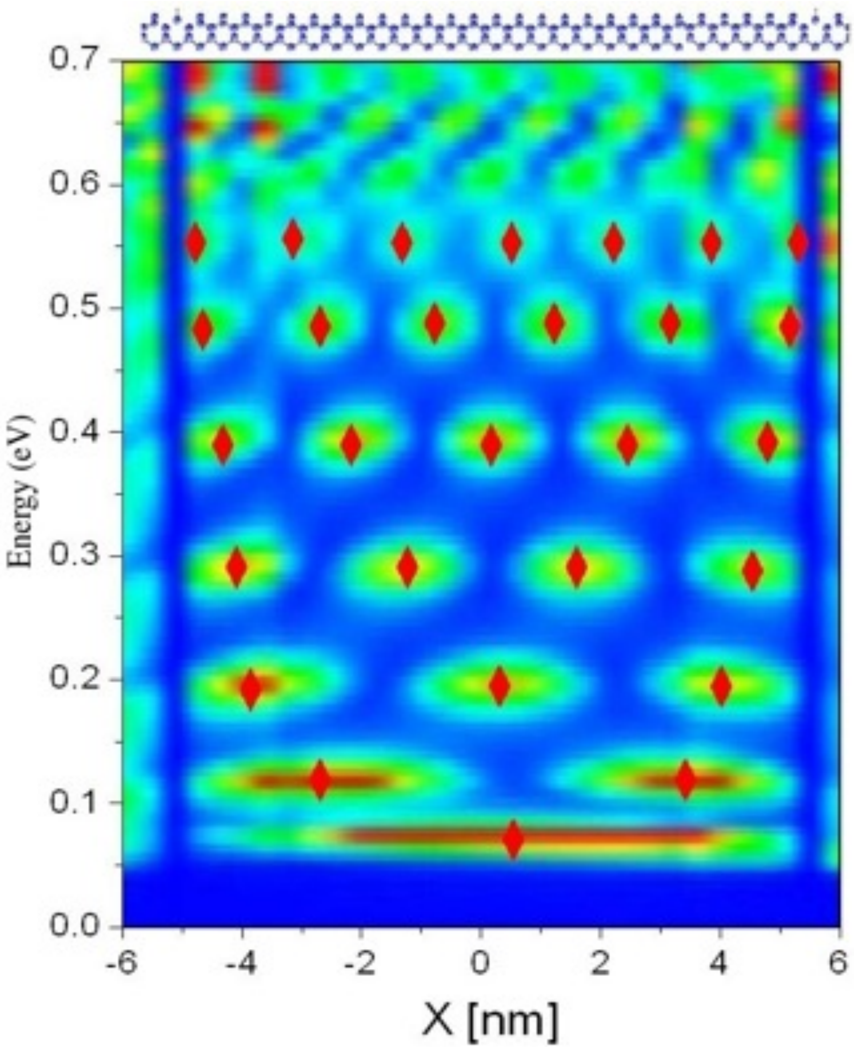
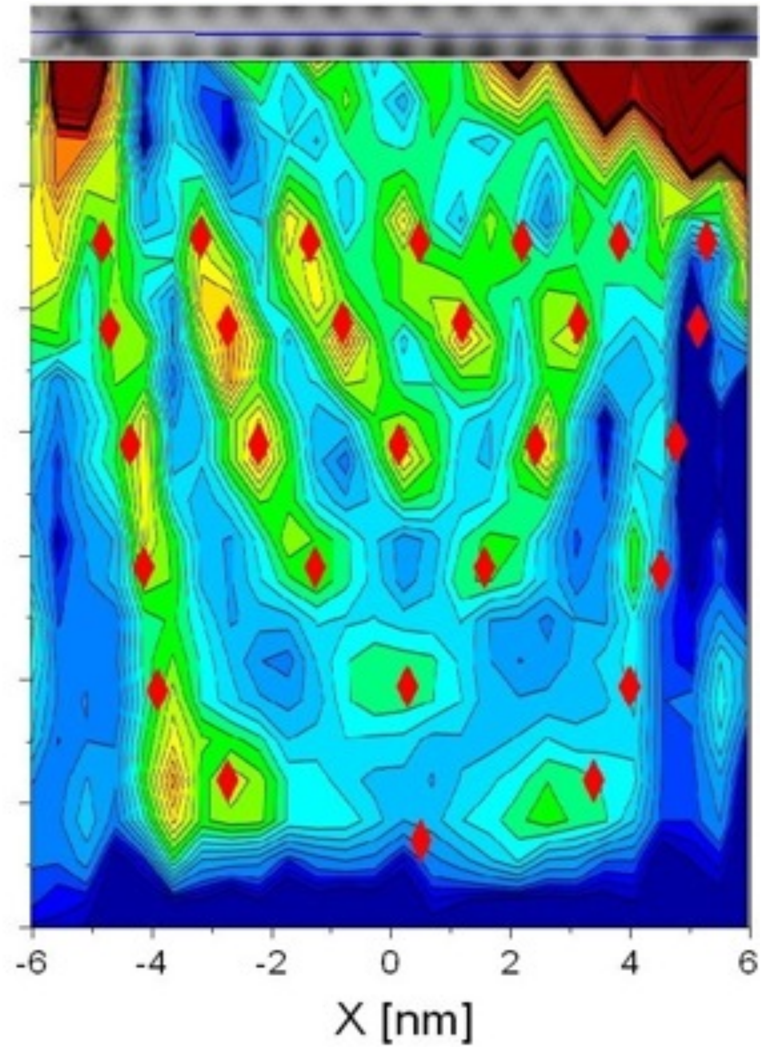
Theory



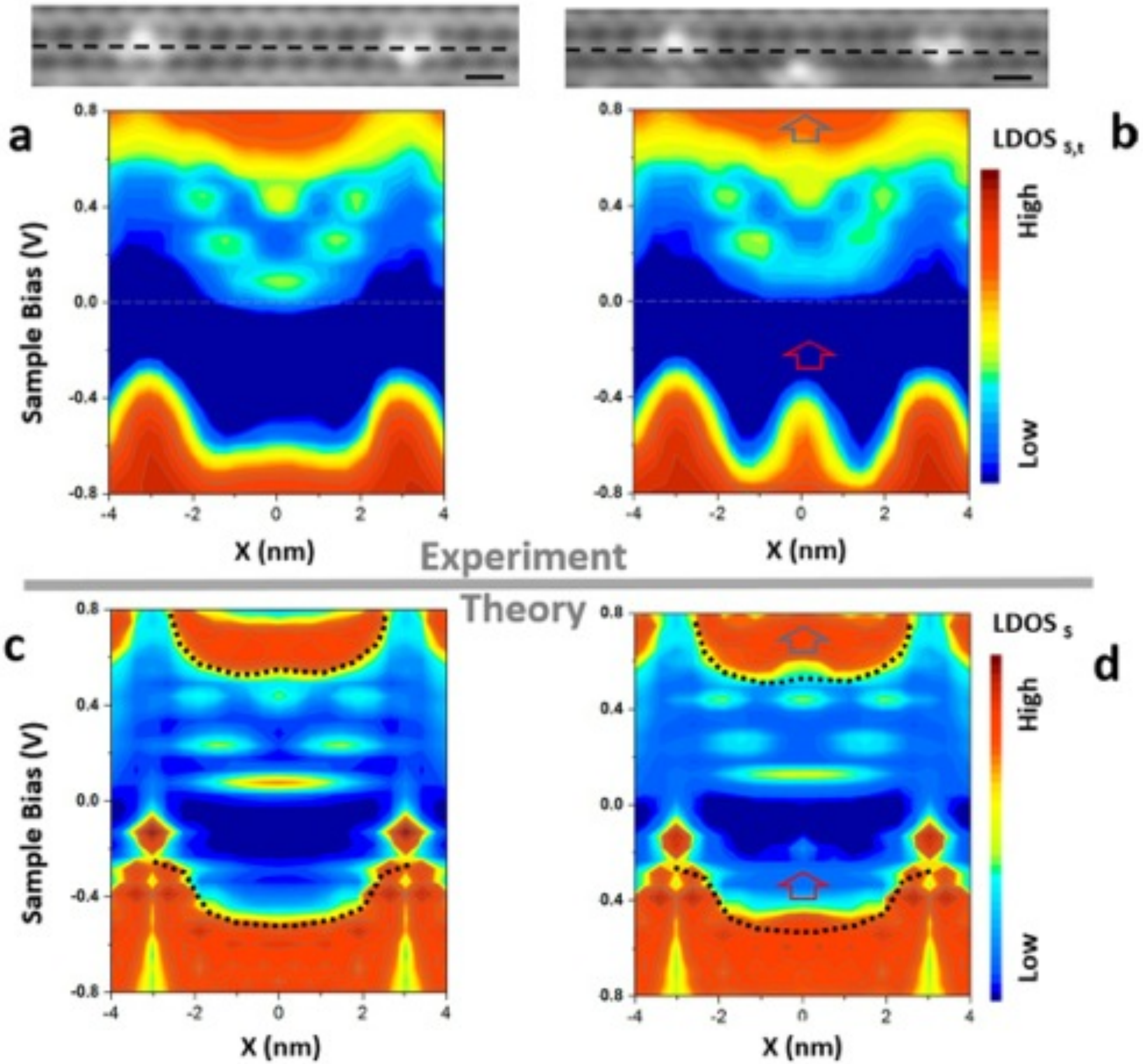
Experiment



H on Si (100): heterostructures

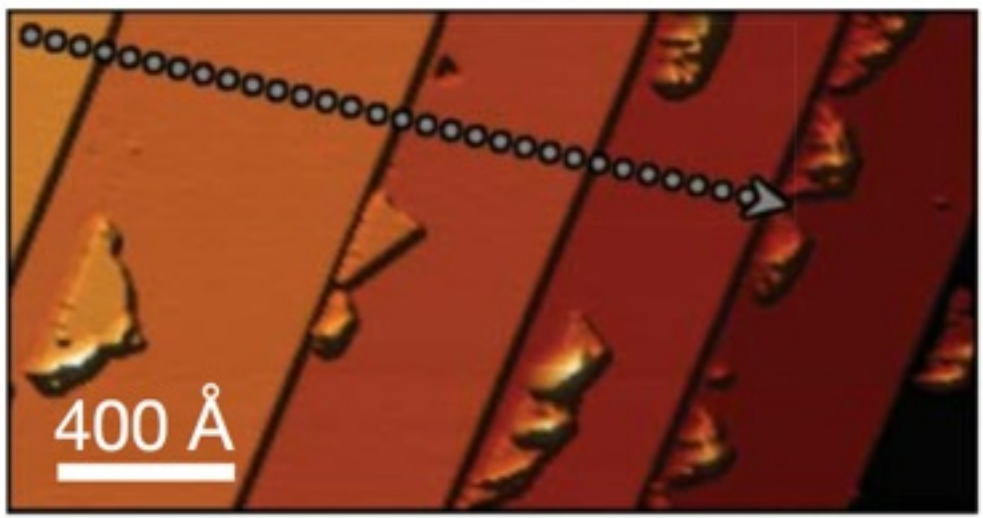
PRB **84**, 195321 (2011)

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



Quantum playground 2

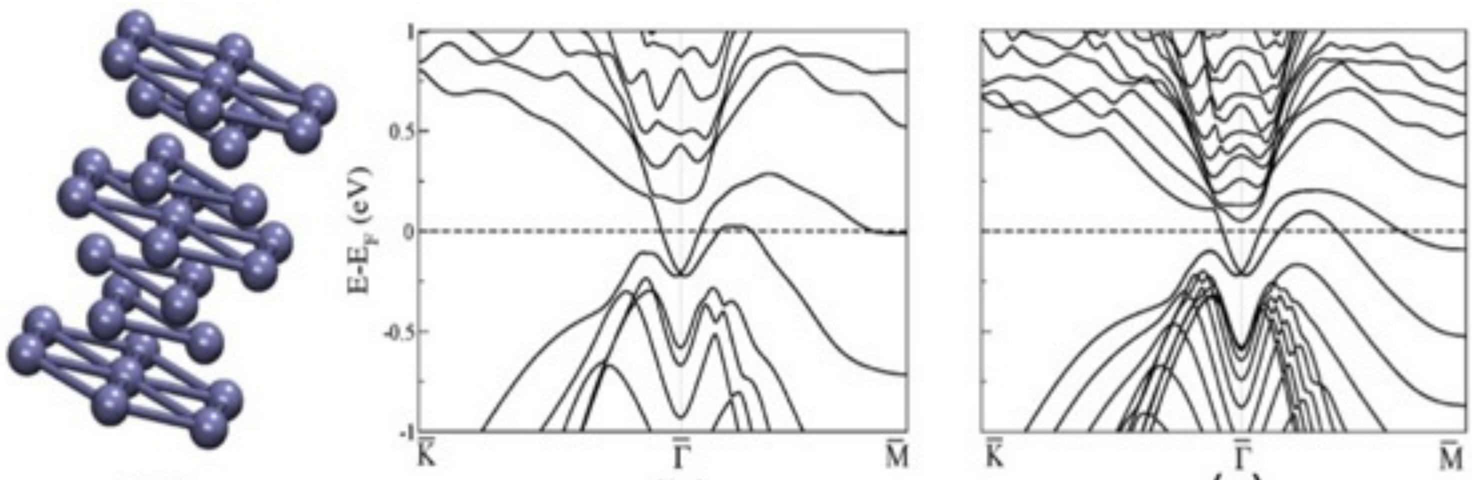
Topological surfaces



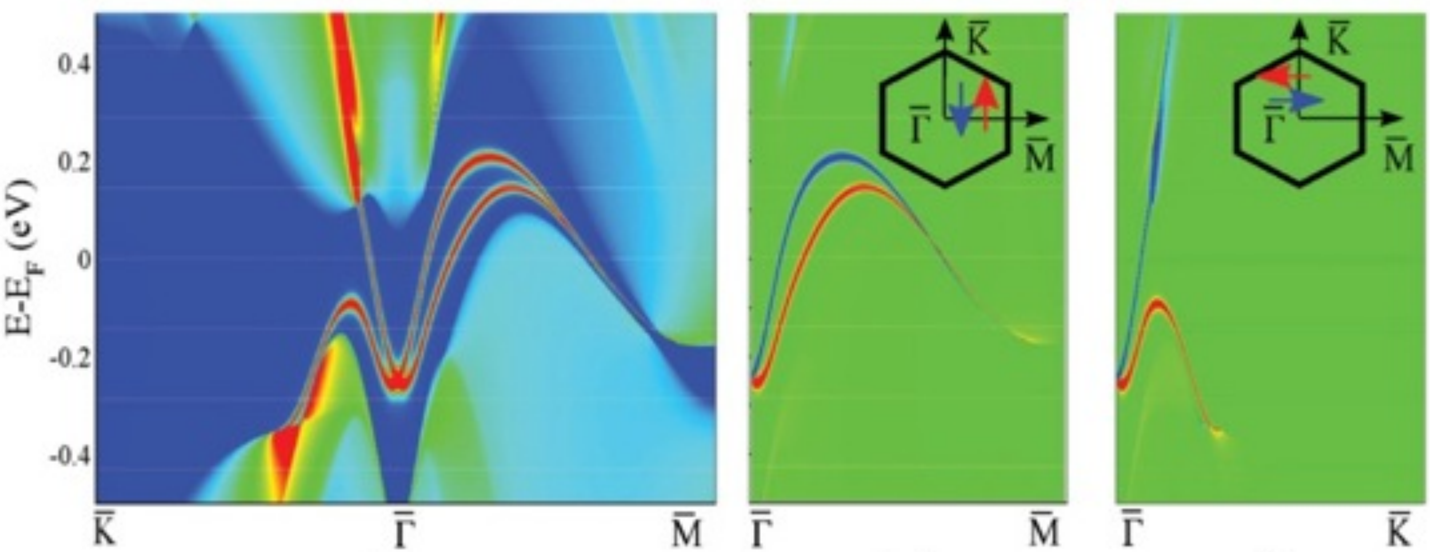
Awadhesh Narayan, Ivan Rungger and SS, PRB **86**, 201402(R) (2012); PRB **90**, 205431 (2014)

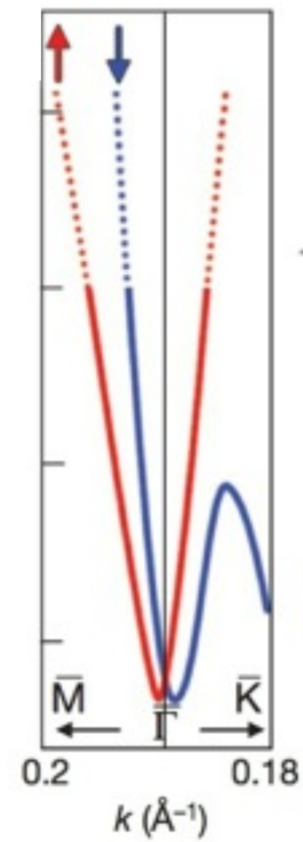
Scattering at topological surfaces

Sb (111)



(a) (b) (c)





Nature **466**, 343 (2012)

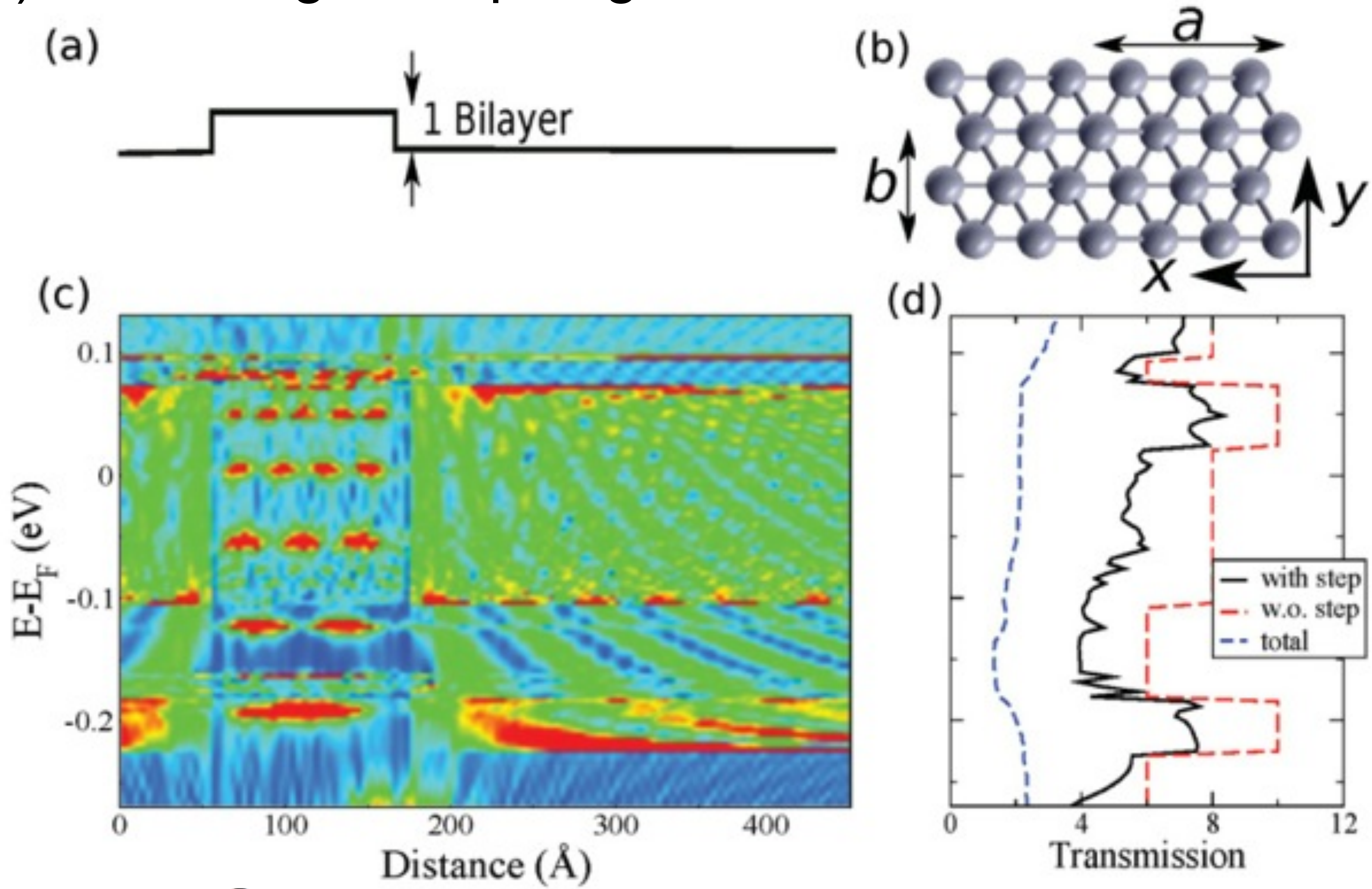
PRB **86**, 201402(R) (2012)

Simulated ARPES

Scattering at topological surfaces

CRANN

Sb (111): scattering at step edge

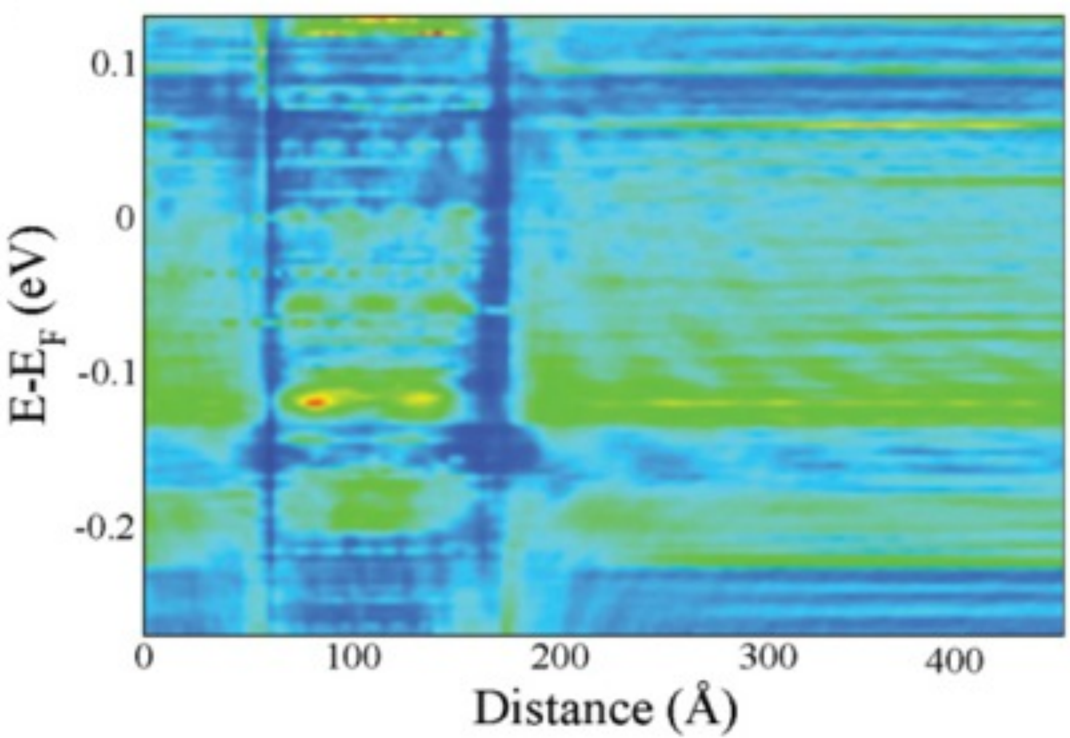


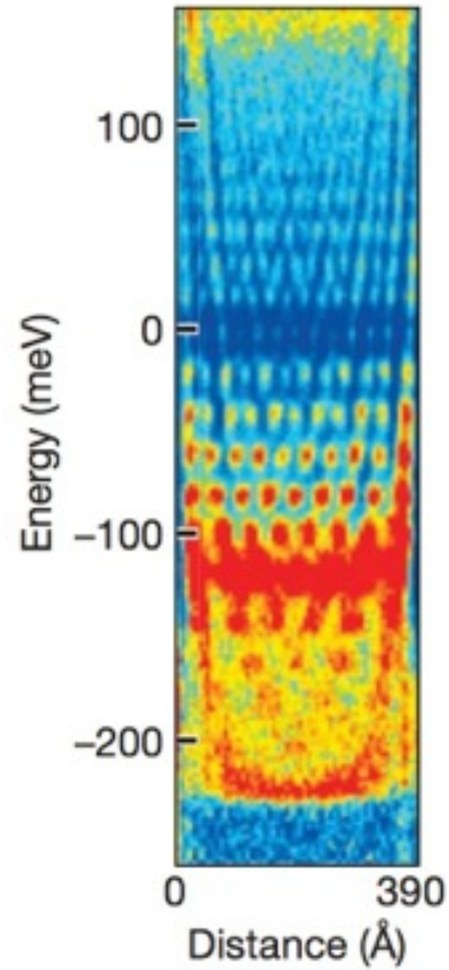
Transport along $\bar{\Gamma}$-$\bar{M}$

Scattering at topological surfaces

CRANN

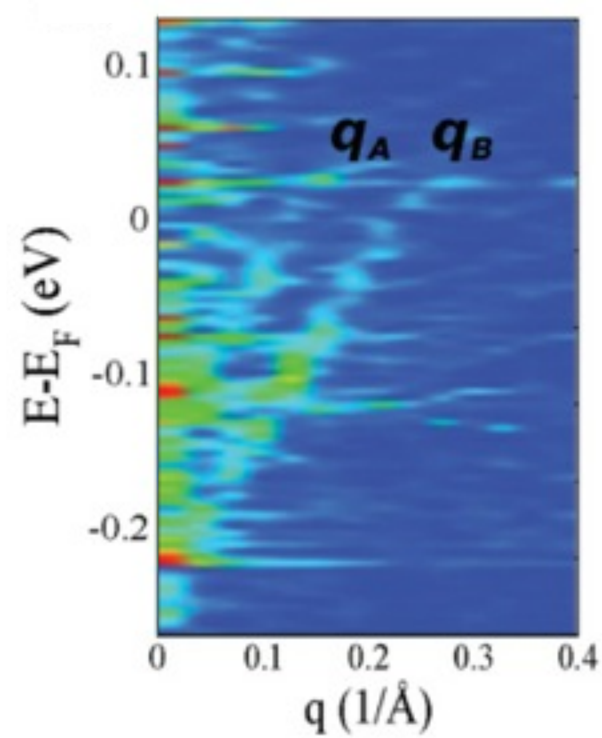
Sb (111): scattering at step edge

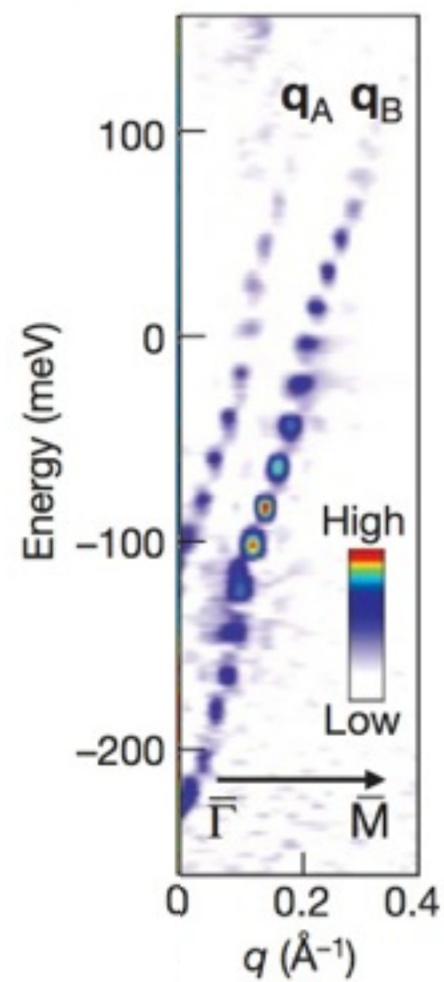




Scattering at topological surfaces

Sb (111): scattering at step edge





Can we find new quantum playgrounds ?

The question

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

Take the example of magnetism ….

Fe, Co, Ni, $Nd_2Fe_{14}B$, $LaMnO_3$, Fe_3O_4 ….

~2,000

Magnetism is rare

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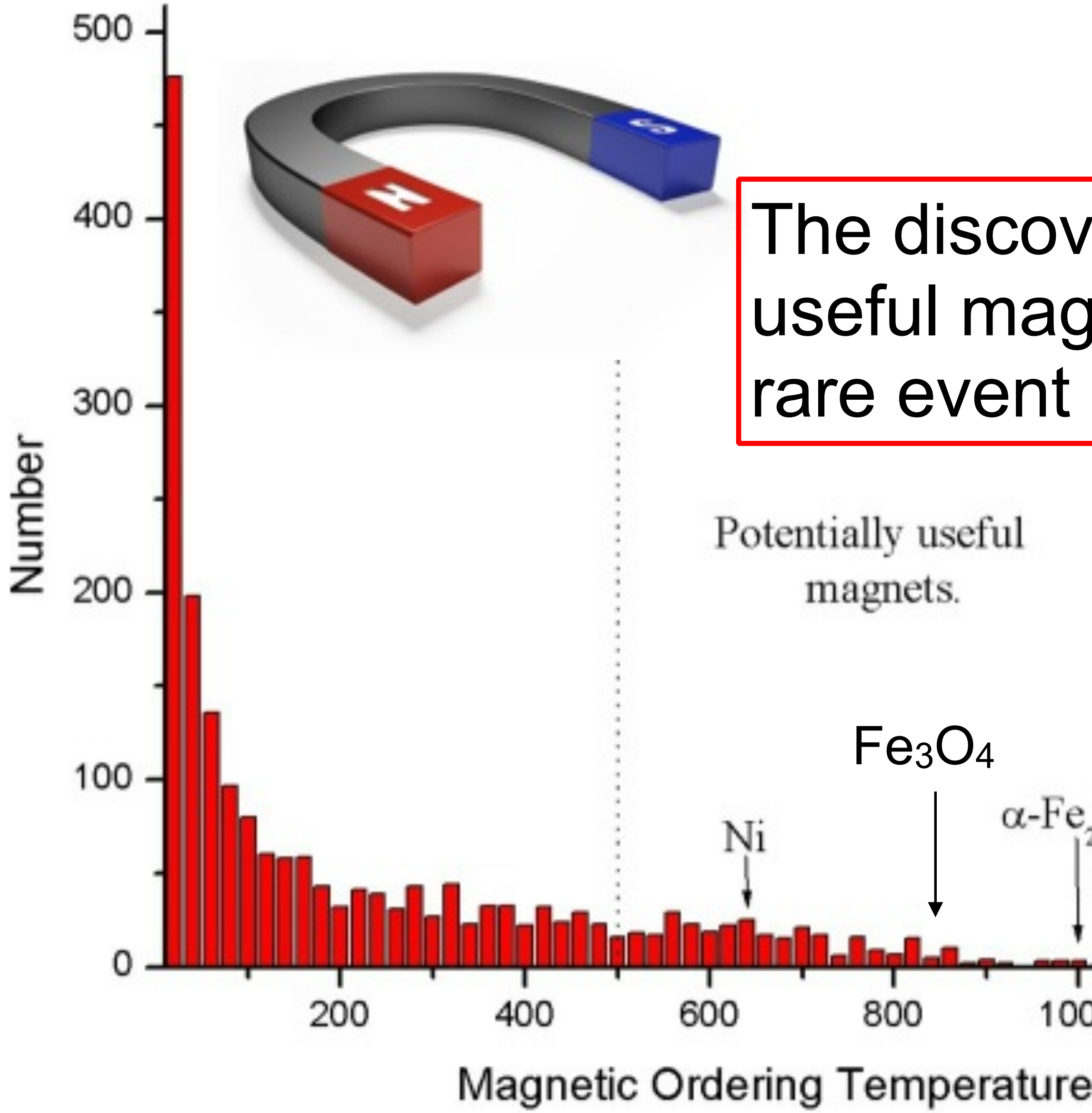
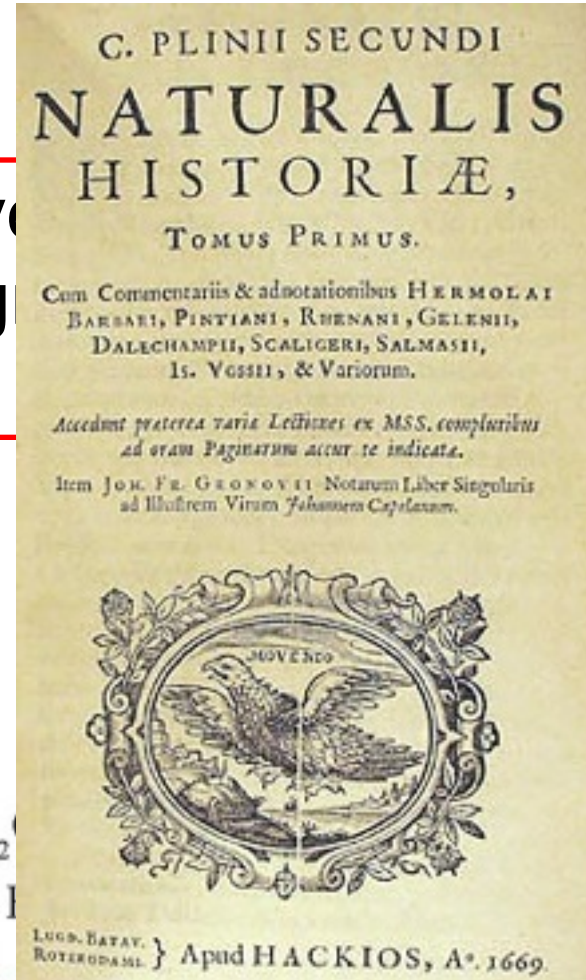


The discove
useful mag
rare event



C. PLINII SECUNDI
NATURALIS
HISTORIÆ,
TOMUS PRIMUS.

Cum Commentariis & adnotationibus HERMOLAI BARBARI, PINTIANI, RHENANI, GELENII, DALECHAMPII, SCALIGERI, SALMASII, Is. VOSSII, & Variorum.

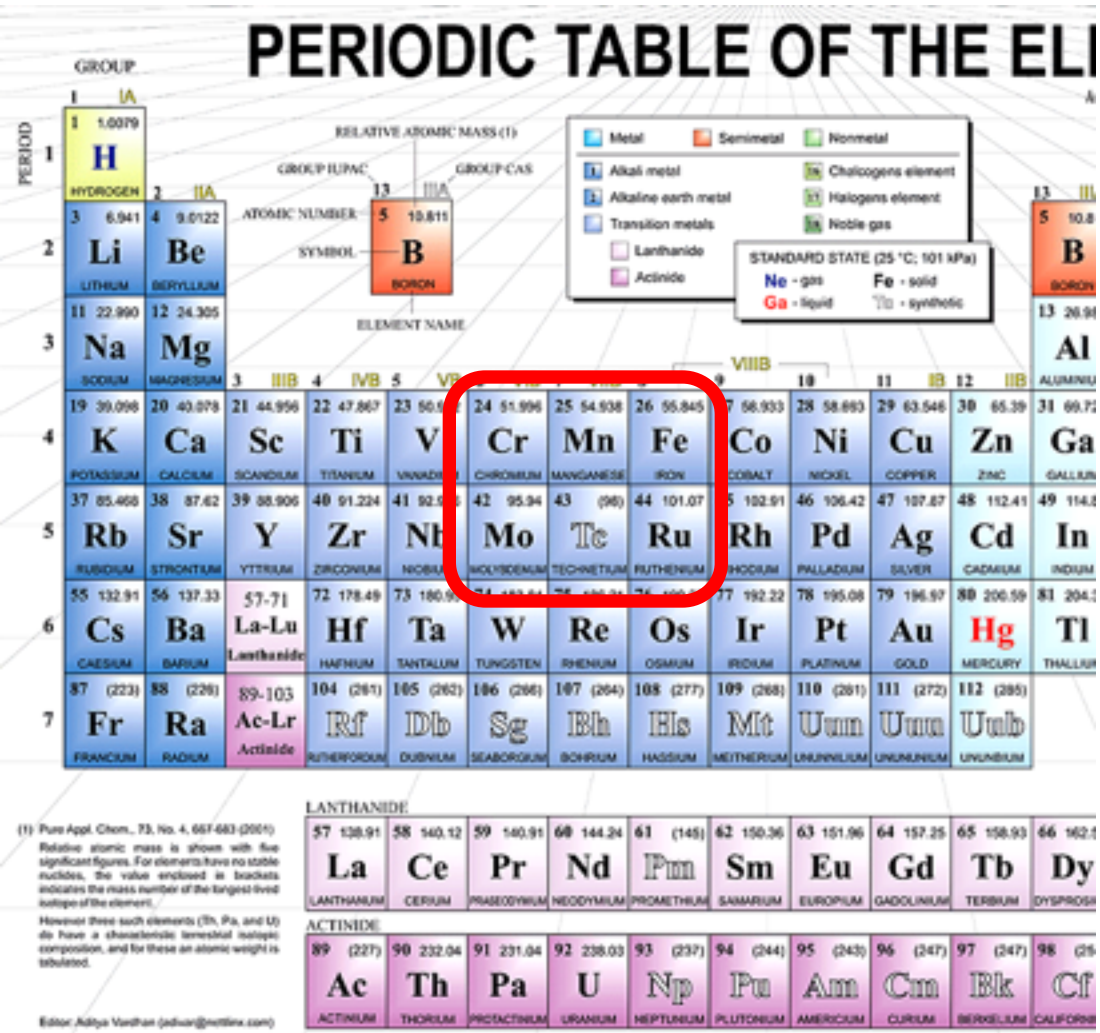
Accedunt praeterea variae Lectiones ex MSS. compluribus ad oram Paginarum accurate indicatae.

Item JOH. FR. GRONOVII Notarum Liber Singularis ad Illustrem Virum *Johannem Capelanum.*

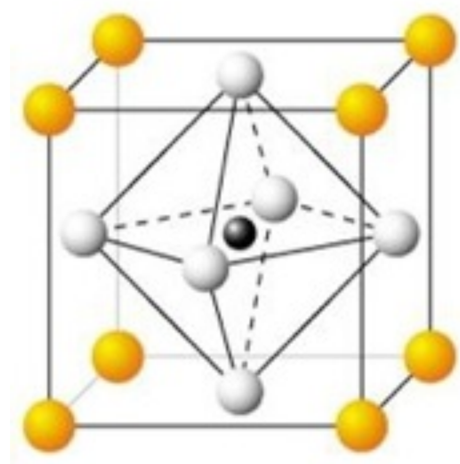
MOVENDO

LUGD. BATAV. ROTERODAMI. } Apud HACKIOS, A°. 1669.

Magnetism is complicated



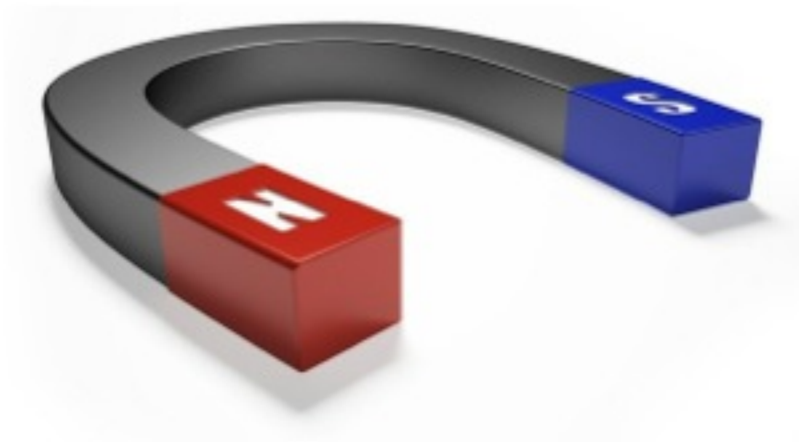
$SrCrO_3$ T_N=-230C	$SrMnO_3$ T_N=-10C	$SrFeO_3$ T_N=-140C
$SrMoO_3$	**$SrTcO_3$ T_N=500C**	$SrRuO_3$ T_C=-100C



$SrMO_3$

C. Franchini, T. Archer, J. He, X.-Q. Chen, A. Filippetti and S. Sanvito, Phys. Rev. B **83**, 220402(R) (2011)

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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...tronic structure method:
...ctional theory (VASP)

The AFLOW consortium

CRANN

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)

CRANN

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 quintenary
- 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

CRANN

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.)

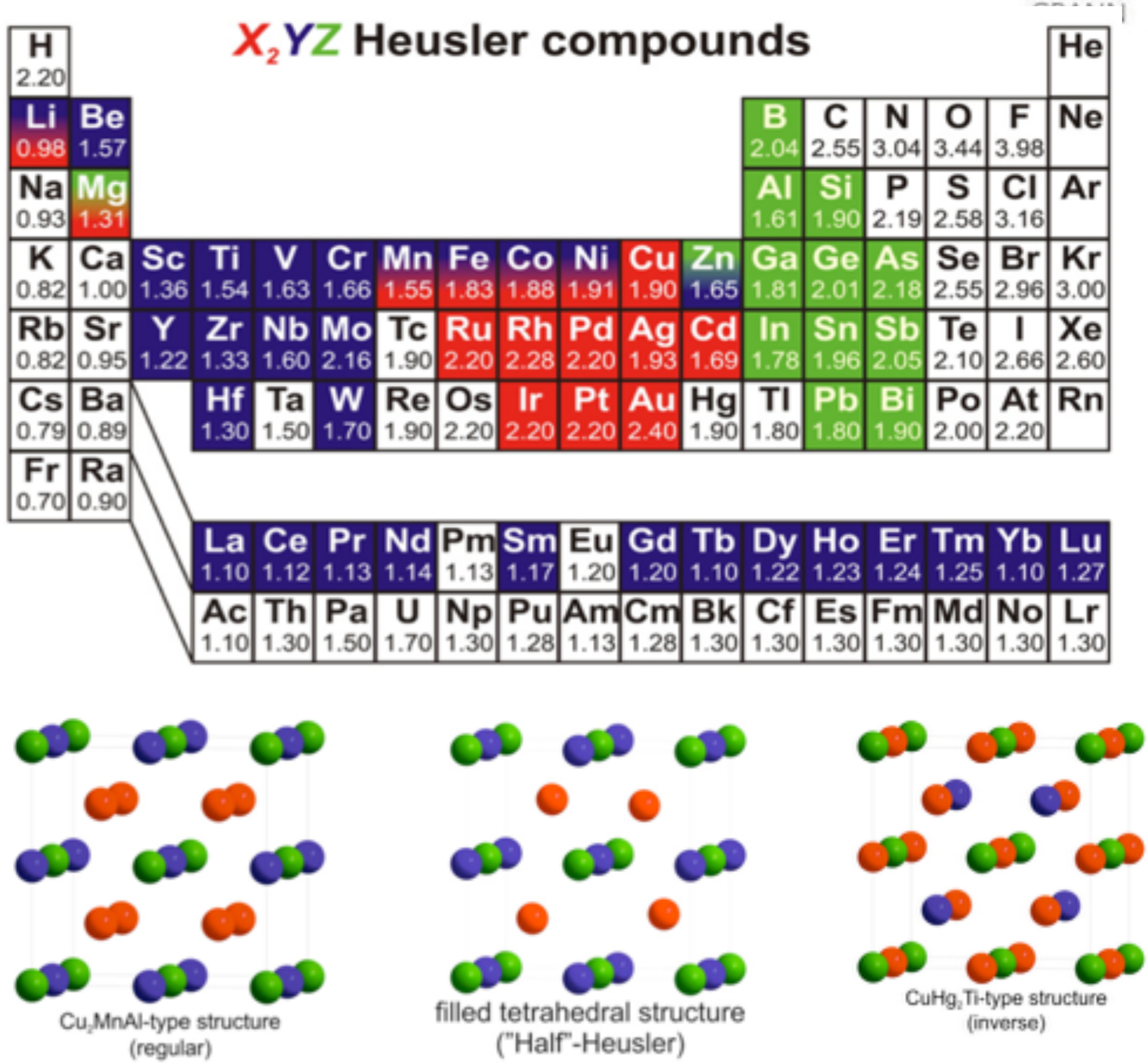
S. Curtarolo, W. Setyawan, G. L. W. Hart, M. Jahnatek, R. V. Chepulskii, R. H. Taylor, S. Wang, J. Xue, K. Yang, O. Levy, M. Mehl, H. T. Stokes, D. O. Demchenko, and D. Morgan, Comp. Mat. Sci. **58**, 218 (2012)

Heusler alloys

~250 known …

~1000 claimed …

~90 magnetic …



Heusler alloys

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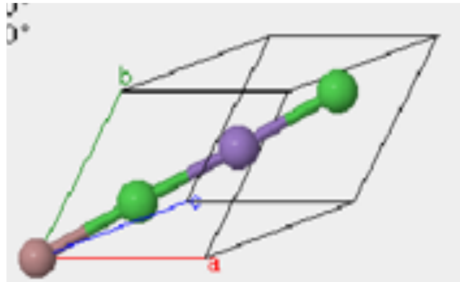
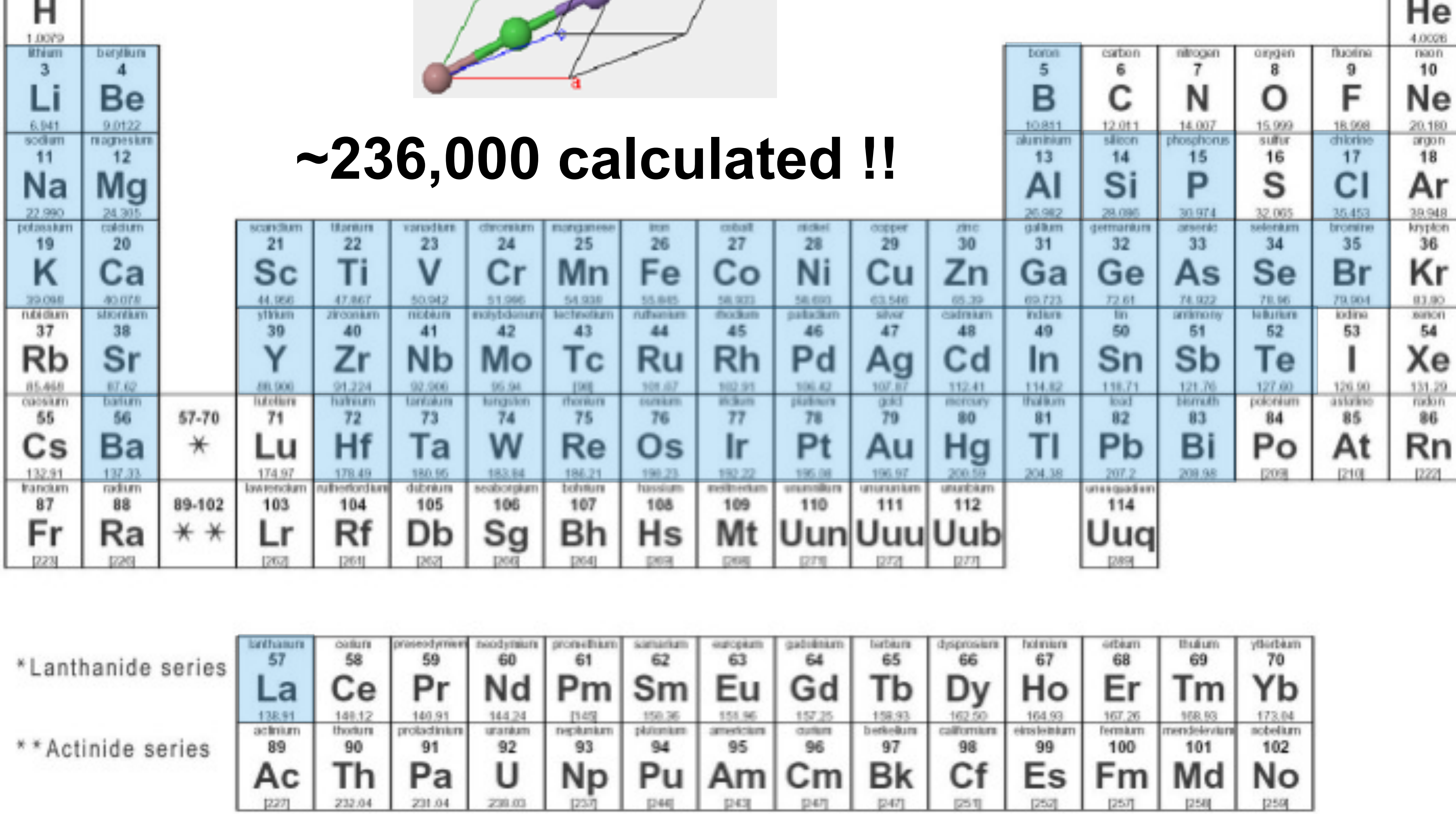


~236,000 calculated !!



The magnetic genome project

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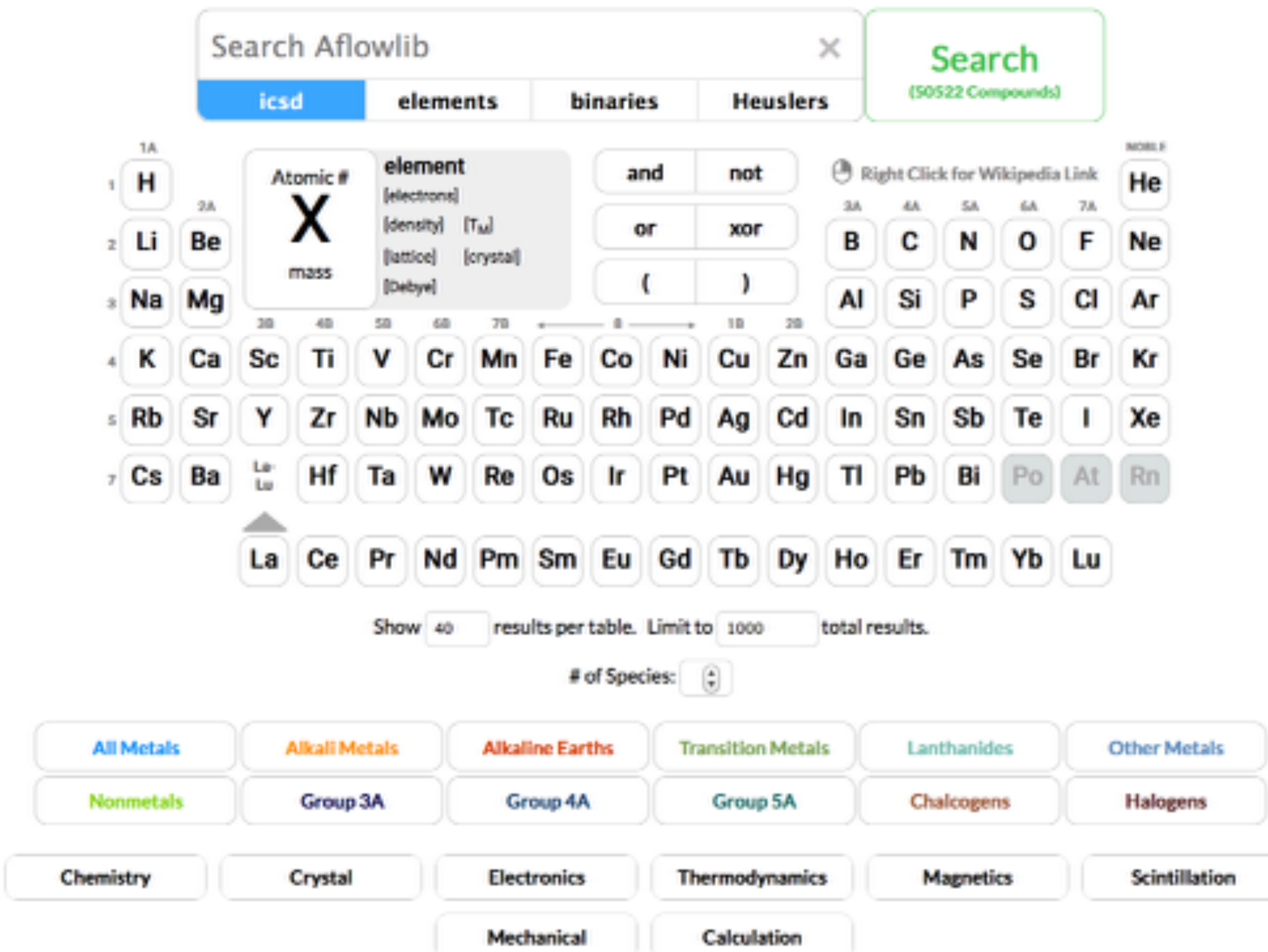
Rational materials storage

www.aflowlib.org



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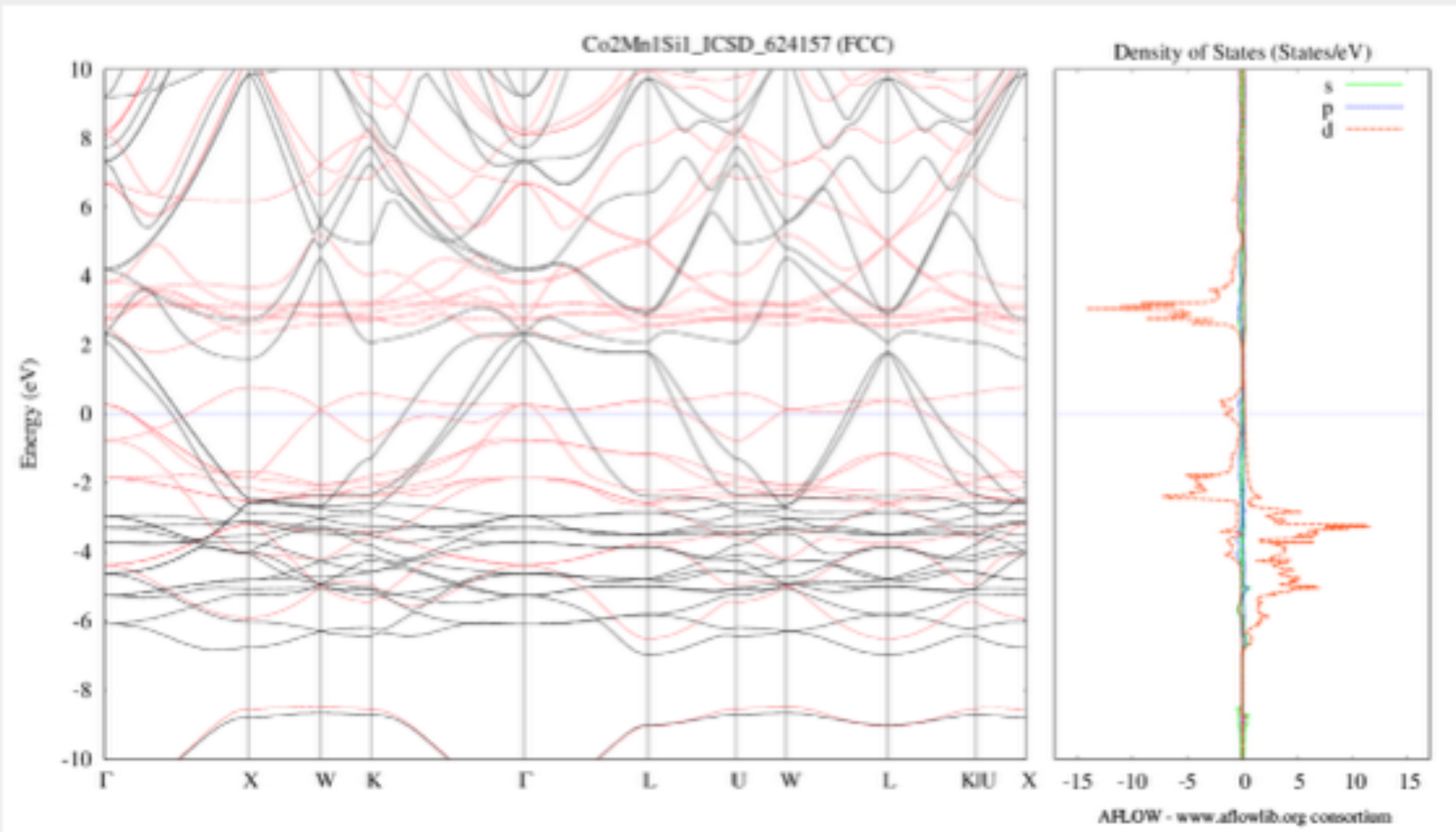
… and one theory for find them all

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:



Comp. Mat. Sci. **49**, 299-312 (2010)

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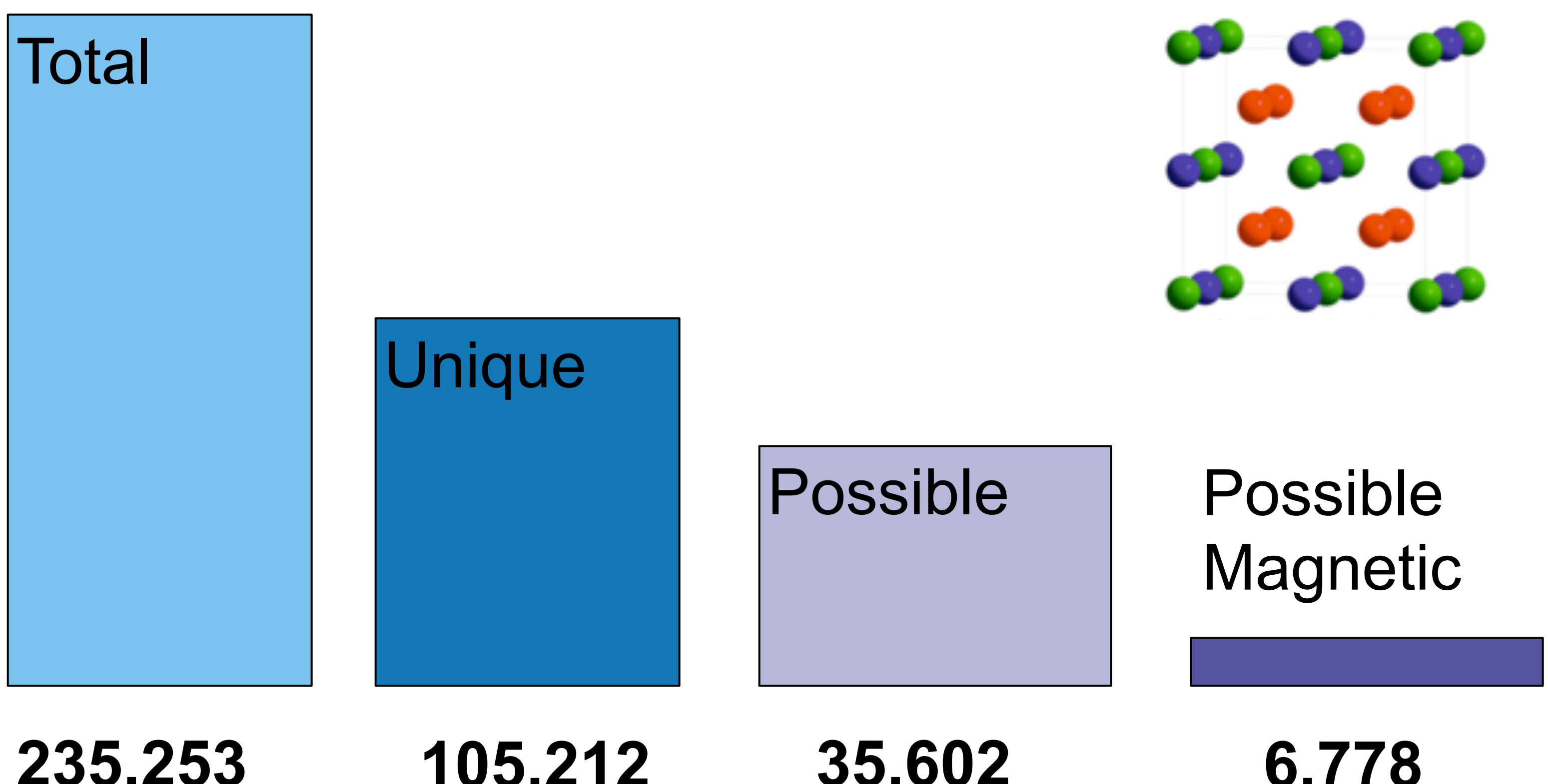
A look at the full database

Property: Can be made ?

Descriptor 0:
Enthalpy of formation

Energy (Ni_2MnAl) < Energy (2Ni + Mn +Al)



Stability analysis

Descriptor 1: Enthalpy of formation

Ni_2MnAl

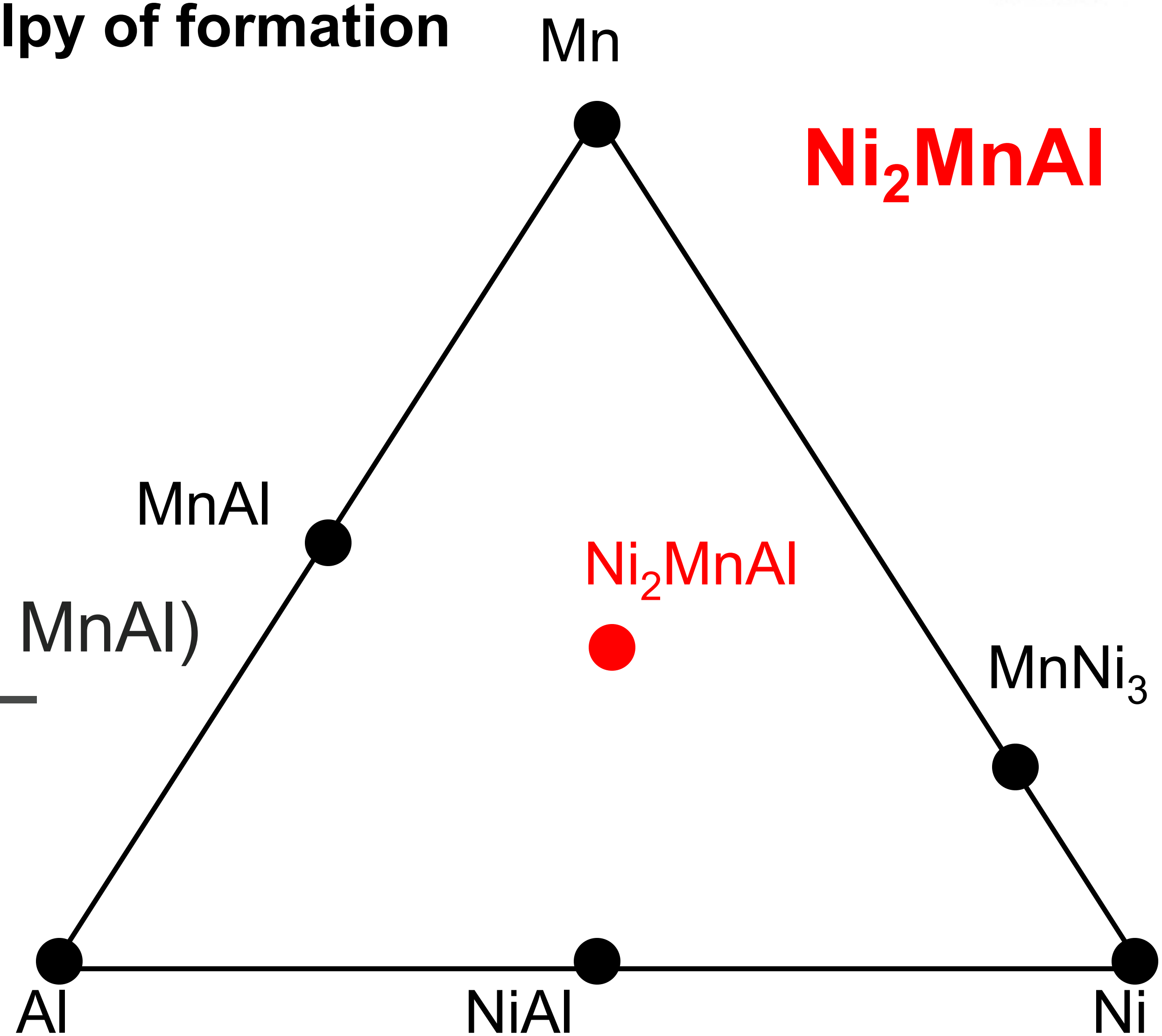
2 Ni + Mn + Al

---

2 Ni + MnAl

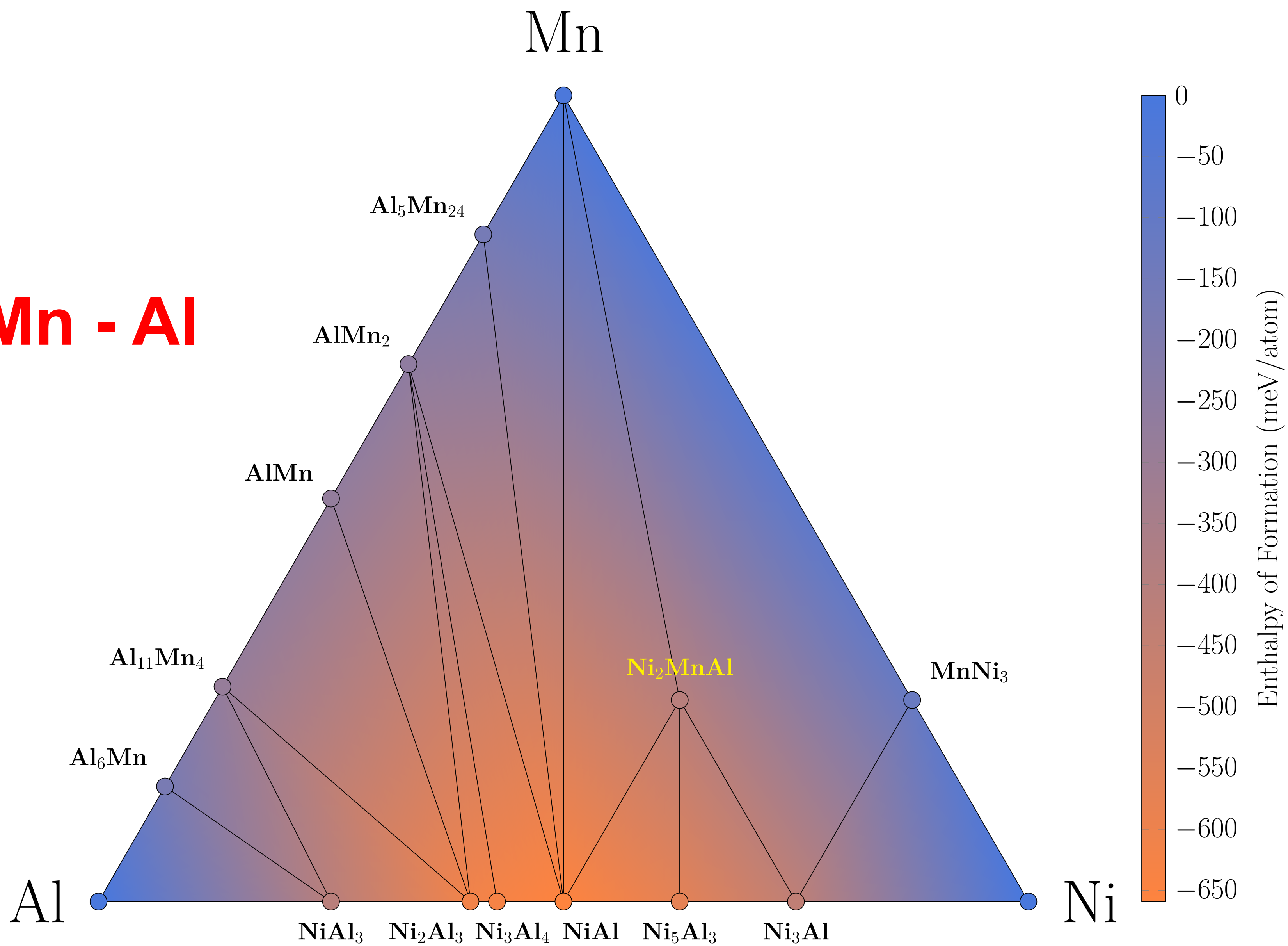
1/2 ($MnNi_3$ + NiAl + MnAl)

Ni_2MnAl



Stability analysis

Ni - Mn - Al



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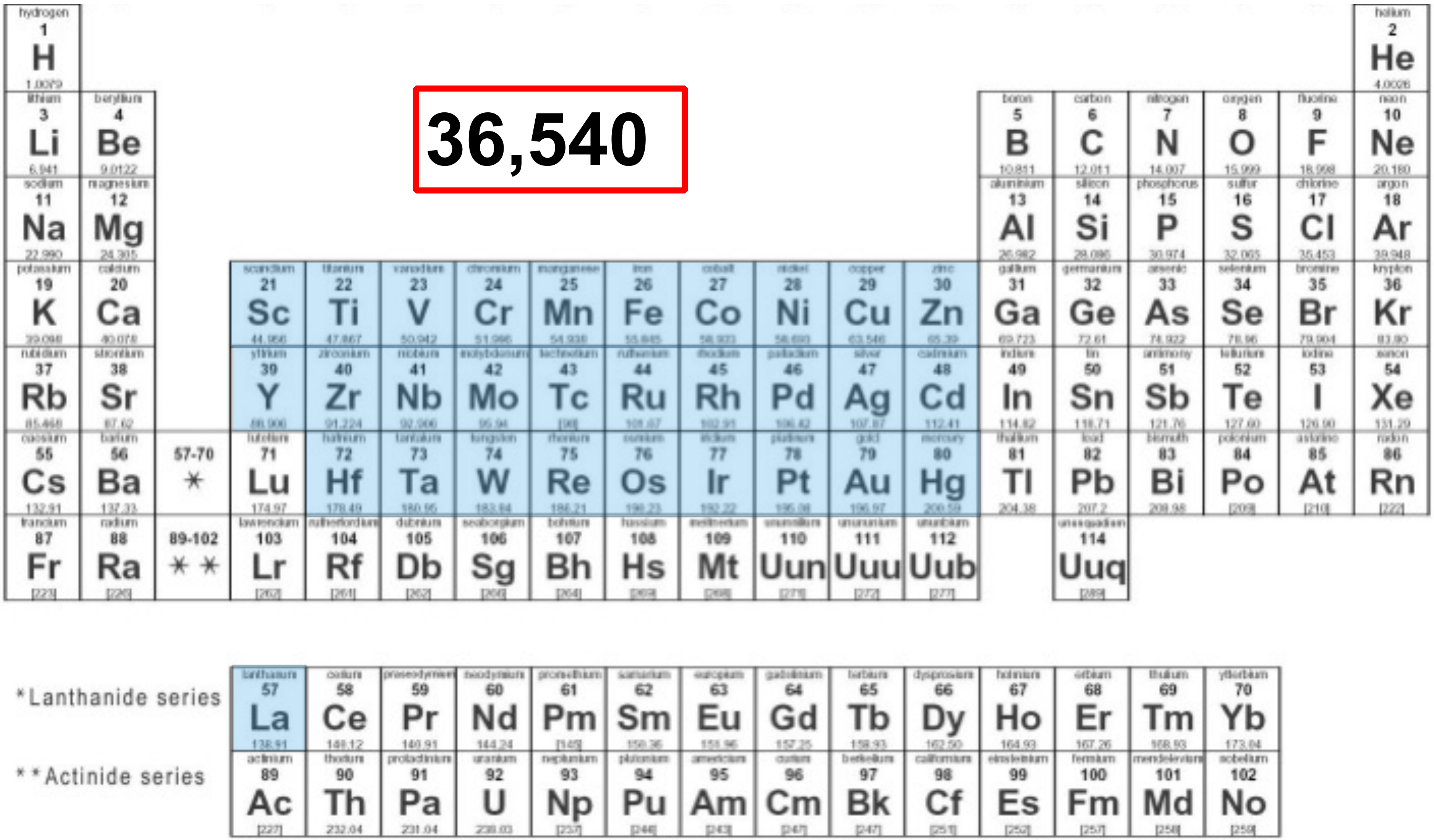
Look at the transition metal intermetallics

36,540



In summary …

36,540 possible → 248 stable

22 magnetic → 8 Robust

↓ Extrapolating

236,000 possible → 1550 stable

138 magnetic → 50 Robust

Entropic temperature

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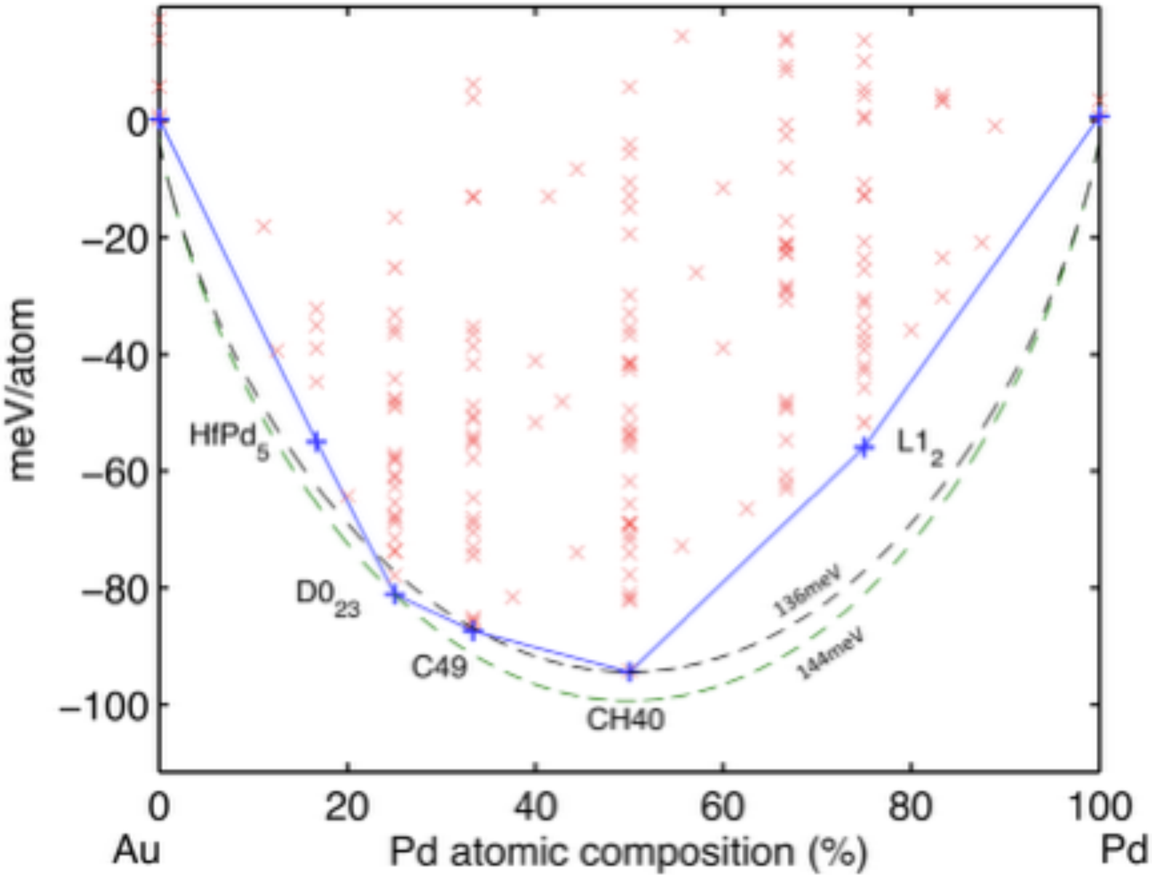
Descriptor 2: Entropic temperature



$$T_{\mathrm{S}} = \max_i \frac{\Delta H(A_{x_i} B_{1-x_i})}{k_{\mathrm{B}}[\log(x_i) + (1-x_i)\log(1-x_i)]}$$

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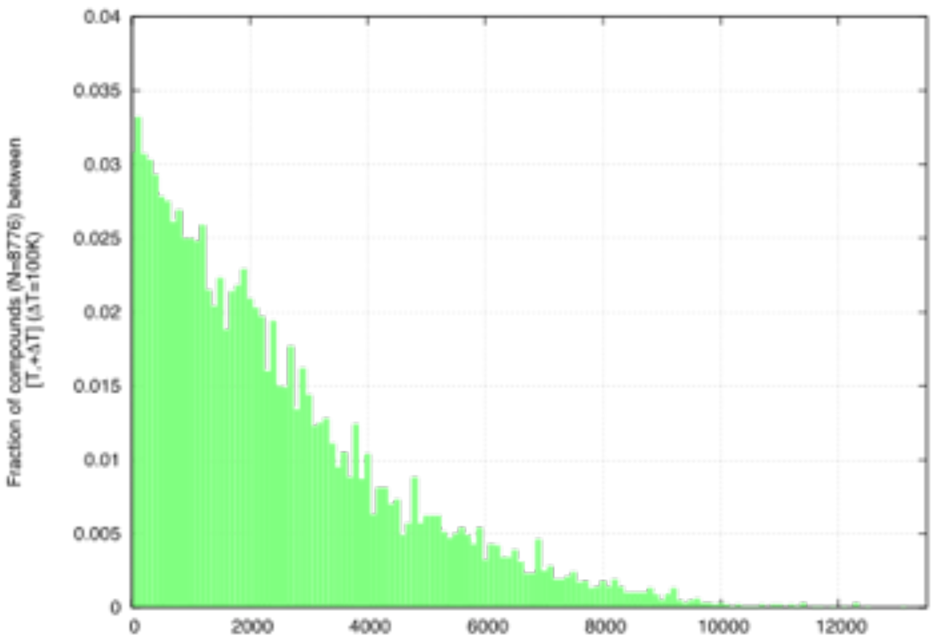
Descriptor 2: Entropic temperature

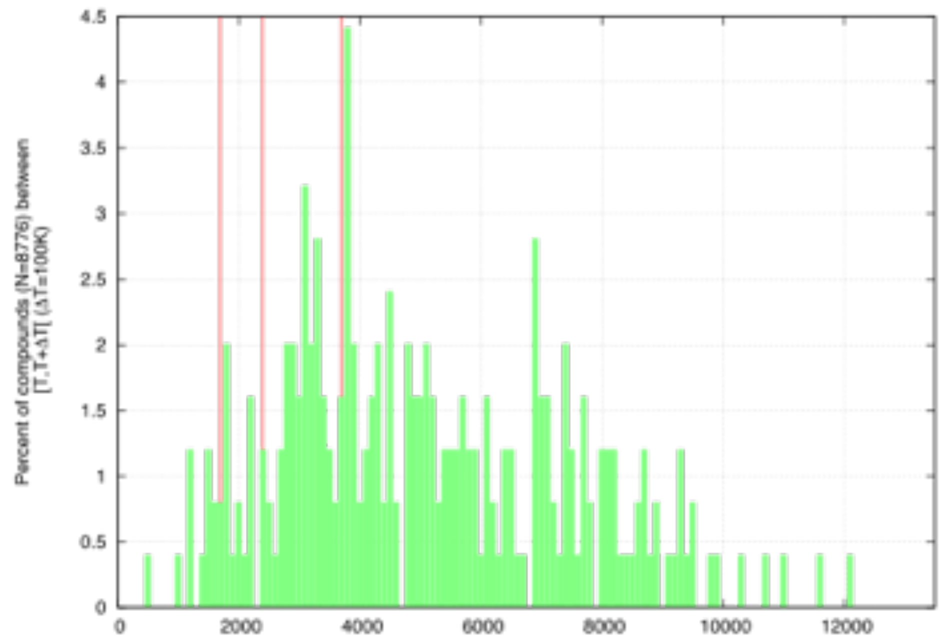
N=8776



T_S

Weibull distribution

N=248



T_S

CRANN

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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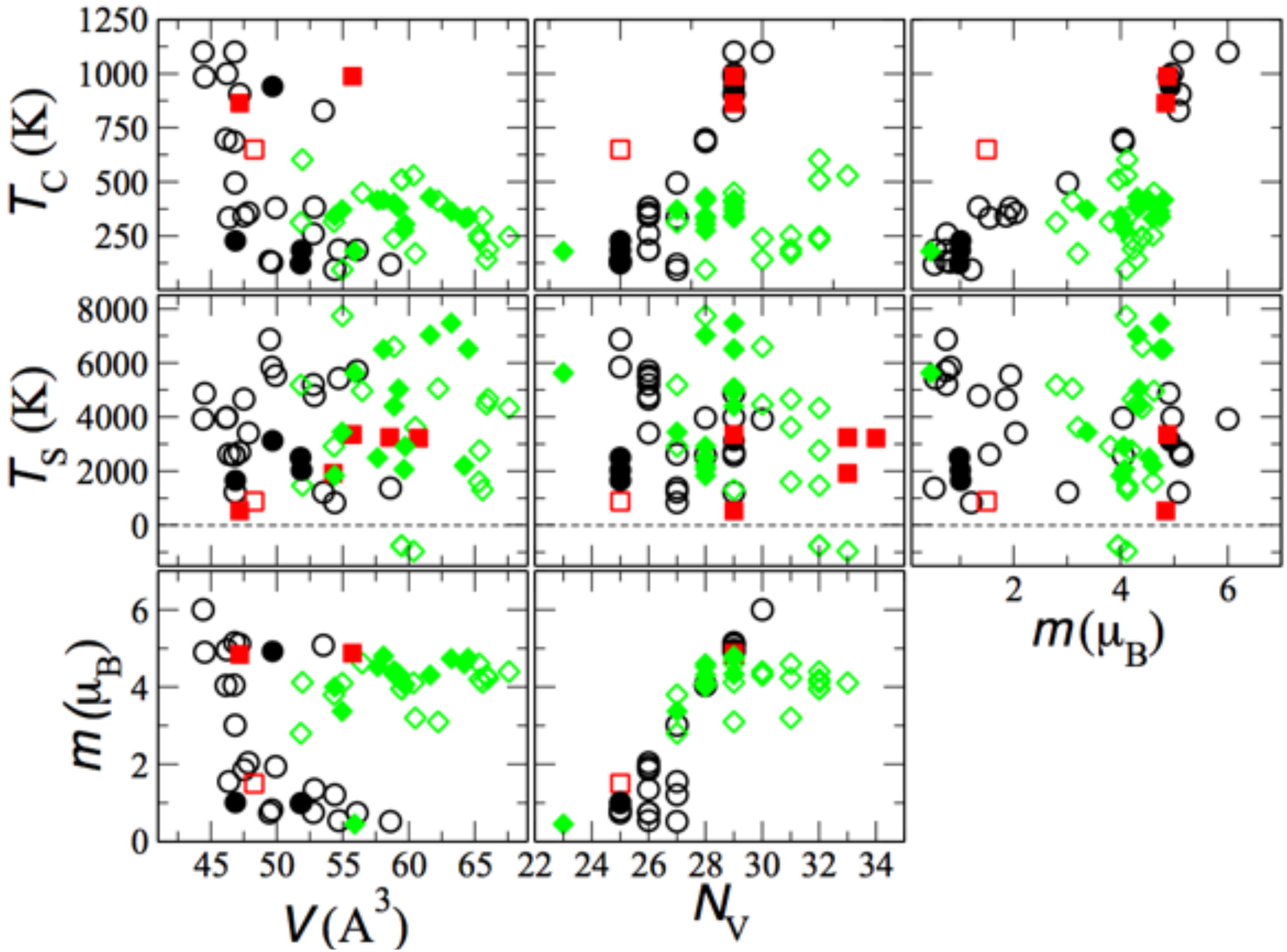
Co_2XY

Mn_2XY

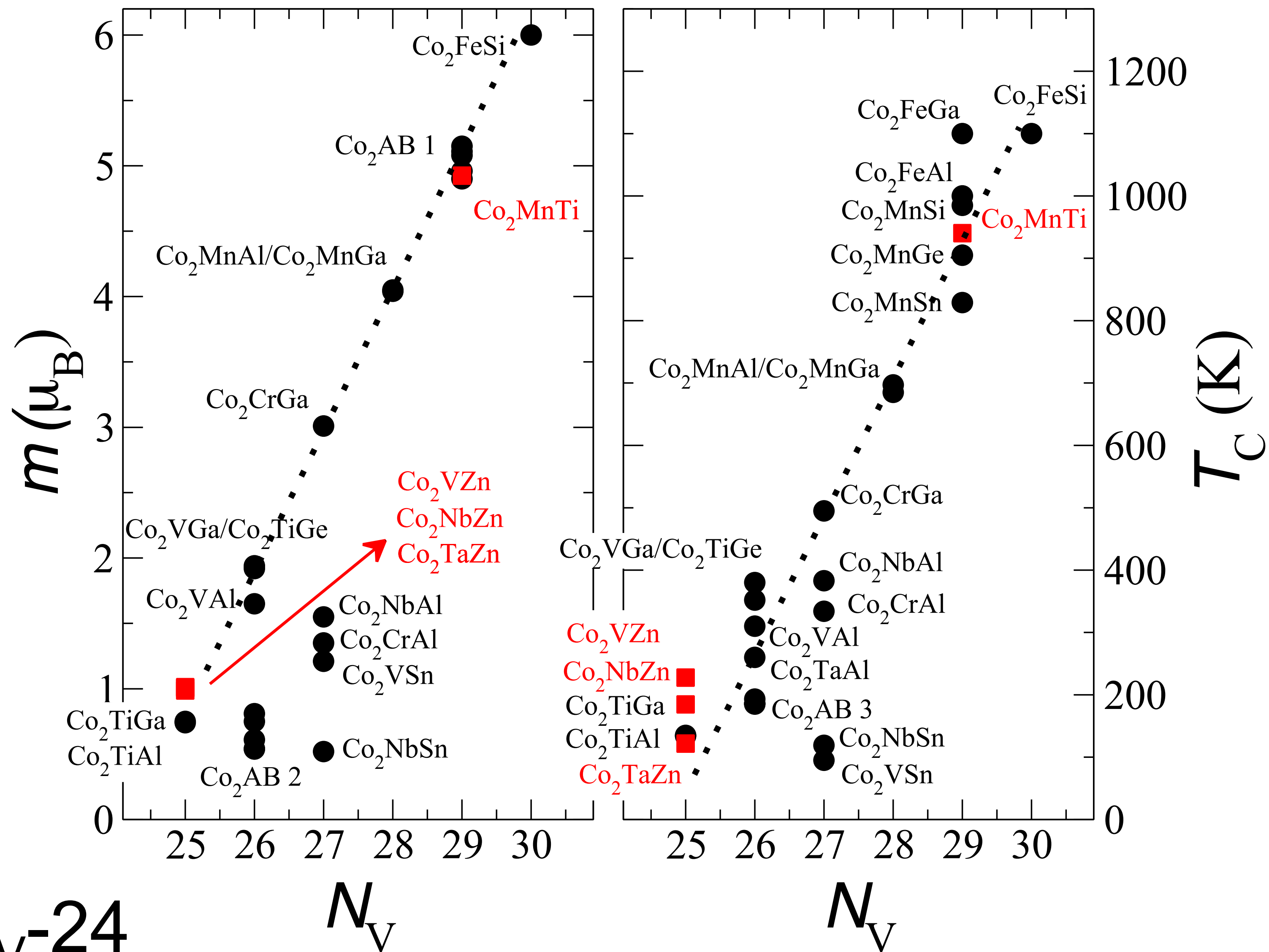
X_2MnY



Co_2YZ

Co_2YZ

Slater-Pauling



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

Co_2YZ

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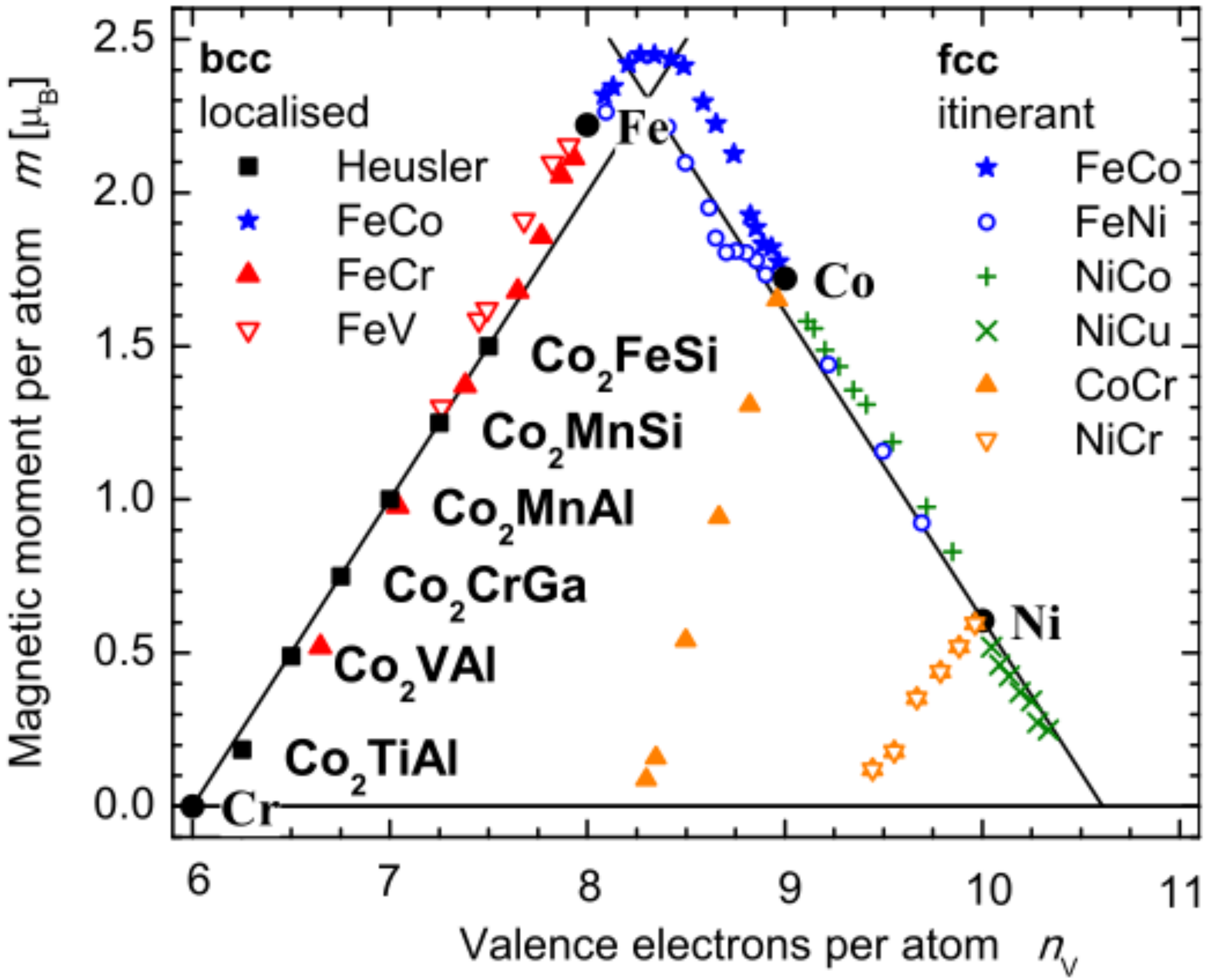
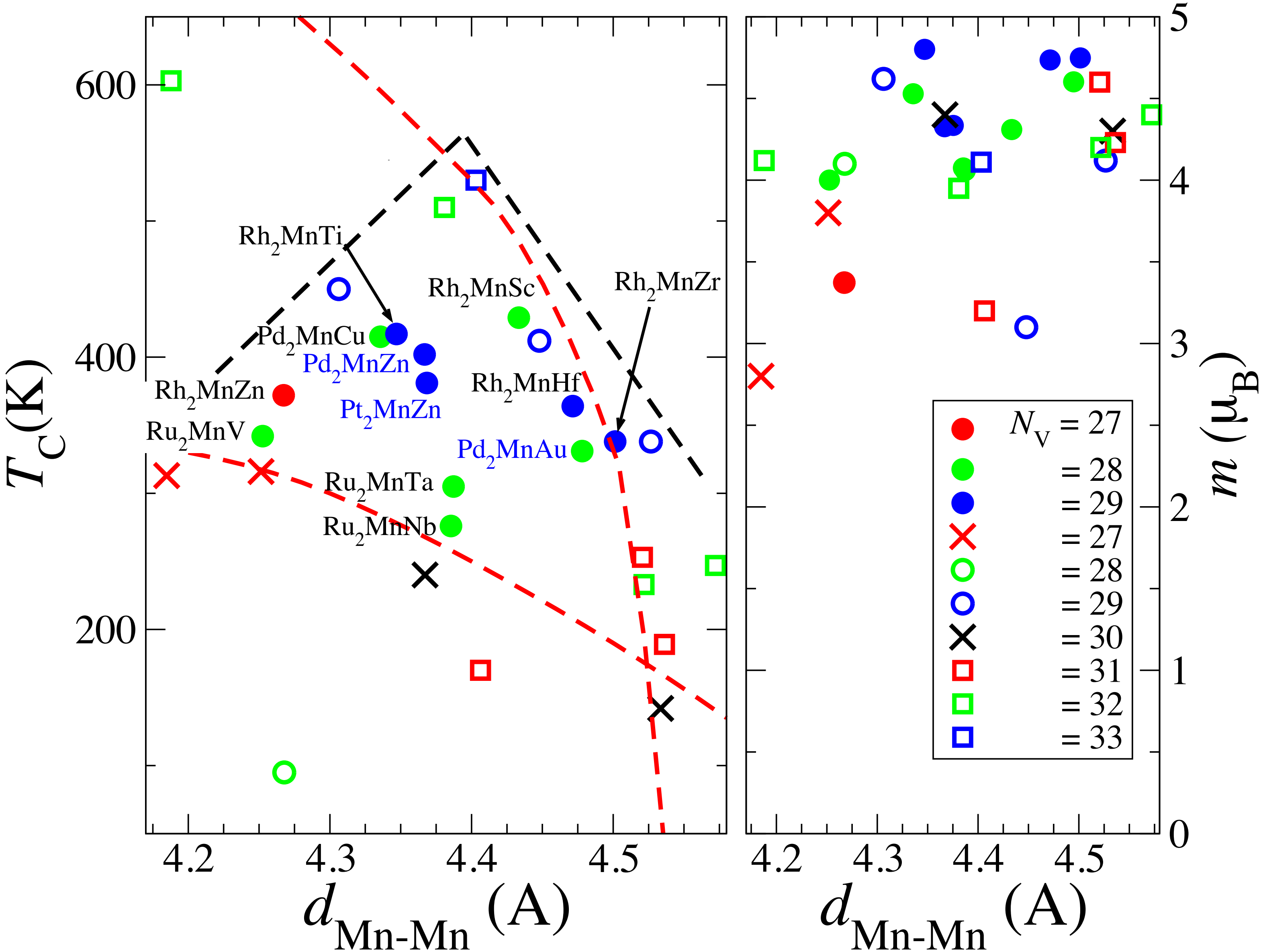


bcc
localised
Heusler
FeCo
FeCr
FeV
fcc
itinerant
FeCo
FeNi
NiCo
NiCu
CoCr
NiCr
Fe
Co
Ni
Cr
Co2FeSi
Co2MnSi
Co2MnAl
Co2CrGa
Co2VAl
Co2TiAl
Magnetic moment per atom m [μB]
Valence electrons per atom nV
0.0
0.5
1.0
1.5
2.0
2.5
6
7
8
9
10
11

X_2MnZ

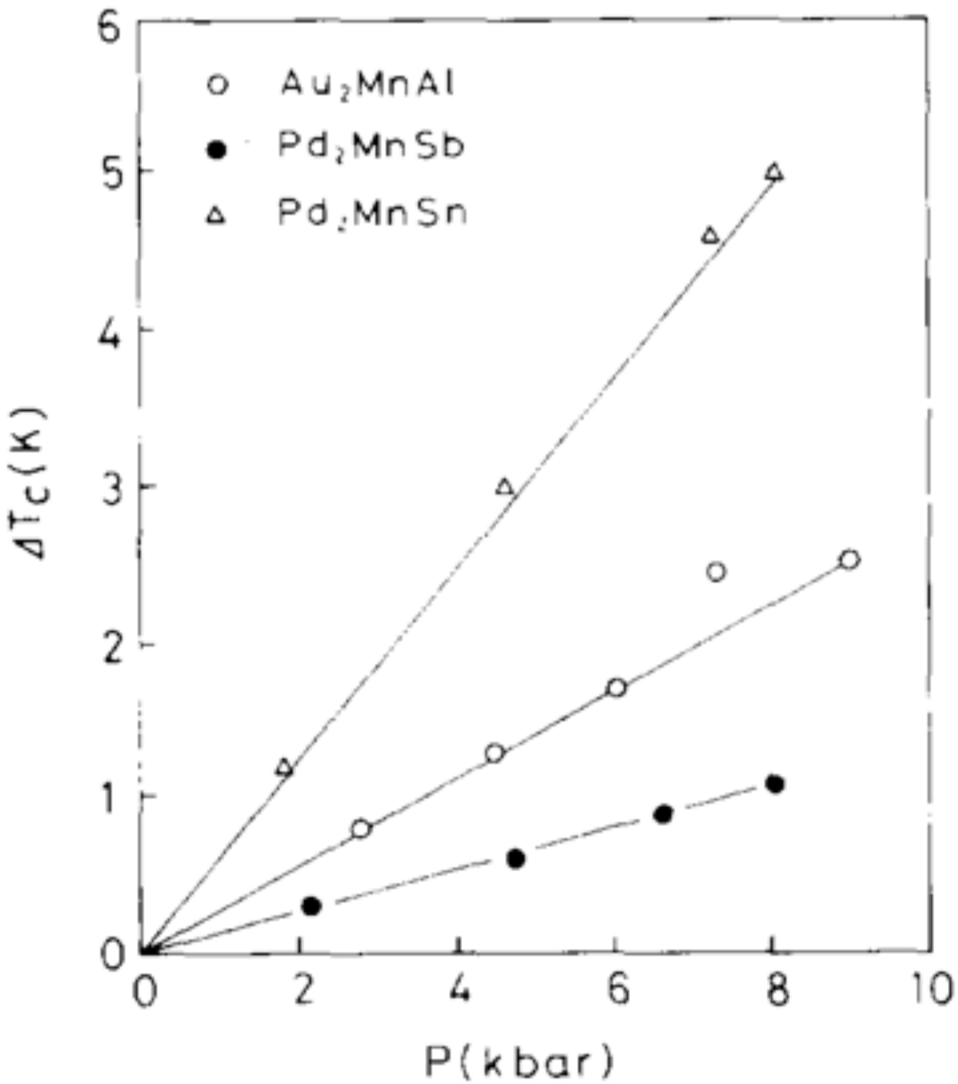
X_2MnZ



Castelliz-Kanomata curve

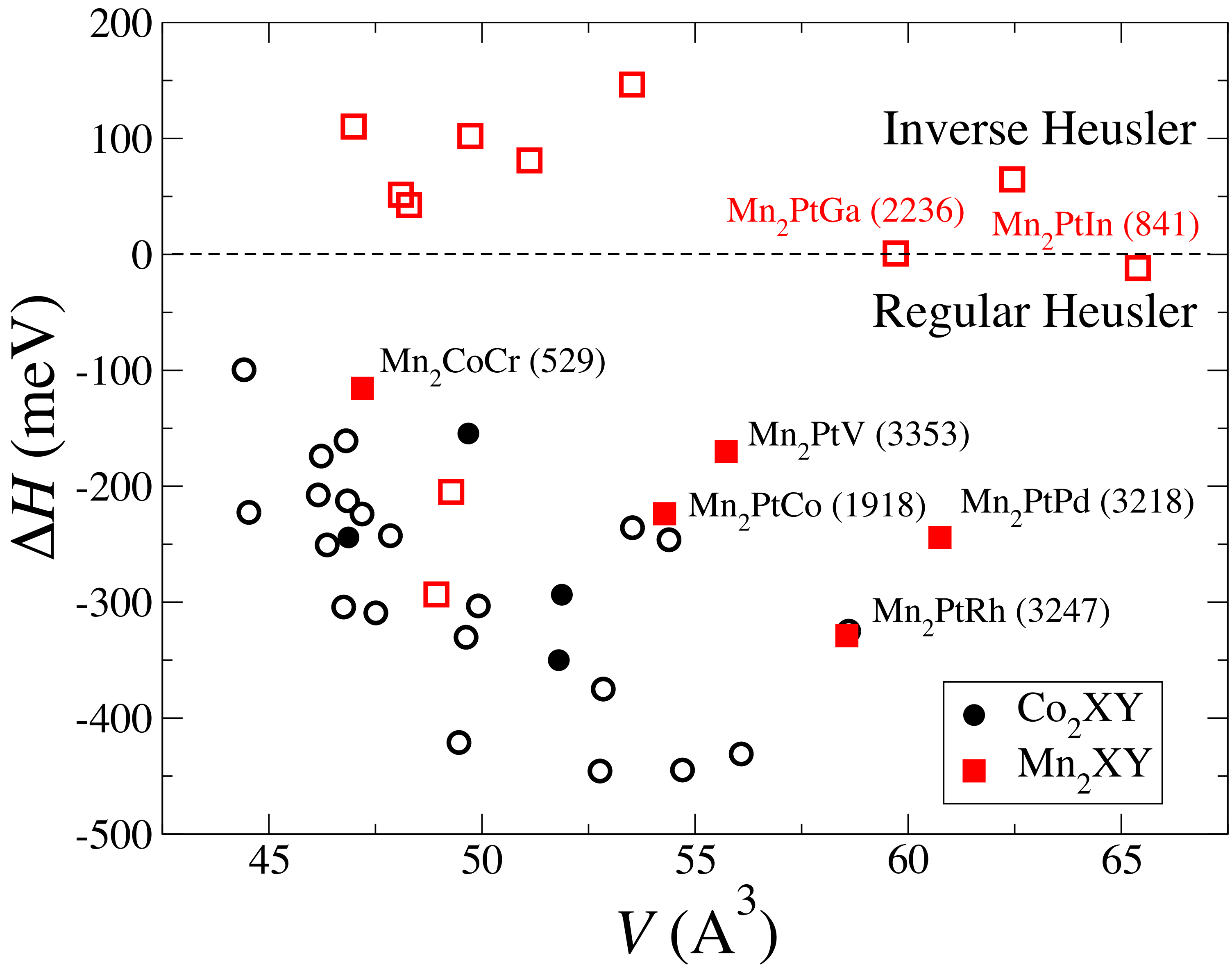
X_2MnZ

X_2MnZ



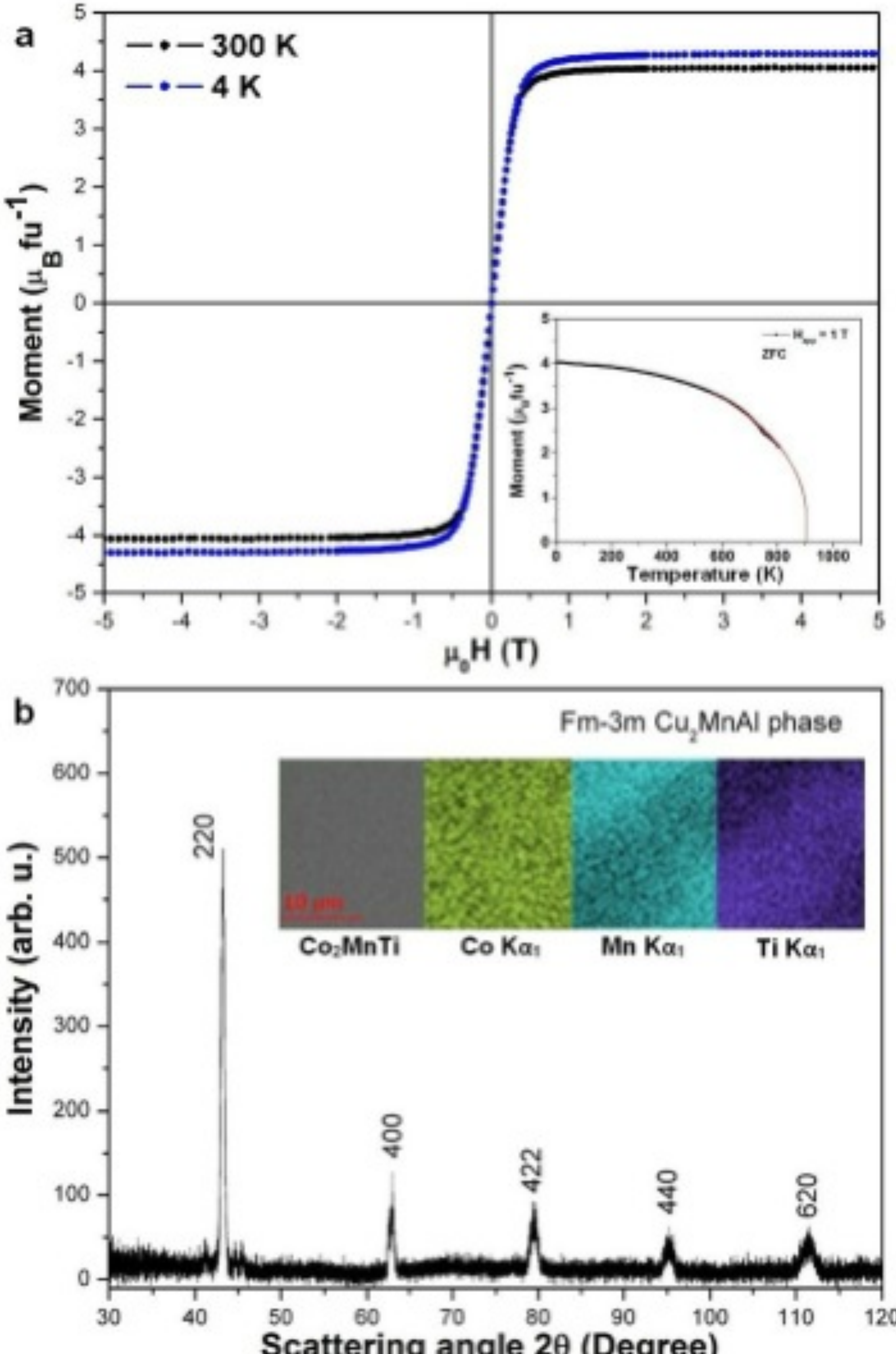
K. Shirakawa et al., J. Magn. Magn. Mater. **70**, 421 (1987)

Mn_2YZ



200
100
0
-100
-200
-300
-400
-500
45
50
55
60
65
ΔH (meV)
V (A3)
Inverse Heusler
Regular Heusler
Mn2PtGa (2236)
Mn2PtIn (841)
Mn2CoCr (529)
Mn2PtV (3353)
Mn2PtCo (1918)
Mn2PtPd (3218)
Mn2PtRh (3247)
Co2XY
Mn2XY

OK, but does all that work?



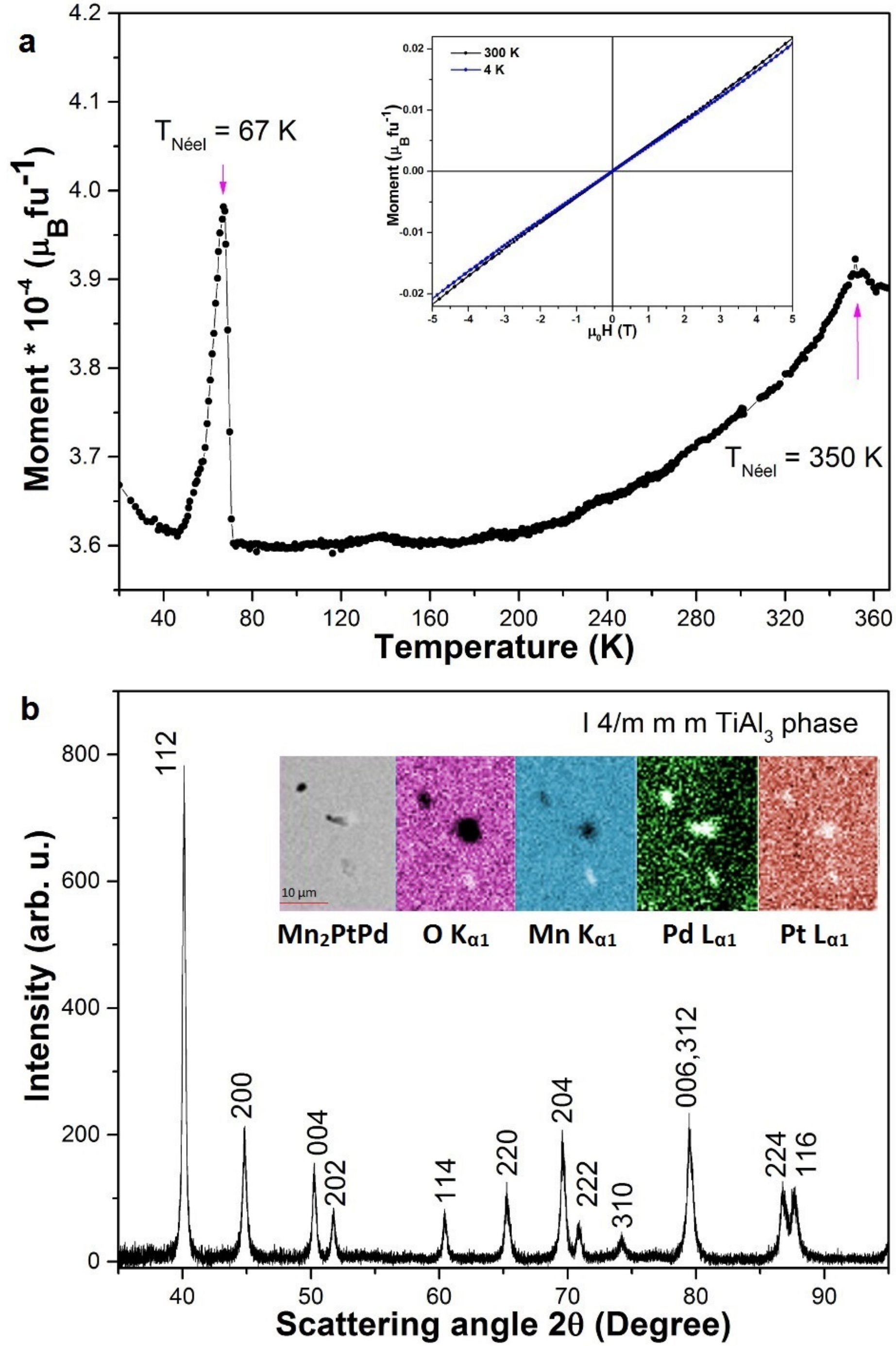
Co_2MnTi

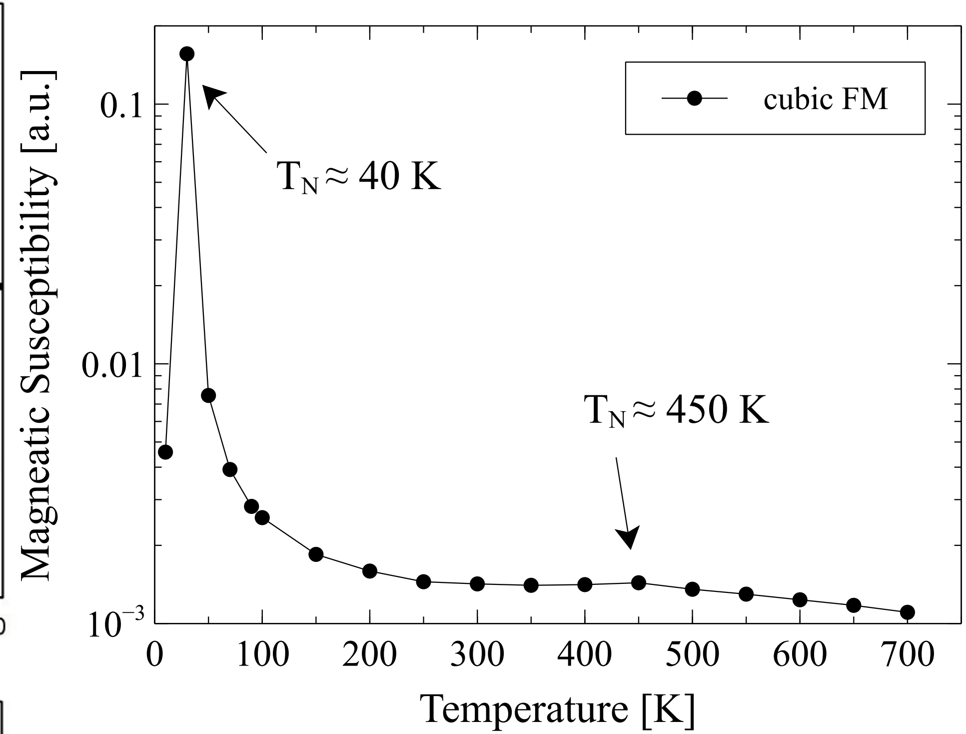
$T_C^{measured} = 940K$

$T_C^{predicted} = 938K$

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 ….

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Did we find one ?

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SEVENTH FRAMEWORK PROGRAMME
KAUST King Abdullah University of Science and Technology
TCHPC
ICHEC Irish Centre for High-End Computing

AICQT, Maynooth June 2016

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

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