Quantitative Predictions by Electronic Structure Theory

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"Our density functional calculations predict iron to be magnetic, in excellent agreement with experimental data published by Gilbert in the year 1600."

This kind of sometimes published phrase is a ridiculous misuse of "prediction".

A quantitative prediction:

- Take the chemical compound A;
- prepare it in the structure B;
- apply the external condition C;
- measure the quantity D;
- you will find the result E.

is meant to **initiate** the related experiment.

I will show four confirmed predictions and two more, yet unconfirmed.

Cooper Minima in the Photoemission Spectra of Solids

Prediction: late transition metals (Pd, Ag) in a lattice will show additional minima in the photo-emission intensity.

Reason: interference of lattice structure and outgoing wave.

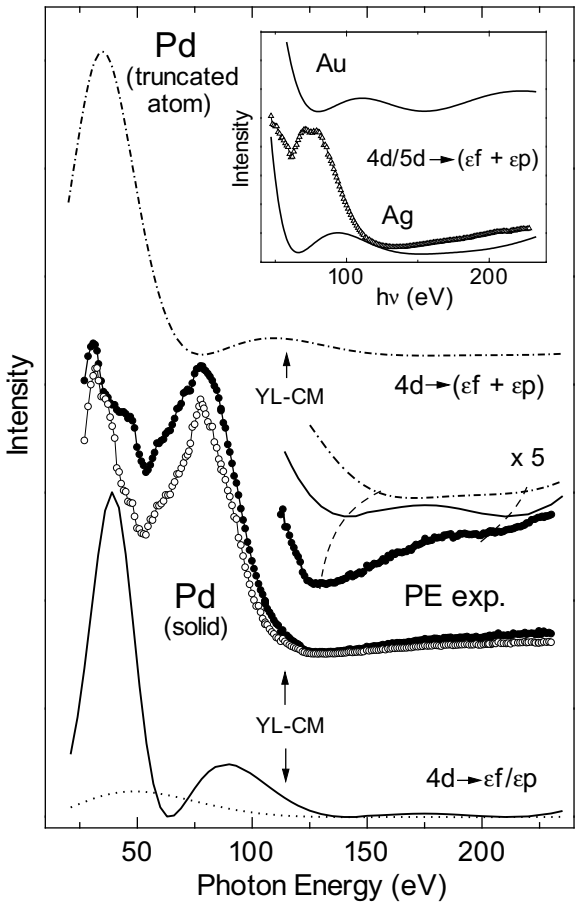
$$w \sim \int (rR_{nl})\, r\, (rR_{\varepsilon,l\pm1})\, dr$$

Confirmation by PE:

PRL **85**, 4184 (2000).

Collaboration: S.L. Molodtsov, S.V. Halilov, V.D.P. Servedio, W. Schneider, S. Danzenbächer, J.J. Hinarejos, C. Laubschat

Fig. 1



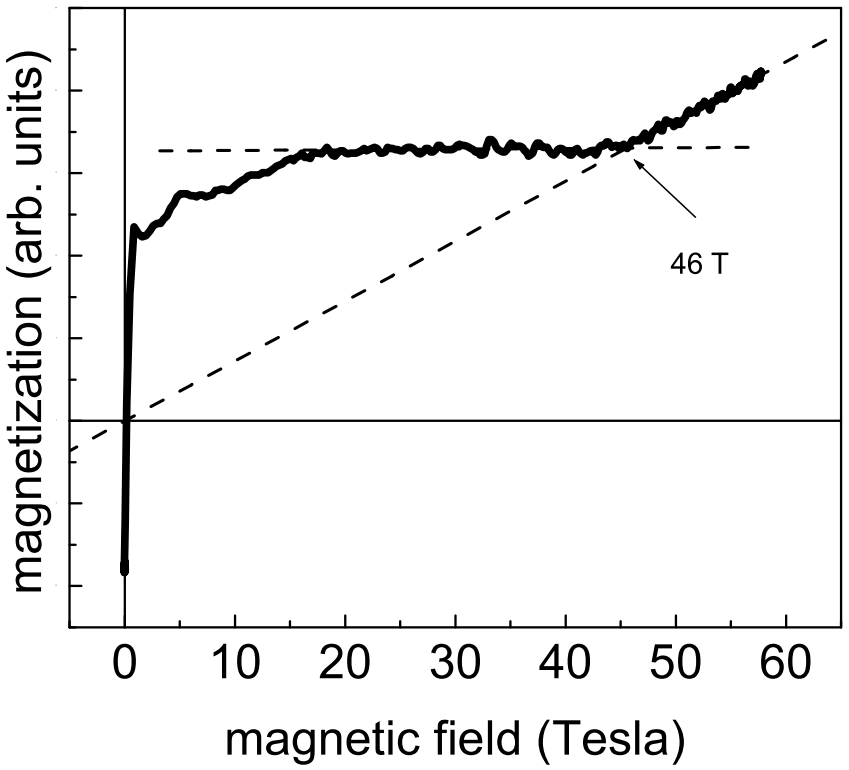
Spin reorientation in high magnetic field in $GdCo_5$

Prediction: The onset of ferrimagnetic-to-ferromagnetic spin-reorientation in $GdCo_5$ will take place close to an external field of 50 Tesla.

Reason: strength of magnetic sublattice coupling estimated from INS and from DFT.

Confirmation by high-field experiments: PRB **70**, 172412 (2004).

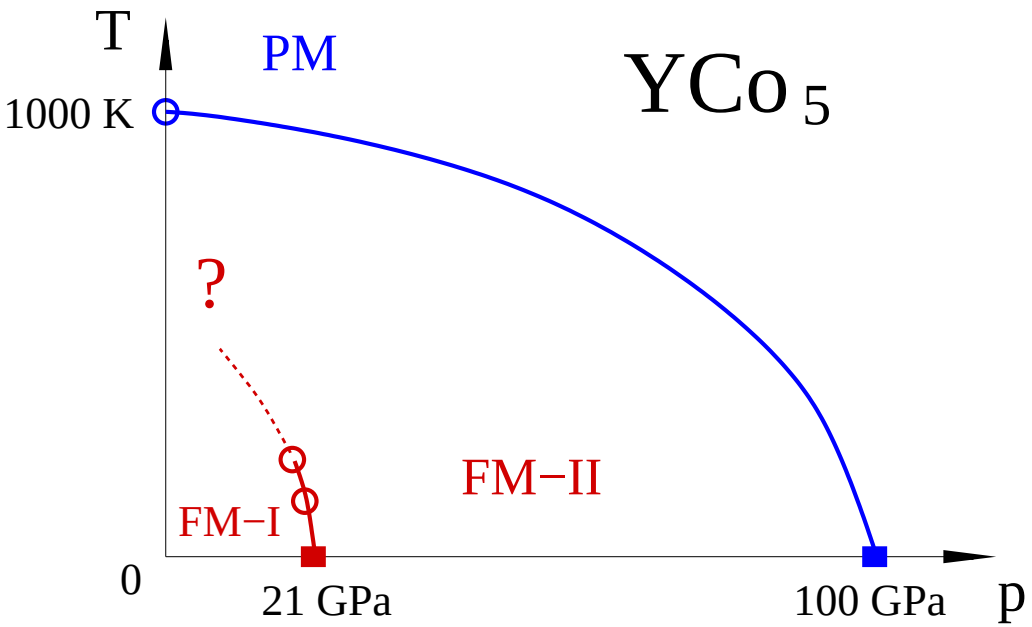
Collaboration: M.D. Kuz'min, Y. Skourski, D. Eckert, K.-H. Müller, K.P. Skokov, I.S. Tereshina.



Magneto-elastic lattice collapse in YCo_5

Prediction: YCo_5 will undergo an isomorphic volume collapse at a pressure between 10 and 25 GPa.

Reason: Lattice instability due to a van Hove singularity crossing the Femi level under pressure.



Confirmation by high-pressure diffraction: Nature Physics **2**, 469 (2006).

Collaboration: H. Rosner, D. Koudela, U. Schwarz, A. Handstein, M. Hanfland, I. Opahle, K. Koepernik, M. Kuz'min, K.-H. Müller, J. Mydosh.

$LaFe_{12-x}Si_x$:

The ideal material for magnetic cooling?

Magnetic cooling:

- the cooling power is proportional to the magnetization change ΔM and to the operation frequency ν,

$$P \sim \Delta M \, \nu$$

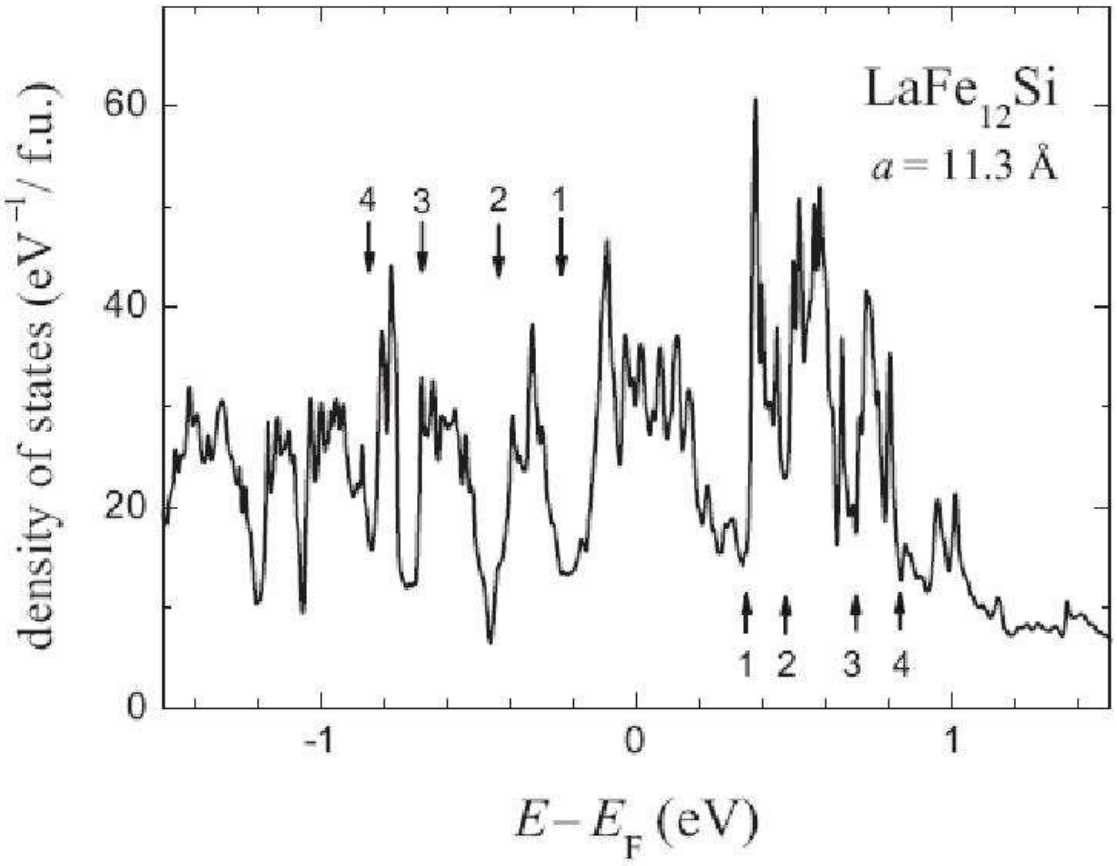
- up to now, all demontrators work with Gd

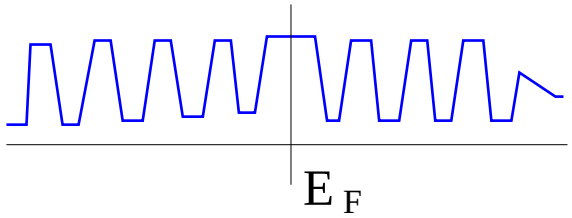
$LaFe_{12-x}Si_x$:

- "almost pure" cubic (*fcc*-like) iron, $x \approx 1$
- almost no hysteresis, if prepared by melt-spinning
- magnetocaloric effect can be larger than in Gd
- operation temperature can be tuned (change x, add Co, add hydrogen)

$LaFe_{12-x}Si_x$:

The reason for its large ΔM and its low hysteresis

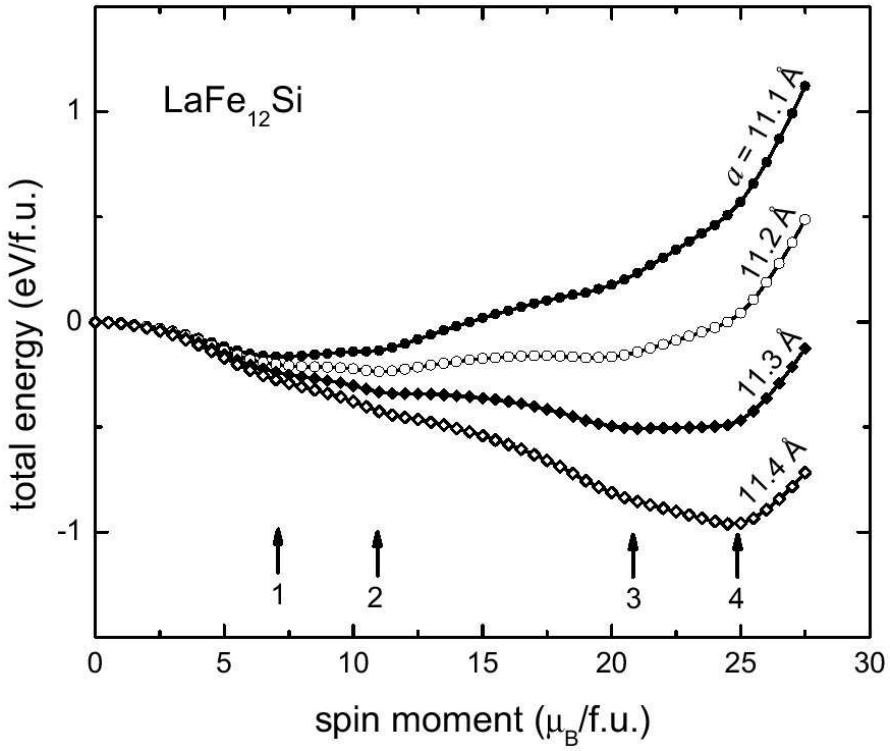


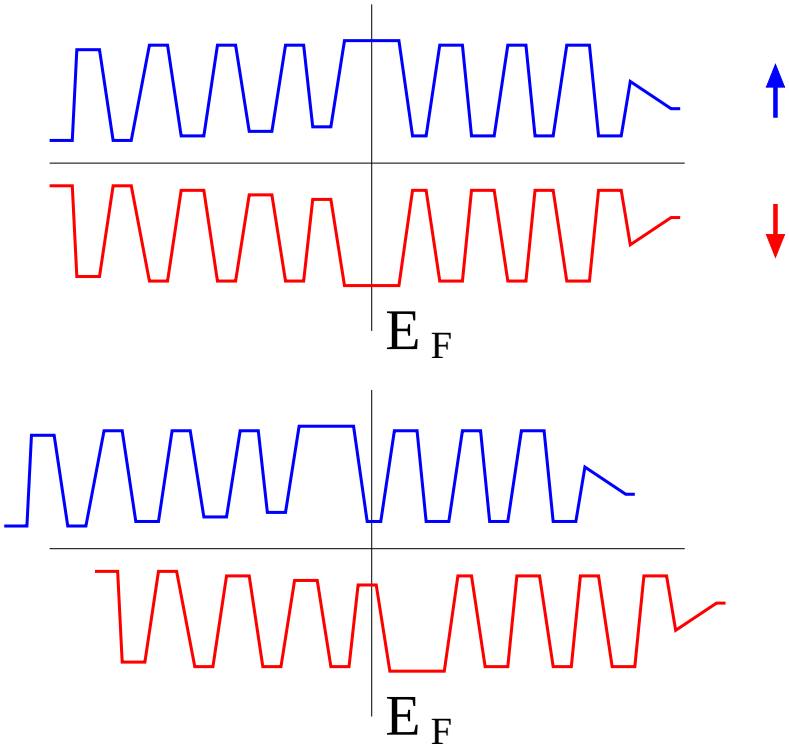


Model of the DOS

$LaFe_{12-x}Si_x$:

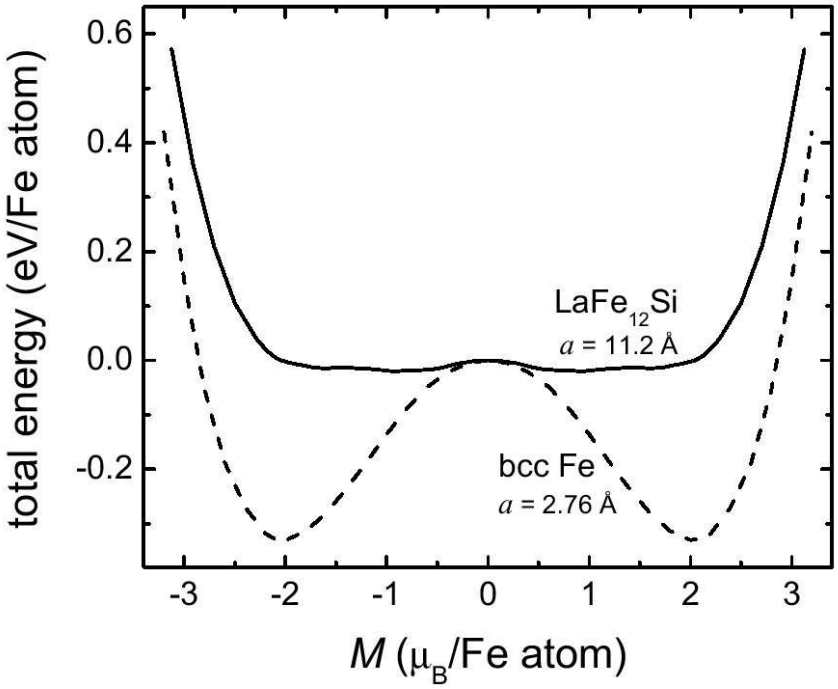
The reason for its large ΔM and its low hysteresis

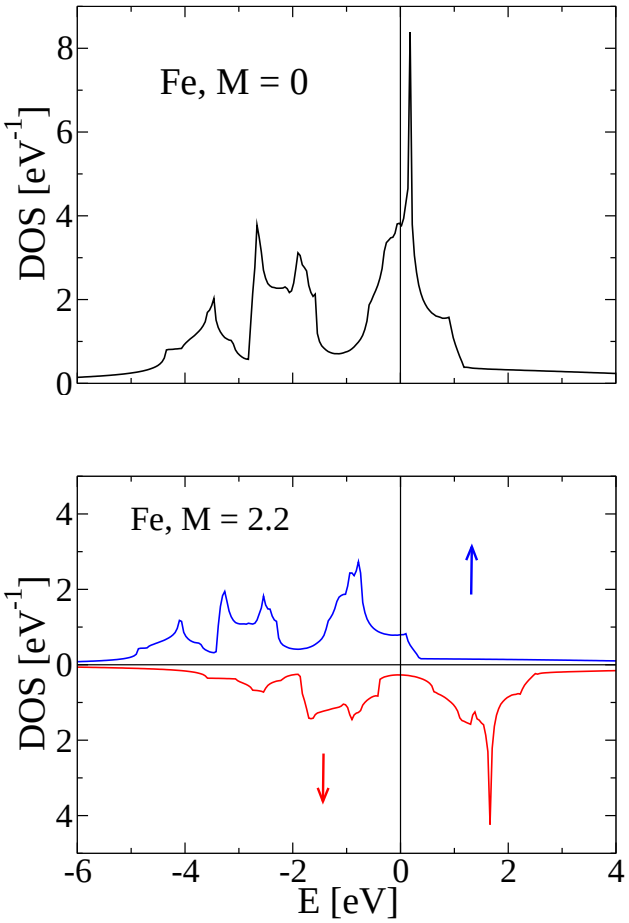




Generalized Stoner criterion: $4\ I\ (1/D(E_{\rm F})^{\uparrow} + (1/D(E_{\rm F})^{\downarrow})^{-1}\ >\ 1$

$LaFe_{12-x}Si_x$: Comparison with bcc iron





very flat $E(M)$:

small external fields produce large ΔM;

small tunnel barriers $\longrightarrow$ small hysteresis

Multiple Metamagnetic Transitions in La(Fe;Si)$_{13}$H$_x$

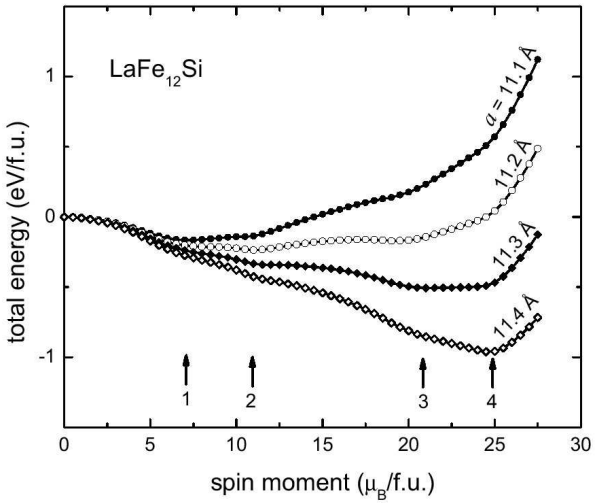
Prediction: La(Fe,Si)$_{13}$ will show a series of up to three metamagnetic transitions in a moderate field.

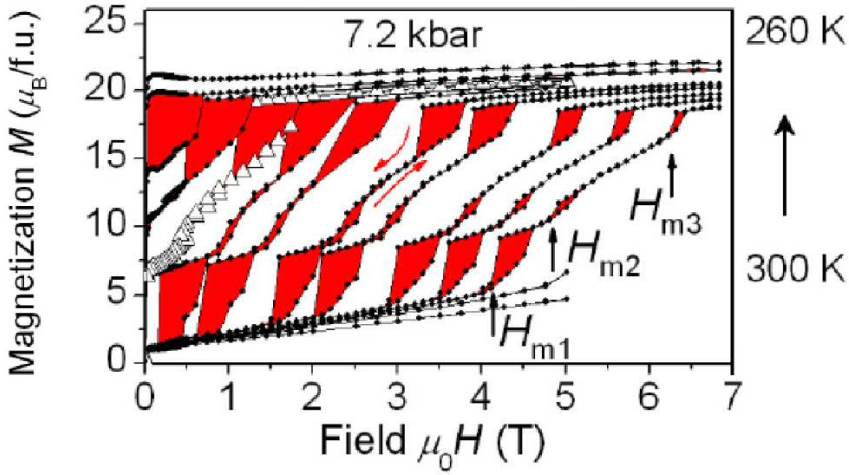
Reason: The peculiar density of states produces four almost degenerate low-energy states with different magnetic moments.

PRB **76**, 092401 (2007), M.D. Kuz'min, M. Richter

Confirmation by magnetization measurements:

PRL **101**, 177203 (2008), J. Lyubina, K. Nenkov, L. Schultz, O. Gutfleisch.

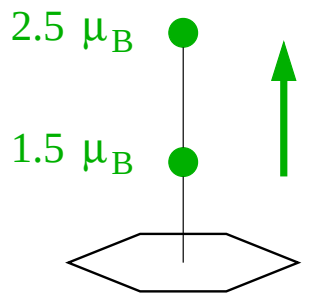




Two more, yet unconfirmed predictions

(already presented at this workshop)

Ruijuan Xiao, Daniel Fritsch, Michael D. Kuz'min,
Klaus Koepernik, Helmut Eschrig, Manuel Richter,
Knut Vietze, Gotthard Seifert
PRL **103**, 187201 (2009)



Stephan Schönecker *et al.*, unpublished

magnetic *bct* uranium

DFT is predictive!

Make use of it!

(Motivate the experimentalists to work on YOUR ideas, not vice versa.)