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National Research Council

Spin fluctuations-corrected DFT for itinerant systems and Fe-based superconductors

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(Experiment)

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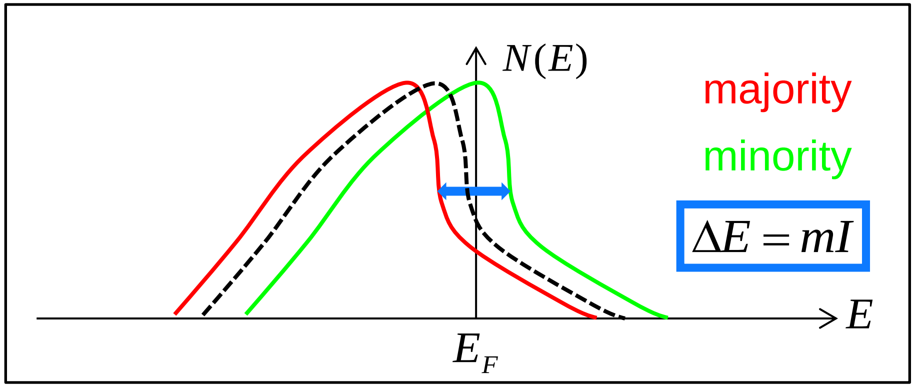
Density Functional Theory for Itinerant Magnets:

Itinerant magnetism: the system is magnetic and metallic (*e.g.* Ni_3Al, Fe pnictides)

Stoner model for ferromagnetism: simple model for describing itinerant systems.
Under the effect of an **external potential** $\mu_B H$ spin up and spin down bands split by ΔE and a finite **magnetic moment** m persists even at zero applied magnetic field.



I is called **Stoner parameter** and governs the magnetic interaction

Problem: DFT implementations (LSDA, magnetic GGA) **overestimate** $\boldsymbol{m}$ in near critical itinerant systems due to the effect of non local spin fluctuations (SF) which tend to destroy the magnetic order over distance ξ leading to an effective reduction of the **Stoner parameter** I.

$$\tilde{I} = I - const \cdot \xi^2$$

One needs to account for this effect within DFT

OUTLINE

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- **Reduced Stoner Theory (RST):** a simple method for correcting the magnetic properties calculated in standard DFT approximations based on the SCR Moriya theory.

- **Ferro-magnetic-paramagnetic transition in Ni_3Al under pressure:** application to a prototypical example of itinerant ferromagnet.

- **Explaining the puzzling behavior of the temperature dependence of local moment in rare earth-doped and P-doped Ca122 family of Fe pnictides.**

- **Conclusion and outlook**

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The Reduced Stoner Theory (RST)

Idea: Introduce a **simple method to simulate** the effect of **spin fluctuations** (beyond LSDA) on the magnetic properties of **near critical itinerant systems**.

$$\tilde{I} = sI = I - const \cdot \xi^2$$

- In practice: **scale the Stoner kernel in V_{xc}** by a constant factor s. **LDA↔LSDA**
- s is a measure of the average amplitude of spin fluctuations ξ.

Link to other approaches

- *s* can be calculated by using the fluctuation dissipation theorem [$\xi \leftrightarrow \chi(\boldsymbol{q},\omega)$].
  T. Moriya (1985); G. G. Lonzarich, L. Taillefer JPC (1985).
- *s* can be estimated through ξ from the band parameters (Fermi velocity, DOS).
  A. Aguayo et al. PRL (2004).

Test case: Ni_3Al archetypal weak itinerant FM.

L. Ortenzi, *I.I. Mazin, P. Blaha, and Lilia Boeri PRB* **(2012).**

RST APPLIED TO Ni_3Al
(a prototypical example)

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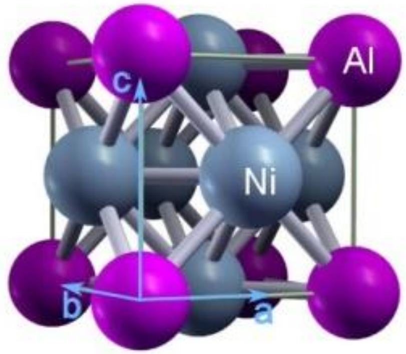

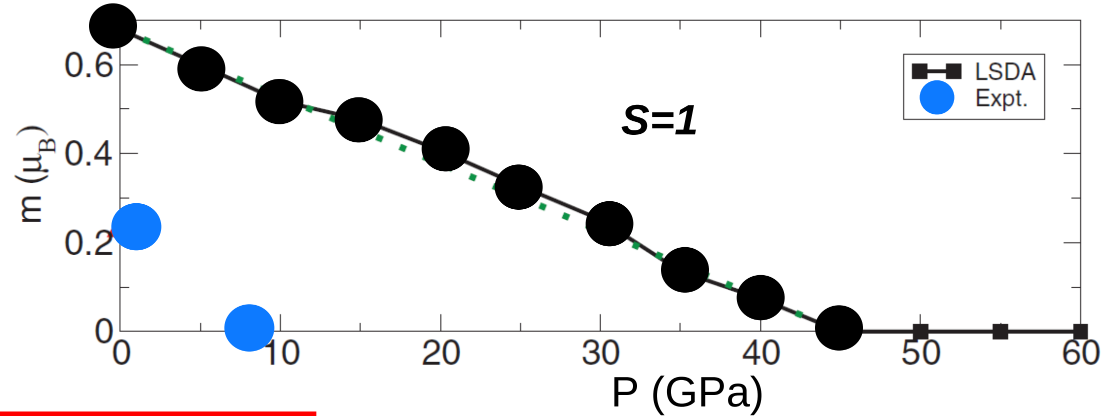

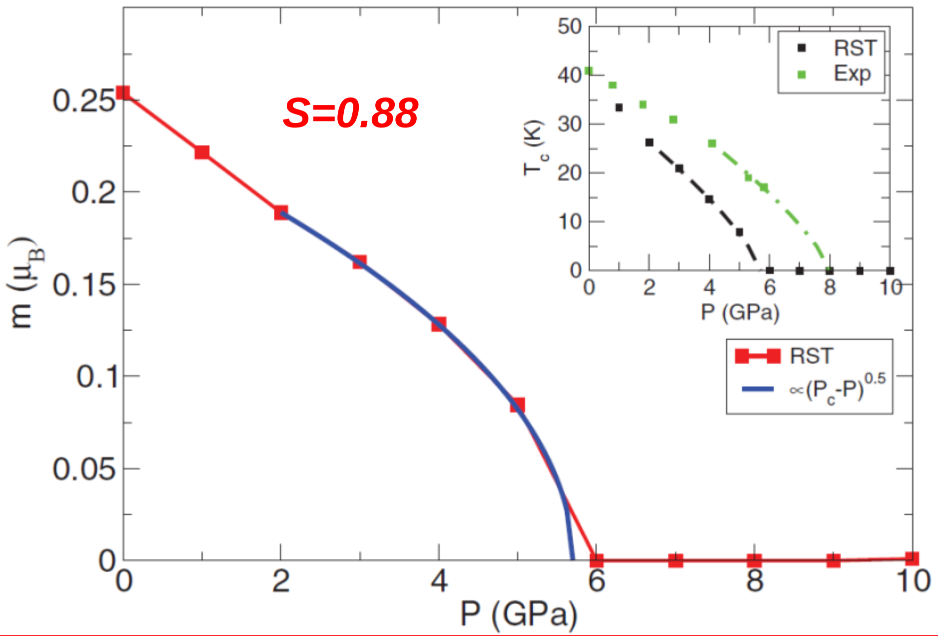

Experiment:

P. G. Niklowitz et al. PRB (2005).

Standard LSDA calculations: overestimate both P_c and *m(0)*

RST calculations:

With one parameter s=0.88 for all pressure we manage reproduce the m(P) curve and the critical exponent ¾ of T_c

L.Ortenzi et al. PRB (2012).

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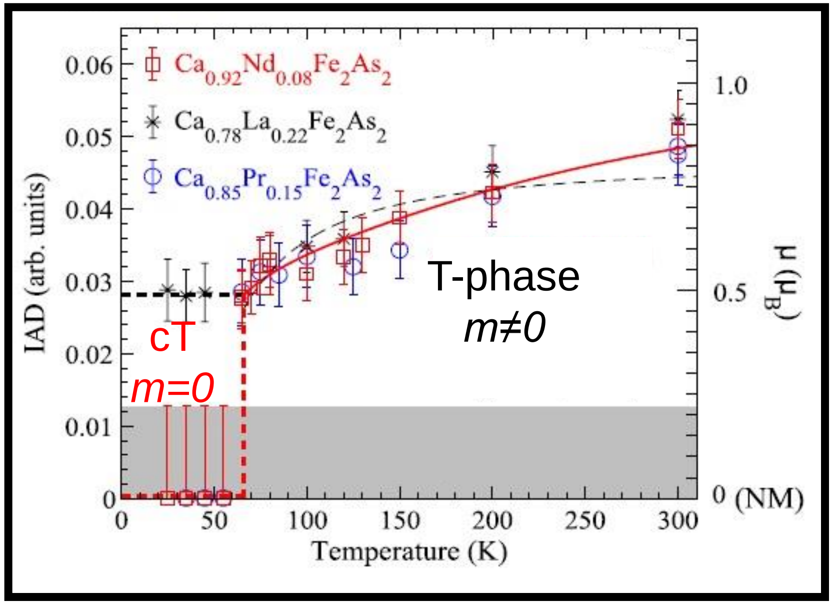
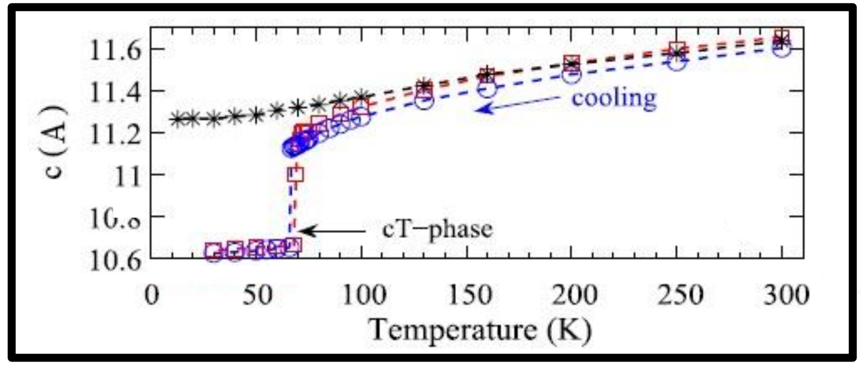
WHAT ABOUT PNICTIDES?

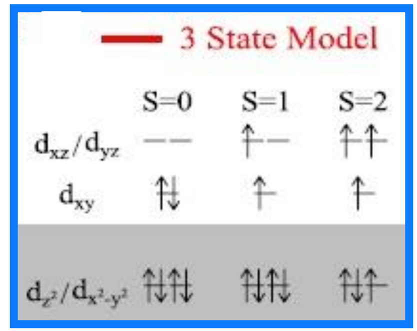
Fe local moment increase with temperature in rare earth-doped $CaFe_2As_2$



Large thermal expansion coefficient of the *c*-axis lattice parameter



Possible explanation: "Spin state transition in Fe-pnictides" as in LaCoO3**?**



H. Gretarsson et al. PRL (2013).

HOWEVER:

- The experimentally measured bandwidth are large
- The system is a metal
- Both crystal field and Hund's rule coupling J are small compared to the bandwidth.

CaF_2As_2: ITINERANT vs LOCAL MODEL

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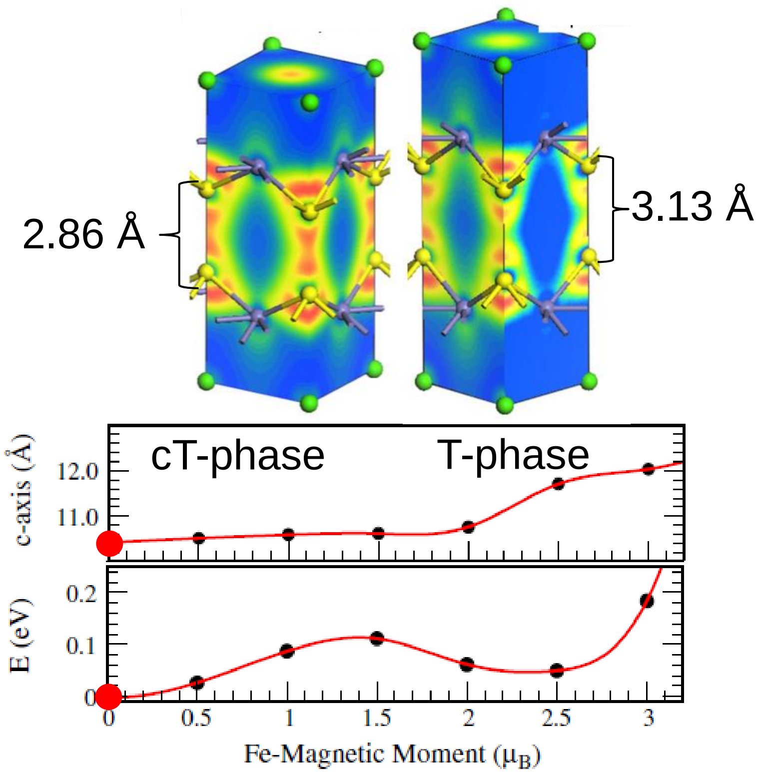
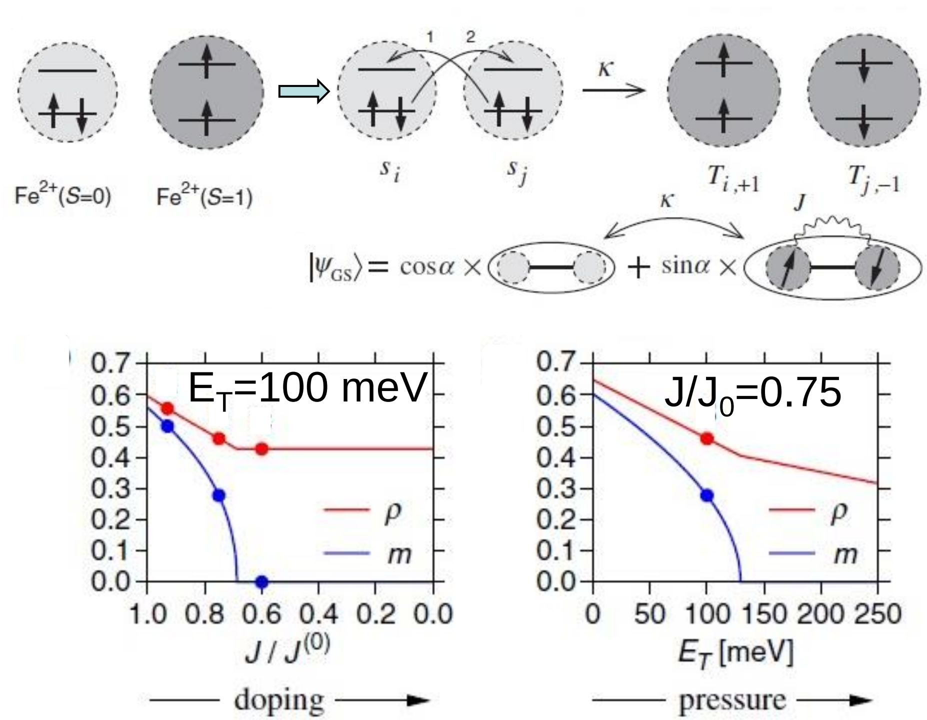
ITINERANT



T. Yildirim PRL (2009).

Fe magnetic moment is tuned by As-As interaction and in the cT phase *m=0* but local moment are too large

LOCAL



J. Chaloupka and G. Khaliullin PRL (2013).

- No localized bands are present
- Fine tuning is needed: cT and T phase need different parameters.

NEW EXPERIMETS ON $CaFe(As_xP_{1-x})_2$

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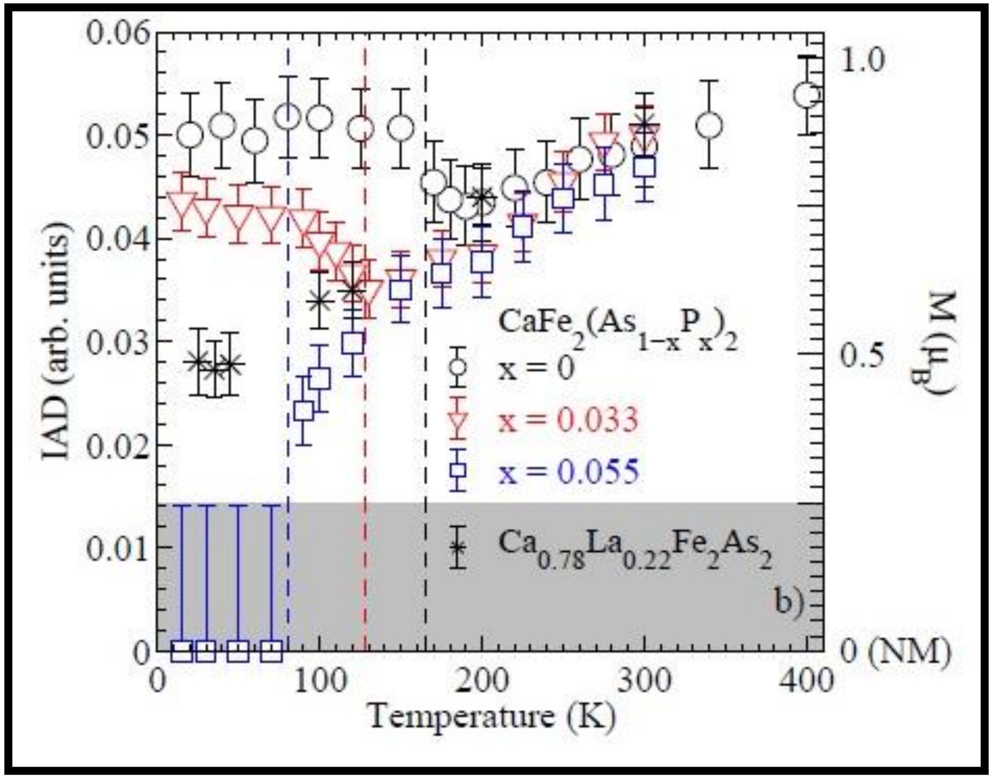

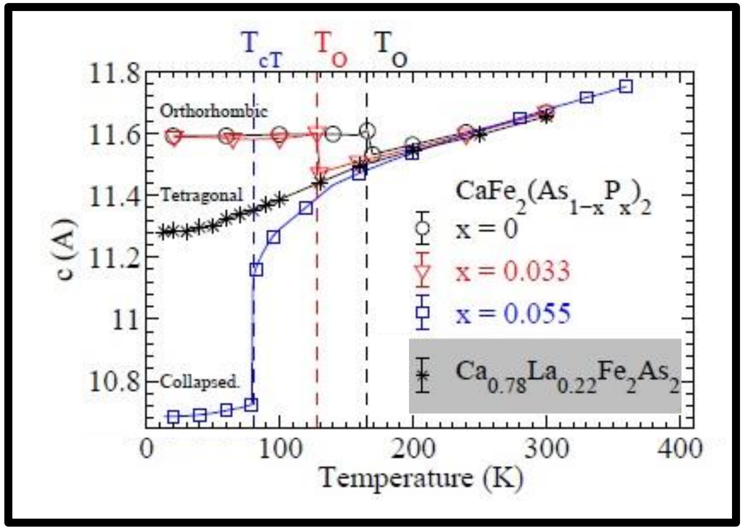

- Large c-axis thermal expansion coefficient
- Strong dependence of m on doping x and temperature T
- The moment is strongly coupled to the lattice.

L.Ortenzi et al. arXiv:1408.4058 (2014).

One needs RST calculations in order to capture the connection between the structural and magnetic properties in this system .

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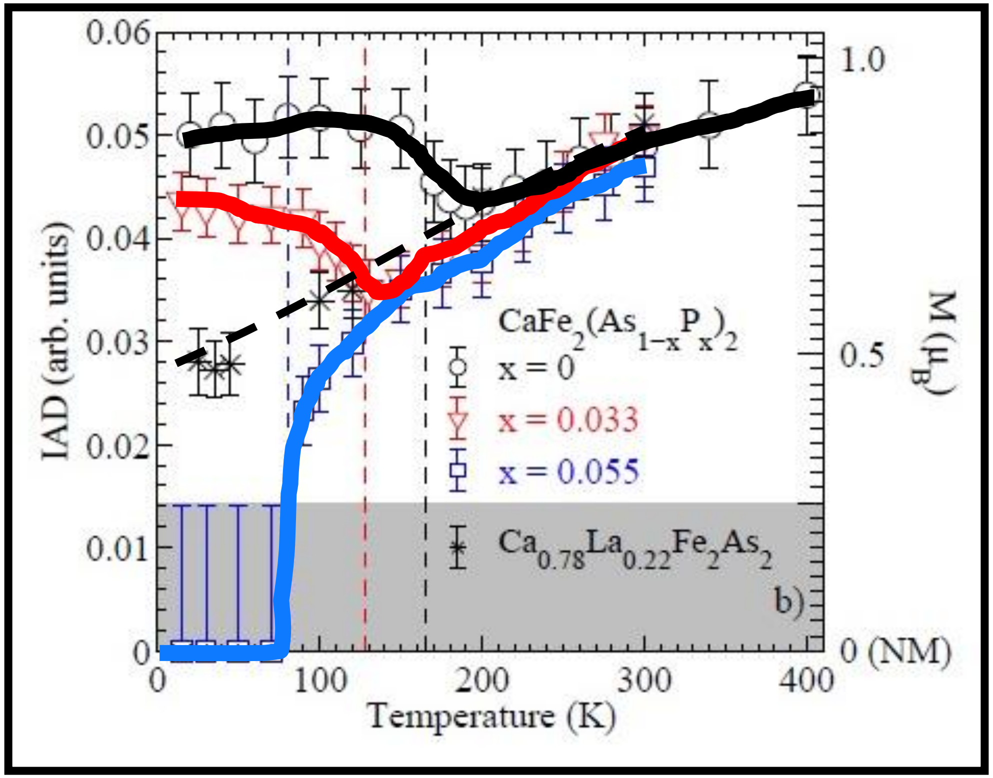

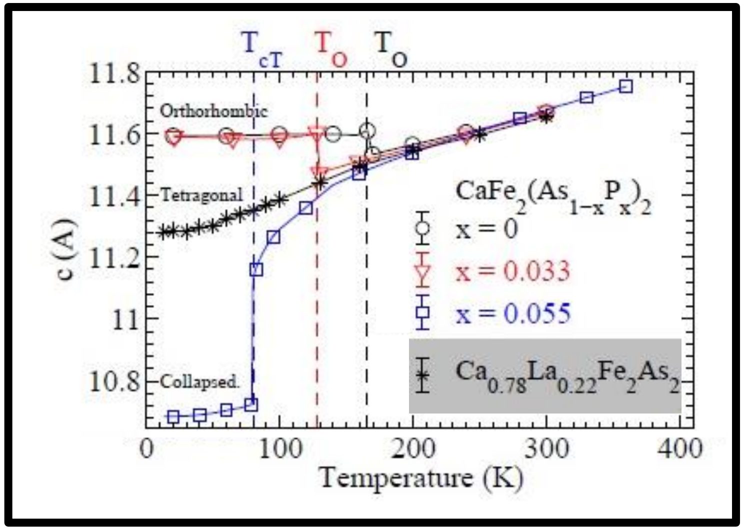

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OUR (NEW) RESULTS!

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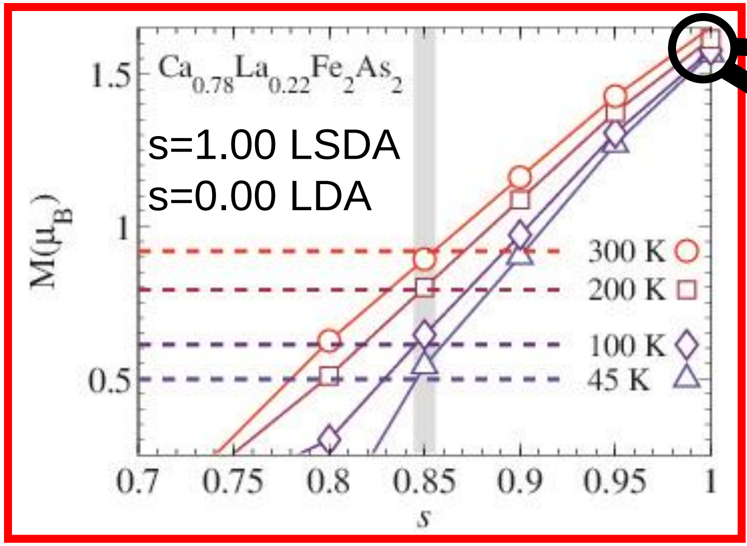
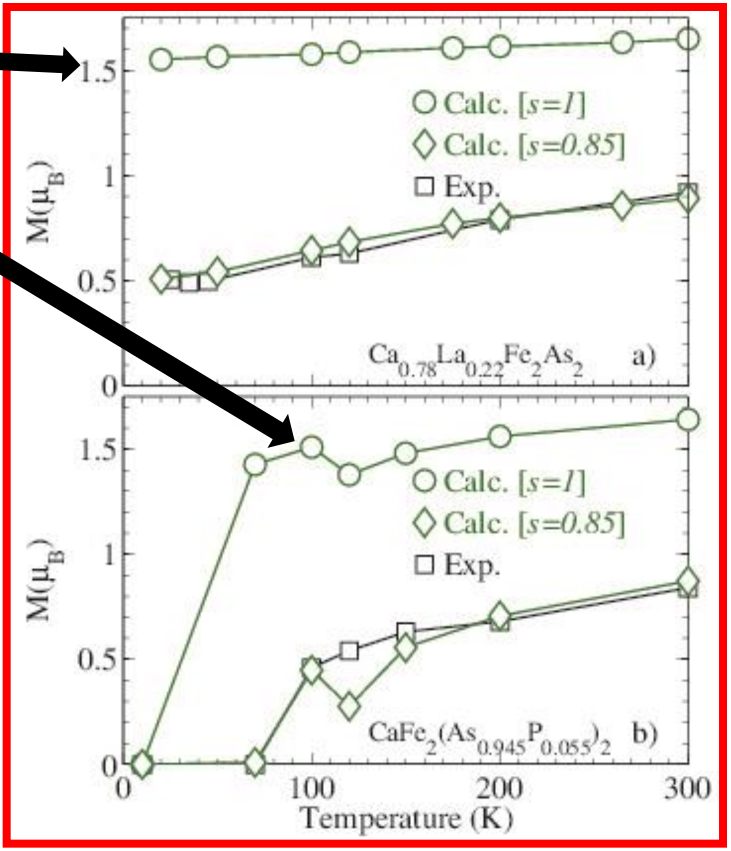
- We simulate the temperature by changing the structure.
- Magnetism is corrected by choosing the "correct" value of *s.*





- LSDA calculations overestimate the magnetic moment
- LSDA moment does not change with T unless cT phase is reached

RST manages to reproduce M(T) both in La-doped and P-doped compound with only one value of s

L.Ortenzi et al. arXiv:1408.4058 (2014).

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CONCLUSIONS

- New simple method (RST) for treating non local spin fluctuations effectively in DFT
- The method allows to describe *ab-initio* the pressure phase diagram of Ni_3Al
- New experiment on $CaFe_2(As_{1-x}P_x)_2$ showing general M(T) behavior
- RST calculations perfectly reproduce M(T) both for the La-doped and P-doped compounds using only one parameter
- Local moment are large but soft and strongly coupled to the lattice
- No thermal excitation BUT thermal expansion.

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THANK YOU!!!!!