Electronic phase diagrams of 1111 oxy-pnictides investigated by means of μ^+ spin spectroscopy

Giacomo Prando Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, Germany and Alexander von Humboldt Stiftung Fellowship for Postdoctoral Researchers



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S. Sanna, P. Carretta

CNISM (UdR Pavia) – Phys. Dept., University of Pavia, Italy R. De Renzi

Phys. Dept., University of Parma, Italy

B. Büchner

Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, Germany

Sample preparation

S. Wurmehl's group Leibniz-IFW Dresden, Germany A. Palenzona's group University of Genova, Italy J. Karpinski's group ETH Zurich, Switzerland V. P. S. Awana's group NPL, New Delhi, India

Review and summarizing discussion of results

Carretta, De Renzi, Prando, Sanna, *arXiv*:1307.8283 (2013, to appear soon on Physica Scripta)

e⁻-doped ReFeAsO: Electronic Phase Diagram



(Sanna et al., PRB 80, 052503; Prando et al., PRB 87, 174519)

Electron doping: the O/F substitution



(Zhao et al., Nat. Mater. 7, 953 - Ce; Sanna et al., PRB 80, 052503 - Sm)



Crucial importance of the intermediate region

RAPID COMMUNICATIONS

PHYSICAL REVIEW B 81, 140501(R) (2010)

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Unconventional pairing in the iron arsenide superconductors

Rafael M. Fernandes,* Daniel K. Pratt, Wei Tian, Jerel Zarestky, Andreas Kreyssig, Shibabrata Nandi, Min Gyu Kim, Alex Thaler, Ni Ni, Paul C. Canfield, Robert J. McQueeney, Jörg Schmalian, and Alan I. Goldman Ames Laboratory, U.S. DOE, and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA (Received 15 February 2010; revised manuscript received 13 March 2010; published 2 April 2010)

We use magnetic long-range order as a tool to probe the Cooper-pair wave function in the iron arsenide superconductors. We show theoretically that antiferromagnetism and superconductivity can coexist in these materials only if Cooper pairs form an unconventional, sign-changing state. The observation of coexistence in $Ba(Fe_{1-x}Co_x)_2As_2$ then demonstrates unconventional pairing in this material. The detailed agreement between theory and neutron-diffraction experiments, in particular, for the unusual behavior of the magnetic order below T_c , demonstrates the robustness of our conclusions. Our findings strongly suggest that superconductivity is unconventional in all members of the iron arsenide family.

A careful investigation of magnetism at the border between **M** and **SC** regions in the electronic phase diagram is required

Beyond macroscopic techniques of investigation



(Prando et al., PRB 87, 174519; Shang et al., PRB 87, 075148)

Microscopic local-probe techniques - NMR



(Lang et al., PRL 104, 097001; Laplace et al., PRB 80, 140501)

NMR: nuclei detect coexistence on nanoscopic or even atomic scale for the different ground states (both static and dynamic features)

<u>Drawbacks</u>

- Strong local fields from magnetic Re ions (Prando et al., PRB 81, 100508(R))
- No information on absolute values of V_m

μ^+ Spin Rotation, Relaxation, Resonance (μ^+ SR)







Spin-polarized beam of μ^+ implanted in sample ${\bf S}$

Once thermalized, Larmor precession around local field ${\bf B}_{\mu}$

Left: experimental setup for GPS spectrometer at Paul Scherrer Institute

μ^+ Spin Rotation, Relaxation, Resonance (μ^+ SR)



After $\langle \tau_{\mu} \rangle \simeq 2.19 \ \mu s$: muon decays as $\mu^{+} \longrightarrow e^{+} + \nu_{e} + \overline{\nu_{\mu}}$ Weak decay \Rightarrow Parity conservation is violated

Positrons from μ^+ decay \Rightarrow Experimental access to the time-dependent autocorrelation function G(t) for the μ^+ spin

$$G(t) = \frac{\langle \mathbf{s}(t) \cdot \mathbf{s}(0) \rangle}{s^2(0)} \equiv \frac{A(t)}{A_0} \qquad \text{where} \qquad A(t) = \frac{N_{\mathsf{B}}(t) - N_{\mathsf{F}}(t)}{N_{\mathsf{B}}(t) + N_{\mathsf{F}}(t)}$$

Single crystals: information about possible anisotropies of G(t)

μ^+ SR: simultaneous presence of different phases



(Prando, Ph. D. Thesis)

 μ^+ randomly and uniformly implanted into the sample % of μ^+ probing features of some electronic environment \updownarrow $V_{\rm m}$ of the sample associated to that environment Disentangle signals: combination of ZF and TF Intrinsic features: low-background spectrometers

μ^+ SR: the paramagnetic phase (SC in ZF!)



No B_{μ} of electronic origin: spin polarization ideally preserved in conditions of zero external field (ZF)

Real case: weak nuclear magnetism leads to a slow depolarization

Weak **H**_{ext} transverse to initial direction of spins (weak-TF): coherent precession damped by nuclei

μ^+ SR: the magnetic phase (powders)



Long-range ordered phase leads to well-defined B_{μ} of electronic origin: 2/3 of spins precess ($\omega = \gamma_{\mu}B_{\mu}, \ \gamma_{\mu} = 2\pi \times 135.54 \text{ MHz/T}$)

Weak nuclear magnetism leads to a slow depolarization

Weak-TF: no effect as long as $H_{ext} \ll B_{\mu}$. ZF and weak-TF are equivalent in strongly-magnetic phases

μ^+ SR: the magnetic phase. Disorder



Distribution of local magnetic fields: damping of oscillations

- $\Delta B_{\mu} \ll B_{\mu}$: (almost) long-ranged order
- $\Delta B_{\mu} \sim B_{\mu}$: disorder, short-ranged order

 μ^+ SR highly sensitive to $V_{\rm m}$ in both the cases

Two sites for muons (DFT - electrostatic potential and zero-point energy):

- Inside FeAs layers (dominant signal)
- Close to Re (clear only for La)

(De Renzi et al., SUST 25, 084009)







Long-range order: coherent precession, $\omega = \gamma_{\mu}B_{\mu}$ ($\gamma_{\mu} = 135.54 \text{ MHz/T}$)

$$\frac{A_{T}(t)}{A_{0}} = \left\{ \left[1 - V_{m}(T) \right] e^{-\frac{\sigma^{2} t^{2}}{2}} + \left[a^{Tr}(T)F(t)D^{Tr}(t) + a^{L}(T)D^{L}(t) \right] \right\}$$

$$V_m(T) = \frac{1}{2} \operatorname{erfc}\left(\frac{T - T_N}{\sqrt{2}\Delta}\right) \qquad \left[\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^{+\infty} e^{-t^2} dt\right]$$



Long-range order: coherent precession, $\omega = \gamma_{\mu}B_{\mu}$ ($\gamma_{\mu} = 135.54 \text{ MHz/T}$)

 $= | \, \textbf{B}_{\mathsf{dip}}(\textbf{r}_{\mu}) + \textbf{B}_{\mathsf{c}}(\textbf{r}_{\mu}) +$

contact

dipolar

B

Lorentz

$$\frac{A_T(t)}{A_0} = \left\{ \left[1 - V_m(T)\right] e^{-\frac{\sigma^2 t^2}{2}} + \left[a^{Tr}(T) \underline{F(t)} D^{Tr}(t) + a^L(T) D^L(t)\right] \right\}$$

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 $= |\mathbf{B}_{dip}(\mathbf{r}_{\mu}) + \mathbf{B}_{c}(\mathbf{r}_{\mu}) + |\mathbf{B}_{c}(\mathbf{r}_{\mu})|$

dipolar

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μ^+ SR: simultaneous presence of different phases



- μ^+ inside domains probe magnetism
- µ⁺ outside domains probe magnetism (dipolar range d ∼ 1 nm)

(Park et al., PRL 102, 117006)

Closely-packed domains $\Rightarrow V_{\rm m} = 100 \%$ Nanoscopic coexistence

Widely-separated domains $\Rightarrow V_{\rm m} < 100$ % Maroscopic segregation





Advantages of μ^+ SR

- Extremely high sensitivity to absolute values of $V_{\rm m}$
- Extremely high sensitivity to SRO magnetism
- Direct access to the magnetic order parameter for LRO phases
- Spin polarization: typically \sim 100% (never the case in NMR)
- Possibility of performing zero-field measurements
- ▶ No need for "suited" materials (e. g., good nuclei for NMR)
- Relatively quick measurements

 Phase diagram upon chemical substitutions (both charge dopings and isovalent substitutions)

Phase diagram upon external/chemical pressures

 Phase diagram upon chemical substitutions (both charge dopings and isovalent substitutions)

Phase diagram upon external/chemical pressures

Nanoscopic coexistence in CeFeAsO_{0.94}F_{0.06}

 $\mu^+ {\rm SR}$ signal: no oscillations! Still, clear signature of SRO magnetism ($V_{\rm m} = 100\%)$

Diamagnetic contribution to $\chi \Rightarrow$ Bulk ${\rm SC}$ coexists with ${\rm M}$



(Sanna et al., PRB 82, 060508(R))

Nanoscopic coexistence in CeFeAsO_{0.94}F_{0.06}

- $V_{\rm m} = 100\%$
- V_{SC} < 100% but still bulk (SQUID magnetometry)

Coexistence of M and SC on the scale of nanometer

QCP ruled out by μ^+ SR



(Sanna et al., PRB 82, 060508(R))



Nanoscopic coexistence in $CeFeAsO_{1-x}F_x$

 μ^+ SR measurements performed across the whole phase diagram Qualitative difference with respect to results of neutrons



(Shiroka et al., PRB 84, 195123; Zhao et al., Nat. Mater. 7, 953)

A posteriori estimate of F⁻ content via quantitative ¹⁹F-NMR

Out-of-plane vs. in-plane doping/disorder. CeFeAsO_{1-x} F_x vs. CeFe_{1-x}Co_xAsO

Electron doping via Fe/Co: still matter of debate (Wadati et al., *PRL* **105**, 157004; Wadati et al., *PRL* **108**, 207003)



(Shiroka et al., PRB 84, 195123; Prando et al., PRB 87, 174519)

Qualitative identical phase diagram (nanoscopic coexistence) In-plane disorder strongly suppresses T_c values

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Qualitative identical phase diagram (nanoscopic coexistence) In-plane disorder strongly suppresses T_c values

Charge doping vs. isovalent substitution No apparent effect of disorder on magnetic phase



(Prando et al., PRB 87, 174519; Bonfà et al., PRB 85, 054518)

LaFe_{1-x}Ru_xAsO. DFT: no magnetic moment on Ru (Tropeano et al., *PRB* 81, 184504)

 \Rightarrow **Spin-dilution model** for Fe moments. $J_1 - J_2$ model

Percolative thresholds (Papinutto et al., PRB 71, 174425)

- > $x \simeq 0.41$, "standard" square lattice (dashed line)
- $x \simeq 0.59$, $J_1 J_2$ square lattice (continuous line)

$Fe_{1-x}Ru_x$ substitution from optimal doping

 $ReFe_{1-x}Ru_xAsO_{0.89}F_{0.11}$: chemical doping kept constant

Increasing x: re-entrant static magnetism for all Re

Ru freezes fluctuations, kills supercondutivity and triggers static magnetism

(Sanna et al., PRL 107, 227003 + PRB 87, 134518)





Conclusions

- Charge doping leads to nanoscopic coexistence of M and SC both for O/F and Fe/Co
- No qualitative difference between magnetic Re ions
- In-plane disorder is detrimental for SC but not for M
- Correlation/localization/frustration are important in 1111 pnictides
- Fe/Ru possibly enlightens strong relation among magnetic fluctuations and SC

 Phase diagram upon chemical substitutions (both charge dopings and isovalent substitutions)

Phase diagram upon external/chemical pressures

 Phase diagram upon chemical substitutions (both charge dopings and isovalent substitutions)

Phase diagram upon external/chemical pressures

Chemical vs. external pressures

Phase diagram: also scanned with P as tuning parameter **avoiding** direct modification of the chemical doping

SC induced even in undoped LaFeAsO ($P \gtrsim 3 \div 4$ GPa)



(Luetkens et al., Nat. Mater. 8, 305 and Chu et al., Physica C 469, 385)

LaFeAs_{1-x} P_xO : same phenomenology induced by chemical pressure resulting from As/P substitution (Wang et al., *EPL* **86**, 47002)

Charge doping vs. external pressures

Similarly to 1111: same effects in $Ca(Fe_{1-x}Co_x)_2As_2$



(Gati et al., PRB 86, 220511(R))

μ^+ SR under hydrostatic pressure ($P \le 2.5$ GPa)

$$A_{T}(t) = A_{0} \left[a_{PC} e^{-\frac{\sigma^{PC^{2}} t^{2}}{2}} \right] + A_{0} \left(1 - a_{PC} \right) \cdot \underbrace{(a_{PC} \simeq 0.5!)}_{\left\{ \left[1 - V_{m}(T) \right] e^{-\frac{\sigma^{2} t^{2}}{2}} + \left[a^{Tr}(T)F(t)D^{Tr}(t) + a^{L}(T)D^{L}(t) \right] \right\}}$$



Long-range order: coherent precession, $\omega = \gamma_{\mu}B_{\mu}$ ($\gamma_{\mu} = 135.54 \text{ MHz/T}$)



Lightly-doped LaFeAsO_{1-x} F_x (x = 0.055)

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p (GPa)

Pressure is highly effective in inducing ${\bf SC}$ and in suppressing ${\bf M}$

The two different phases strongly compete for volume

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(Khasanov et al., PRB 84, 100501(R))
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- Undoped ReFeAsO (Re = La, Ce, Pr, Sm)
- Undoped ReCoAsO and ReCoPO



- Undoped ReFeAsO (Re = La, Ce, Pr, Sm)
- Undoped ReCoAsO and ReCoPO



(Shang et al., PRB 87, 075148)

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(Shang et al., PRB 87, 075148)

Undoped ReFeAsO (Re = La, Ce, Pr, Sm)







Almost linear correlation of pressure effects and ionic radii

LaFeAsO is "softer" than SmFeAsO

- ► T_N and ground state B_µ: almost linear decrease with P Sizeable dependence on Re ion
- DFT calculations. Inputs: structural parameters (c/a), Re ionic radii, stripelike magnetic ground state of Fe

(see also Opahle et al., PRB 79, 024509 and Yang et al., JAP 106, 073910)



No quantitative agreement on :

- Abs. value of μ_{Fe} (neutrons): DFT strongly overestimates
- ▶ % amount of reduction: DFT strongly underestimates

DFT: band-width increased by P (De Renzi et al., SUST 25, 084009)



Site A: $B_{\mu}(T) = |\mathsf{B}_{\mathsf{dip}}(\mathsf{r}_{\mu}) + \mathsf{B}_{\mathsf{c}}(\mathsf{r}_{\mu}) + \mathsf{B}_{\mathsf{L}}|$

DFT: band-width increased by P (De Renzi et al., SUST 25, 084009)





DFT: band-width increased by P (De Renzi et al., SUST 25, 084009)



 $\mu_{Fe} = 0.68 \pm 0.02 \ \mu_B$ - agreement with NMR and neutron diffraction (Grafe et al., NJP 11, 035002 and Qureshi et al., PRB 82, 184521)

- Undoped ReFeAsO (Re = La, Ce, Pr, Sm)
- Undoped ReCoAsO and ReCoPO



(Shang et al., PRB 87, 075148)

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- Undoped ReCoAsO and ReCoPO



(Shang et al., PRB 87, 075148)



(Prando et al., PRB 87, 064401)

Sizeable differences with respect to ReFeAsO

- Magnetic critical temperatures enhanced by P
- LaCoPO much more sensible than LaCoAsO in spite of stronger chemical pressure
- Clearly discontinuous behaviour is displayed in LaCoPO



(Prando et al., PRB 87, 064401)

Comparison among external and chemical (La/Pr) pressures

- External and chemical pressure play the same role
- Magnetic critical temperatures enhanced by P
- Internal field strongly suppressed
- Pr does not magnetically contribute only shrinkage



Pr does not magnetically contribute - only shrinkage



(Prando et al., PRB 87, 064401)

Comparison among external and chemical (La/Pr) pressures

- External and chemical pressure play the same role
- Magnetic critical temperatures enhanced by P
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Pr does not magnetically contribute - only shrinkage



(Prando et al., PRB 87, 064401)

- Pr: biasing internal pressure ($P_{\rm B} \simeq 16.5$ kbar)
- Discontinuity at P ~ 5 kbar: which origin?

FM ordering: $B_{\mu}(T) = |\mathbf{B}_{dip}(\mathbf{r}_{\mu}) + \mathbf{B}_{c}(\mathbf{r}_{\mu}) + \mathbf{B}_{L}|$ Change in the electron density: $\mathbf{B}_{c}(\mathbf{r}_{\mu})$ modified accordingly

- DFT calculations: electronic band crossing $E_{\rm F}$ at $P \simeq 40$ kbar
- Likely modification of the hyperfine contact term

Conclusions

- Undoped ReFeAsO (Re = La, Ce, Pr, Sm)
- Undoped ReCoAsO and ReCoPO



(Shang et al., PRB 87, 075148)

Conclusions

 $\mu^+ {\rm SR}$ + Pressure: useful to access phase diagram of 1111 pnictides

- Lightly-doped LaFeAsO_{1-x}F_x
 - Macroscopic segregation of M and SC
 - Possible change of pairing symmetry between La1111 and Ce1111, Sm1111 ?
- Undoped ReFeAsO (Re = La, Ce, Pr, Sm)
 - Negative effect of pressure on both μ_{Fe} and T_N
 - Sizeable Re dependence: linear scaling with ionic radii (qualitative agreement from DFT)

Undoped ReCoAsO and ReCoPO

- ▶ Positive effect of pressure on T_C and negligible effect on μ_{Co}
- Clear equivalence of external and chemical pressures
- \blacktriangleright DFT suggests non-trivial sudden modifications of the electronic band structure modifying hyperfine coupling to μ^+ in turn
- Planned: x-rays and ³¹P-NMR under P (investigate structure and hyperfine term at the nuclei)

Out-of-plane vs. in-plane doping/disorder. CeFeAsO_{1-x} F_x vs. CeFe_{1-x}Co_xAsO



Enhancement of Ce^{3+} ordering on the top of SC dome

LaFe_{1-x}Ru_xAsO – Hints for magnetic frustration

Superexchange paths on the Fe square lattice: $J_{nn} \sim J_{nnn}$. Competition of interactions leading to a fully-frustrated g.s. (Yildirim, *PRL* **101**, 057010)

 J_1-J_2 model: good agreement with experimental value of μ_{Fe}





Selection of g.s. possibly associated with orthorombic-tetragonal structural phase transition ($T_{str} \gtrsim T_N$)

$LaFe_{1-x}Ru_xAsO$ – Hints for localization

- Ab-initio calculations: proximity to a Mott-like transition (Cao et al., PRB 77, 220506; Si et al., PRL 101, 076401)
- Experimental Wilson ratio $R = \frac{\pi^2 k_B^2}{3\mu_B^2} \frac{\chi_P}{\gamma} = 2.5 \div 6 \ (> 1).$ (Brüning et al., *PRL* 101, 117206; Baker et al., *NJP* 11, 025010)

Electronic correlations: $U \sim t$ in one-band Hubbard Hamiltonian

$$\mathcal{H}_{Hubb} = -t\sum_{\langle i,j
angle,\sigma}c^{\dagger}_{i,\sigma}c_{j,\sigma} + U\sum_{i}\prod_{\sigma}c^{\dagger}_{i,\sigma}c_{i,\sigma}$$



Pnictides: multi-band scenario

SDW band: possible localization effects. Analogies with $J_1 - J_2$ model in cuprates and vanadates (Melzi et al., *PRL* **85**, 1318)

$Fe_{1-x}Ru_x$ substitution from optimal doping

Possibly in favour of $\ensuremath{\text{SC}}$ mediated by spin-fluctuations

⁷⁵As-NQR gives support to nanoscopic coexistence of phases

(Sanna et al., *PRL* **107**, 227003 + *PRB* **87**, 134518)

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$Fe_{1-x}Ru_x$ substitution from optimal doping

Possibly in favour of **SC** mediated by spin-fluctuations

⁷⁵As-NQR gives support to nanoscopic coexistence of phases

Weight of the 2 peaks as a function of x scale with the two characteristic critical T (Sanna et al., PRL 107, 227003 + PRB 87, 134518)





Chemical vs. external pressures

Sizeable f - d hybridization is at work (Prando et al., PRB 81, 100508(R))

Competition between superconductivity and Kondo effect Exemplary case: CeFeAs_{1-x}P_xO (Jesche et al., PRB **86**, 020501(R))



Magnetic features are qualitatively reproduced by application of pressure on CeFeAsO (Zocco et al., PRB **83**, 094528)

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As/P substitution: V and T_K enhancement

$$T_{K} \equiv \frac{W_{F}}{k_{B}} \exp\left(-\frac{|\varepsilon_{f}|}{2V^{2}n(E_{F})}\right)$$

(Pourovskii et al., EPL **84**, 37006) (Sun et al., EPL **91**, 57008)

Neither chemical nor external pressure induce bulk SC in CeFeAsO (Zocco et al., PRB 83, 094528)



(Prando et al., PRB 87, 064401)

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- Discontinuity at P ~ 5 kbar: which origin?

FM ordering: $B_{\mu}(T) = |\mathbf{B}_{dip}(\mathbf{r}_{\mu}) + \mathbf{B}_{c}(\mathbf{r}_{\mu}) + \mathbf{B}_{L}|$

- Magnetic moment of Co is not affected by P
- DFT calculations: structure is negligibly modified by P

Still: experimental x-rays vs. P missing!



(Prando et al., PRB 87, 064401)

- Pr: biasing internal pressure ($P_{\rm B} \simeq 16.5$ kbar)
- Discontinuity at $P \simeq 5$ kbar: which origin?

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