Magnetism, Electronic Transport and Magneto-Structural Coupling in Sr_2IrO_4

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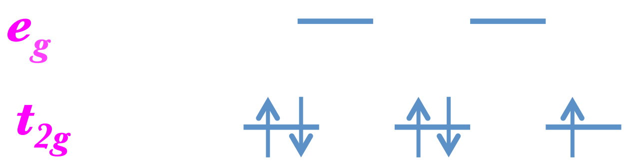
JNU, Frustrated Magnetism, Feb 13, 2015

Our Group at JNU

- ❑ Work in experimental condensed matter physics.
- ❑ Most work in low temperature regime.
- ❑ Do prepare materials, characterize them and study physical properties.
- ❑ At present group of 7 people: 3 Ph.D students and 3 M.Sc students.
- ❑ Transition metal oxides (4d & 5d) based materials.

Sr_2IrO_4 (214) : Overview

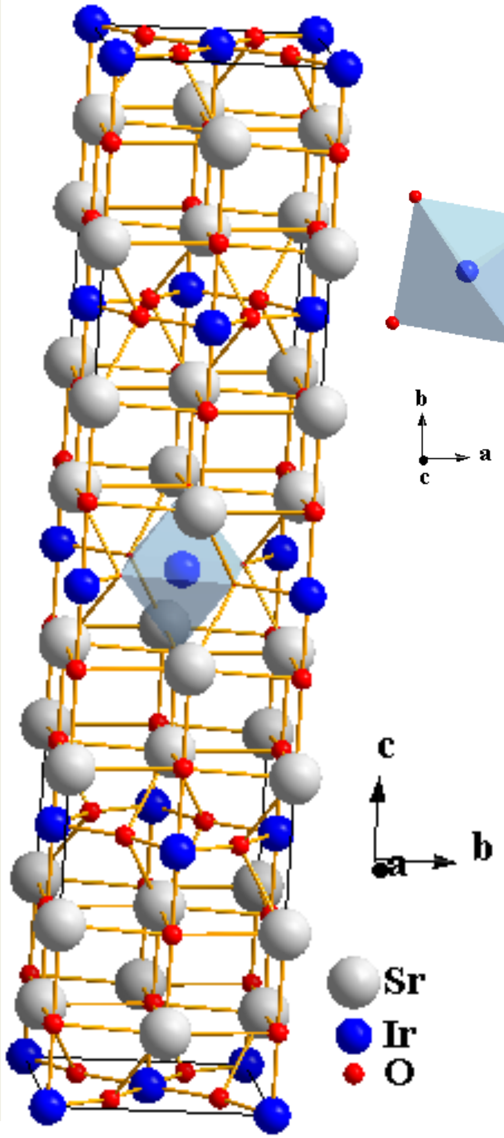
- ❑ $Sr_2^{2+}Ir^{4+}O_4^{2-}$ is 5*d* based Transition Metal Oxide
- ❑ Electronic configuration: **Ir^{4+}** → **$4f^{14}5d^5$**
- ❑ Significant Crystal Field effect → Low spin state

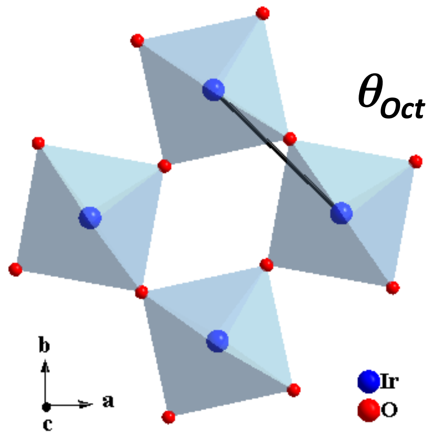


- ❑ Half filled t_{2g} band.
- ❑ Extended nature of 5*d* orbitals.
- ❑ Reduced electronic correlation effect than 3*d* and 4*d* counterpart.
- ❑ Therefore, 5d oxides expected to be metallic.
- ❑ Heavy character of Ir (77) atom.
- ❑ Significant spin-orbit coupling (SOC) effect ($\propto z^4$, atomic number)
- ❑ Comparable energy scale of Coulomb interaction and SOC ~ 0.5 eV

Sr_2IrO_4 (214) : Structural Overview

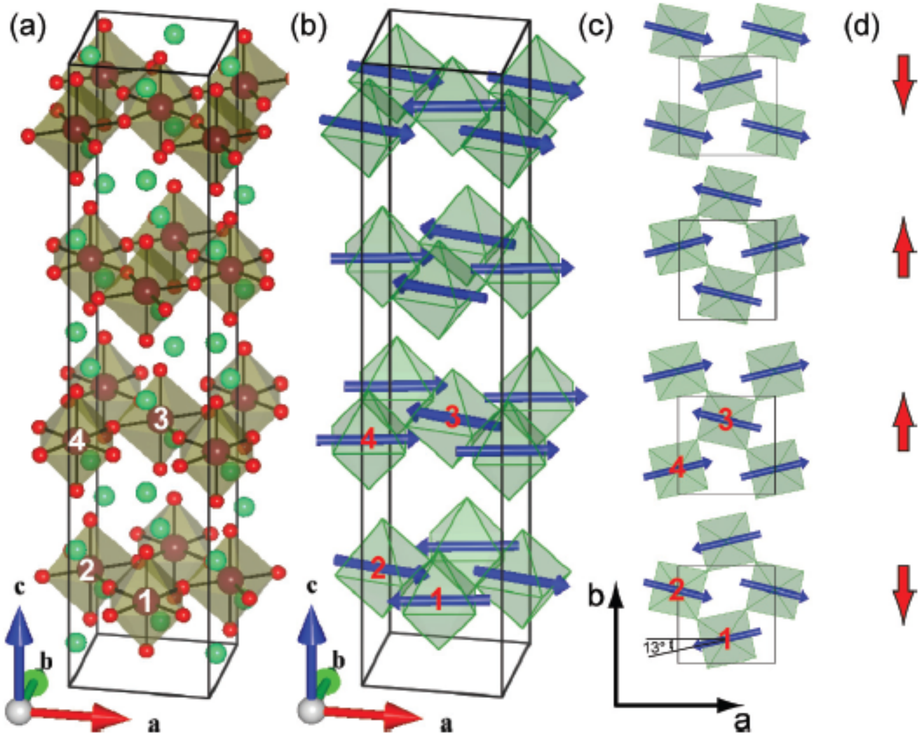
- Member of Ruddlesden-Popper series **$Sr_{n+1}Ir_nO_{3n+1}$** with ***n* = 1**.
- Layered (K_2NiF_4) structure.
- Crystalizes in tetragonal structure
  Space group : *$I4_1/acd$*.
- Alternate tilting of IrO_6 octahedra
  along *c*-axis ($\theta_{Oct} \sim 11^{o}$) .
- Iso-structural with
  La_2CuO_4 and Sr_2RuO_4
- Possible superconductivity !!!
  Wang, PRL, 106, 136402 (2011)
  Yang, PRB 89, 094518 (2014)



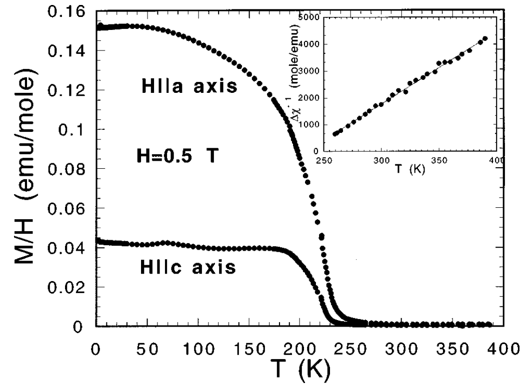


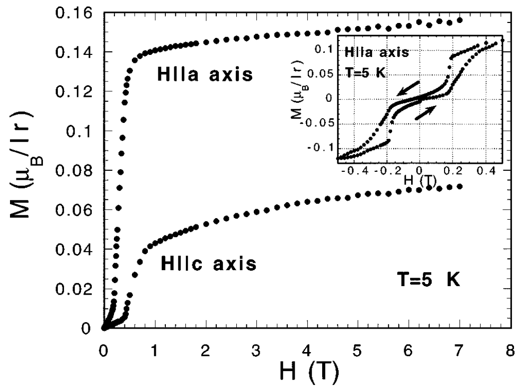
Sr_2IrO_4 (214) : Magnetic Overview

Ye, PRB, 87, 140406, (2013)



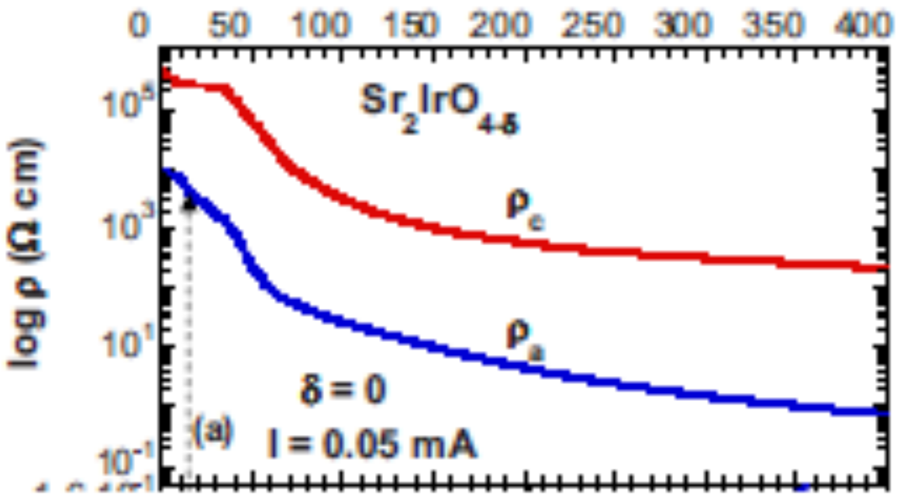
Cao, PRB, 57, 11039, (1998)





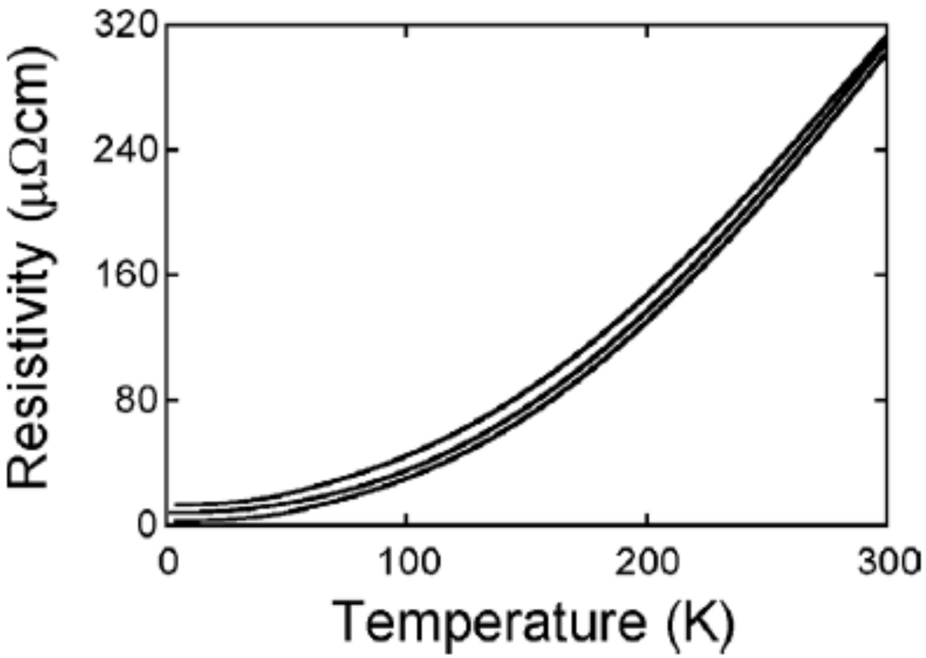
- ❑ Canted Antiferromagnet with $T_N \sim 240$ K.
- ❑ Structural distortion induced Dzyaloshinsky-Moriya (DM) interaction.
- ❑ Weak ferromagnetism with much lower moment than spin-only value (1 μ_B/f.u) for $S = ½$

Sr_2IrO_4 (214) : Electronic Transport



Sr_2IrO_4

Korneta, PRB, 82, 115117 (2010)



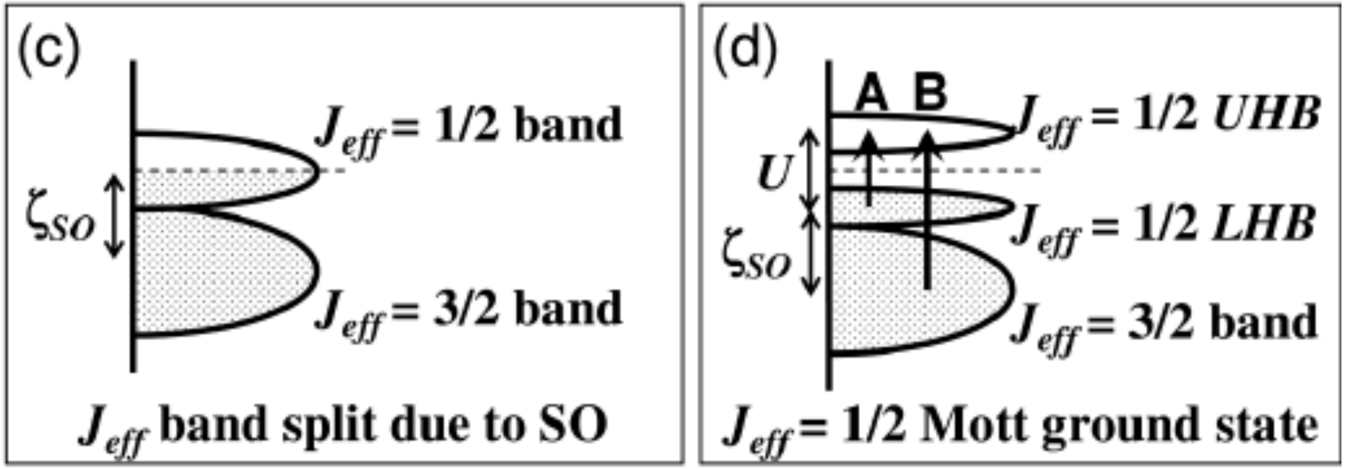
Sr_2RhO_4

Perry, JPCM, 8, 175 (2006)

Sr_2IrO_4 (214) : Insulating behaviour

J_{eff} Mott Insulator : Electronic correlation driven

- Interplay between SOC, W and U gives novel ground state.
- SOC splits t_{2g} band onto $J_{eff} = 1/2$ and $J_{eff} = 3/2$ band.
- $J_{eff} = 1/2$ band is half-filled and narrow.
- Moderate U can lead to Mott gap.



B. J. Kim, PRL 101, 076402 (2008); Science, 323, 1329 (2009)

Sr_2IrO_4 (214) : Insulating behaviour

Slater Insulator : Magnetic Order driven

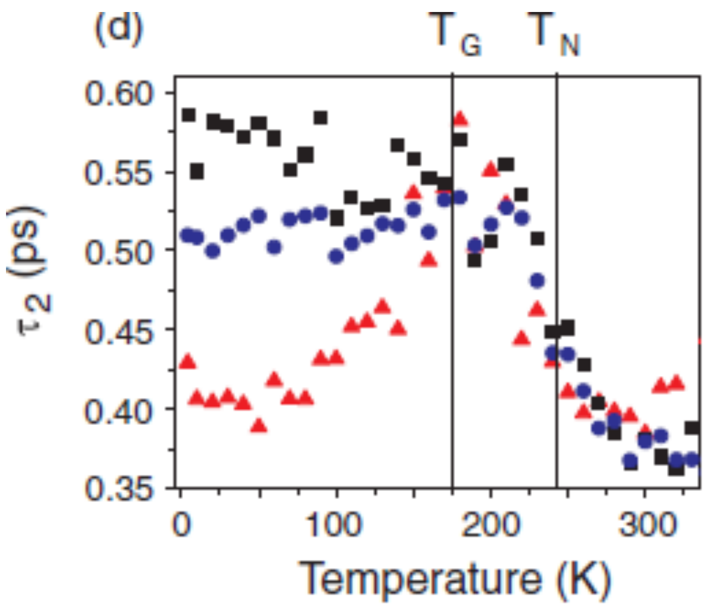
PRL **108,** 086403 (2012) PHYSICAL REVIEW LETTERS week ending 24 FEBRUARY 2012

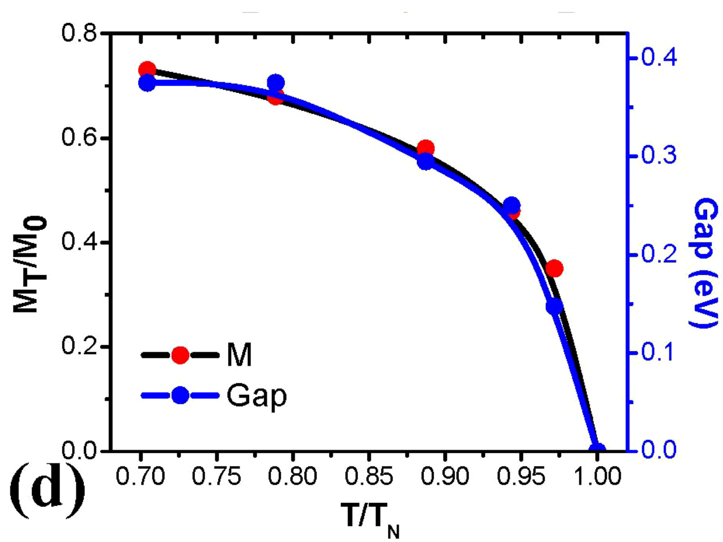
Ab initio **Studies on the Interplay between Spin-Orbit Interaction and Coulomb Correlation in Sr_2IrO_4 and Ba_2IrO_4**

R. Arita,[1,2,3] J. Kuneš,[4] A. V. Kozhevnikov,[5] A. G. Eguiluz,[6] and M. Imada[1,3]

Time resolved optical study
Hsieh, PRB, 86, 035128(2012)

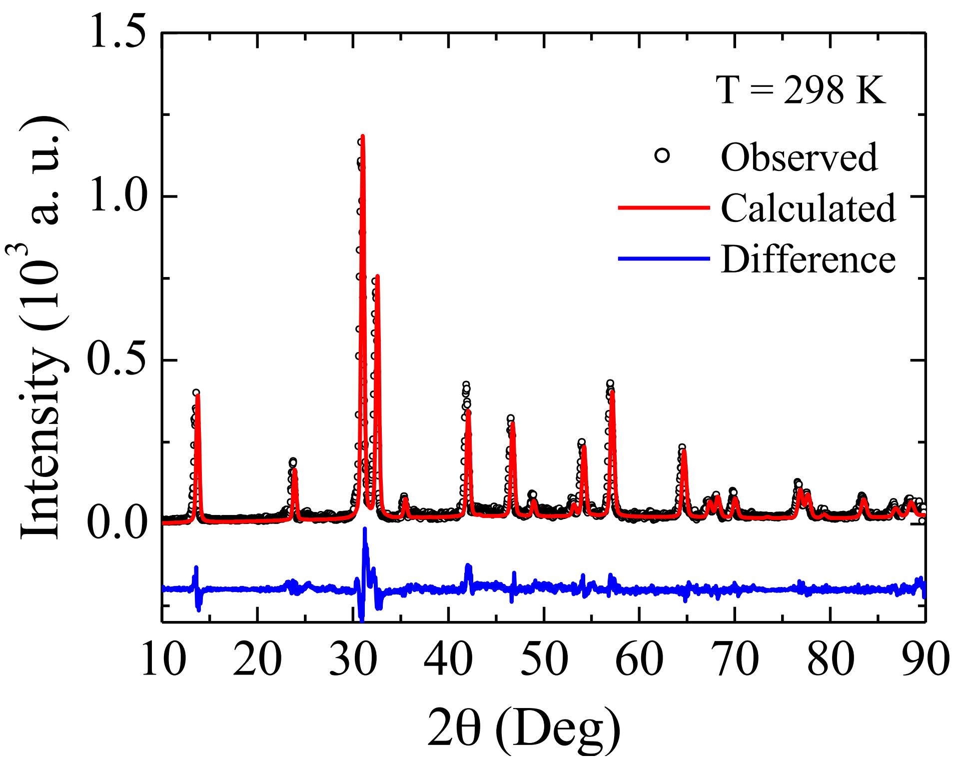
STM/STS investigation.
Li, Scientific Reports, 3, 3073 (2013)





Sr_2IrO_4 (214) : Material Synthesis

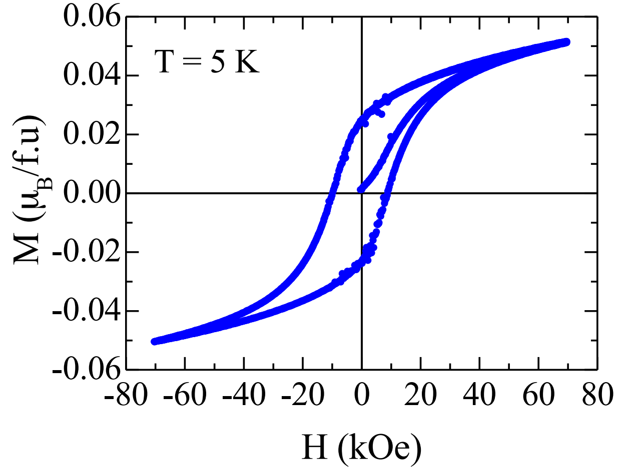
- Single-phase polycrystalline material prepared using solid state method.
- Materials are characterized using XRD and allied Rietveld analysis.
- Sample crystallizes in tetragonal structure with *I4/acd* symmetry.
- Lattice parameters; a = 5.4980(2) Å and c = 25.779(1) Å.

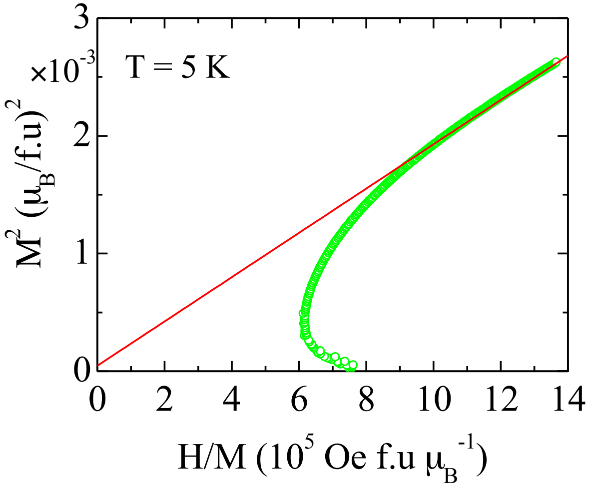


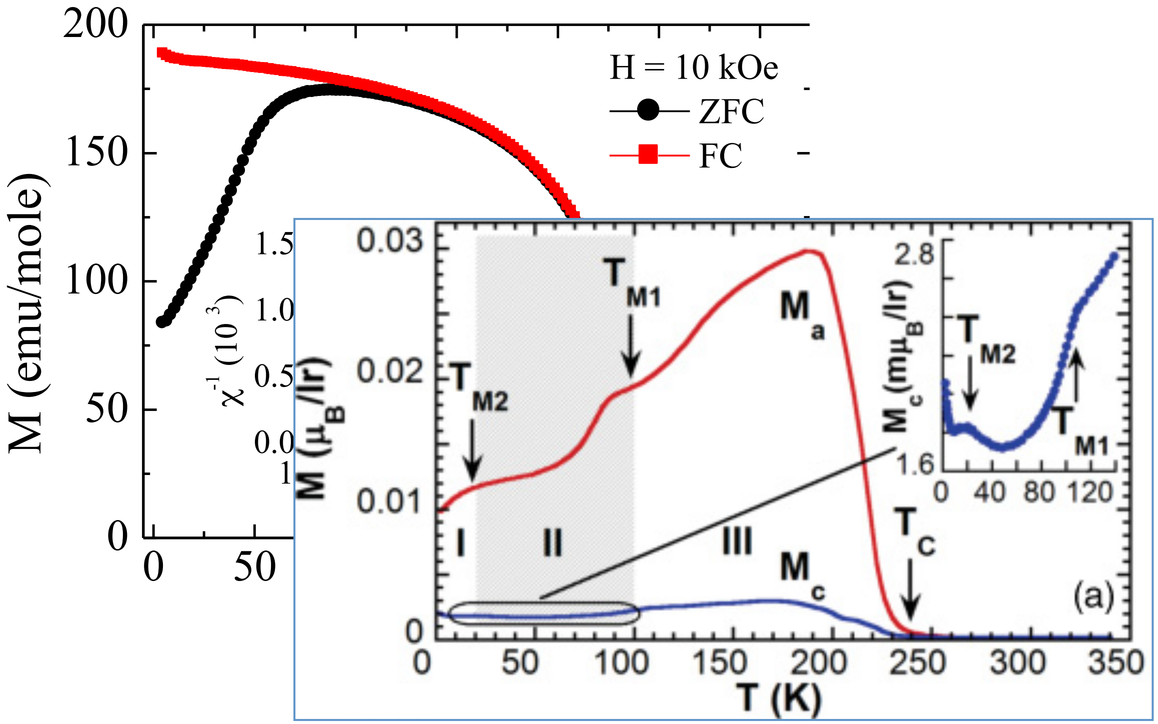
Bhatti, AKP, JPCM, 27, 016005 (2014)

Sr_2IrO_4 (214) : Magnetic Properties

- Weak FM transition around 238 K (dM/dT).
- Steep decrease in $M_{ZFC}(T)$ below ~ 95 K.
- Curie-Weiss behaviour in limited temperature.
- Estimated θ_P = 233 K and μ_{eff} = 0.56 μ_B/f.u.
- Expected μ_{eff} = 0.57 and μ_H = 0.33 μ_B/f.u ($g_{\mathcal{J}}$ = 2/3)



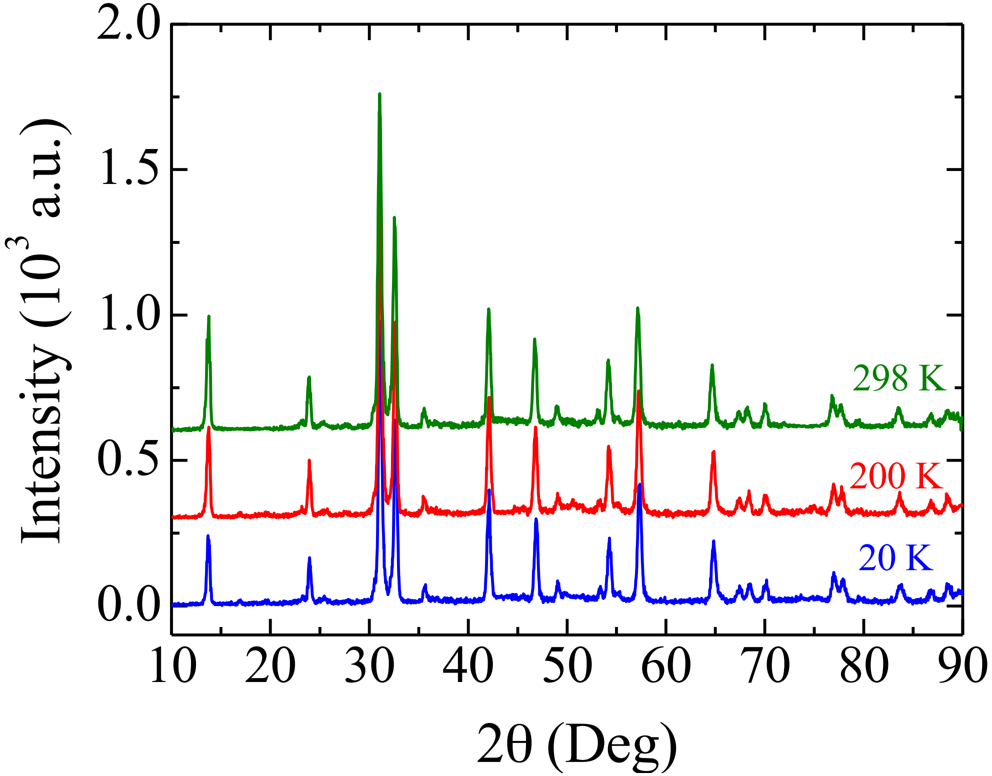




Ge, PRB, 84, 100402 (2011).

Sr_2IrO_4 (214) : Temperature Dependent Structure

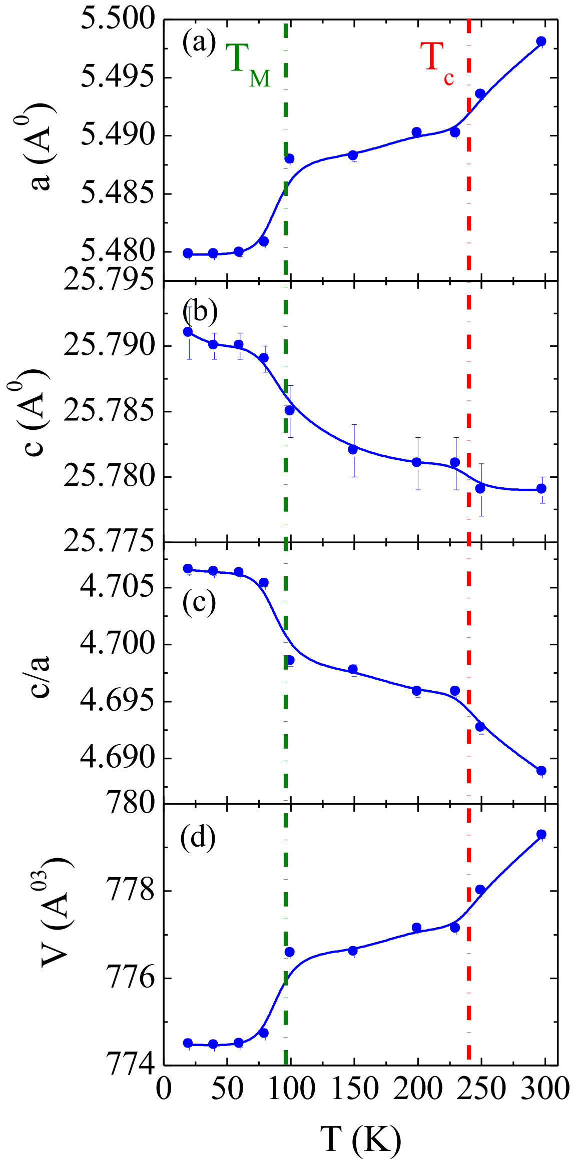
- ❑ Representative XRD data in PM, FM and low temperature state.
- ❑ No structural phase transition down to 20 K.

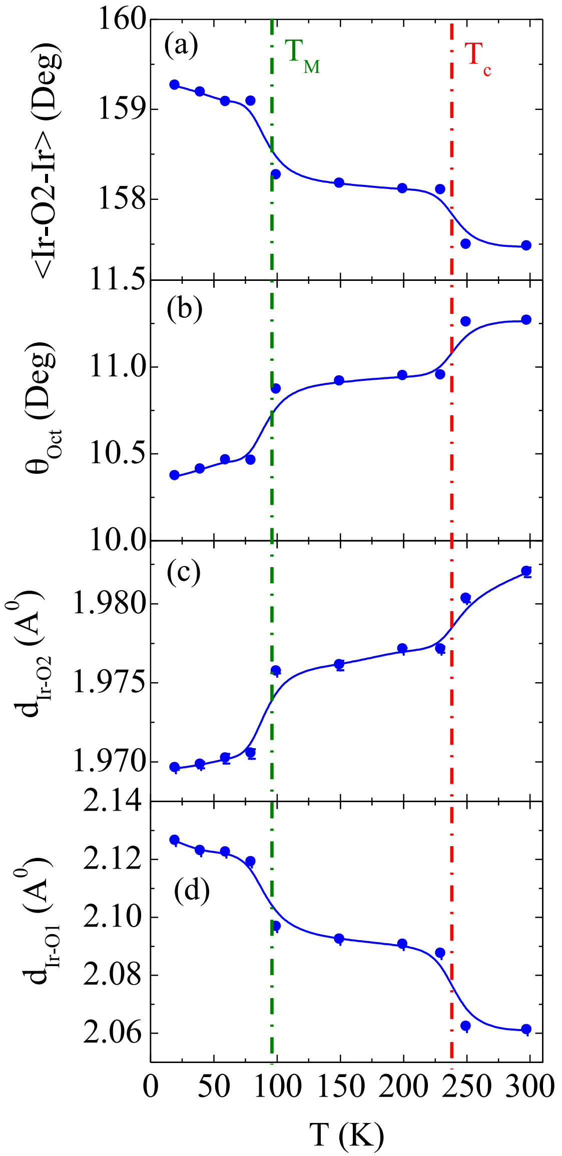


Sr_2IrO_4 (214) : Temperature Dependent Structure

Temperature dependent changes in structural parameters.

Unit Cell

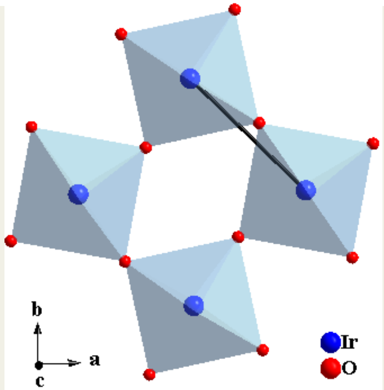


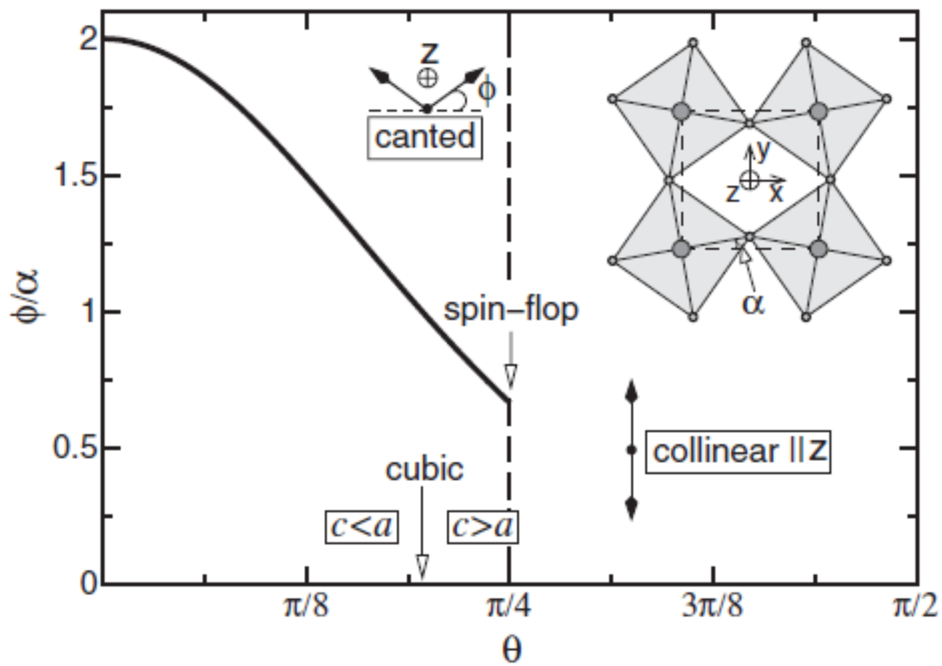


IrO_6 Octahedra

Sr_2IrO_4 (214) : Prediction for Magneto-Structural correlation

- ❑ Magnetism is linked to IrO_6 octahedra distorsion.
- ❑ α - IrO_6 octahedra distortion angel.
- ❑ Φ - spin canting angle.
- ❑ θ - tetragonal distortion parameter.

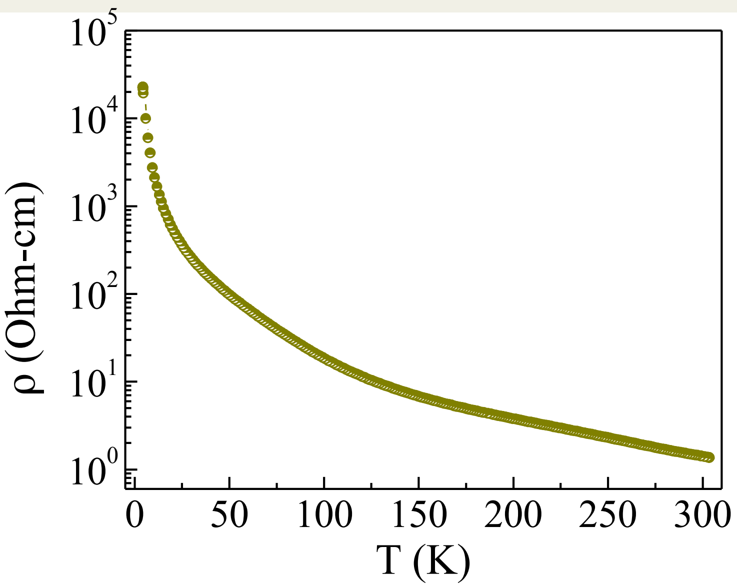


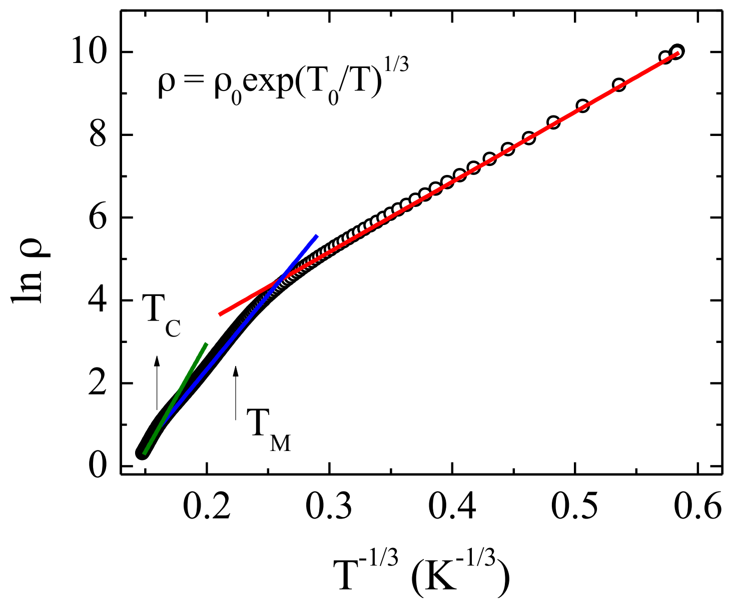


Jackeli, PRL, 102, 017205 (2009)

Sr_2IrO_4 (214) : Electronic Transport

- Resistivity shows insulating behaviour ($d\rho/dT < 0$).
- Resistivity increases by five orders at low temperature.
- Electronic transport can be understood using 2D Mott variable range hopping model.



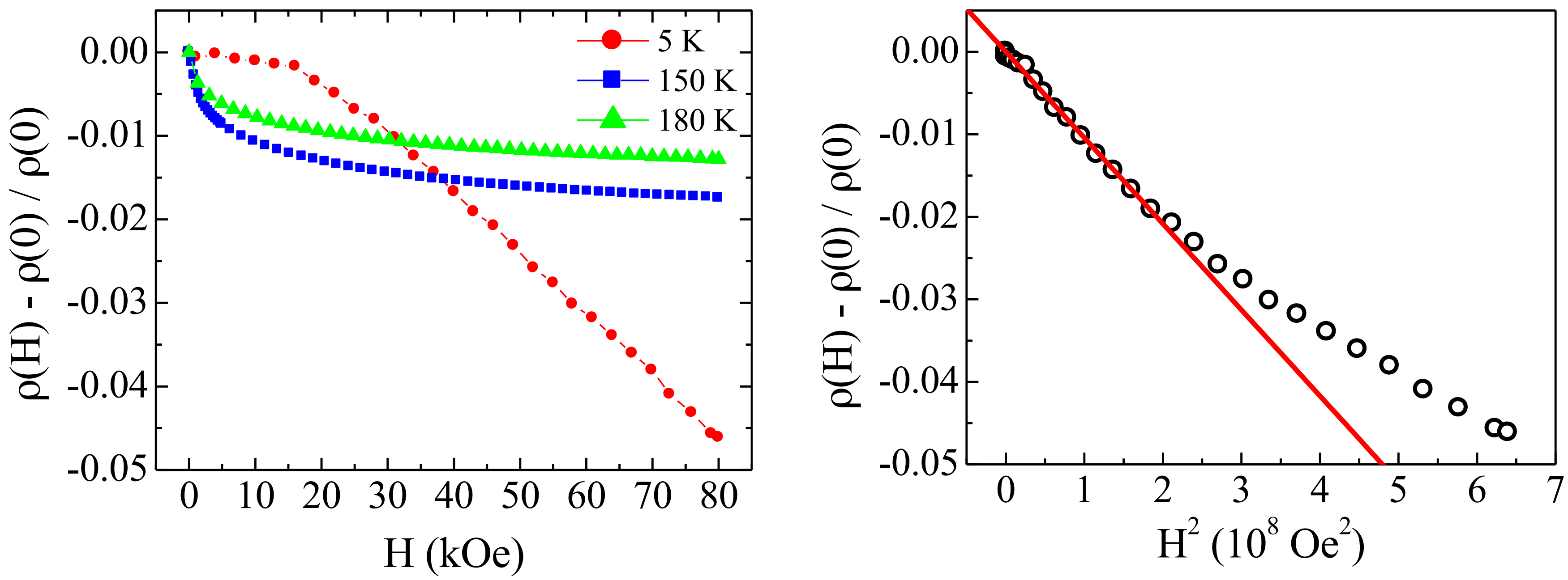


Temperature range (K)	T_0 (K)	ξ (Å)
300–240	1.44×10^5	3.04
240–70	4.68×10^4	4.42
40–5	4.82×10^3	9.44

Sr_2IrO_4 (214) : Magneto-transport

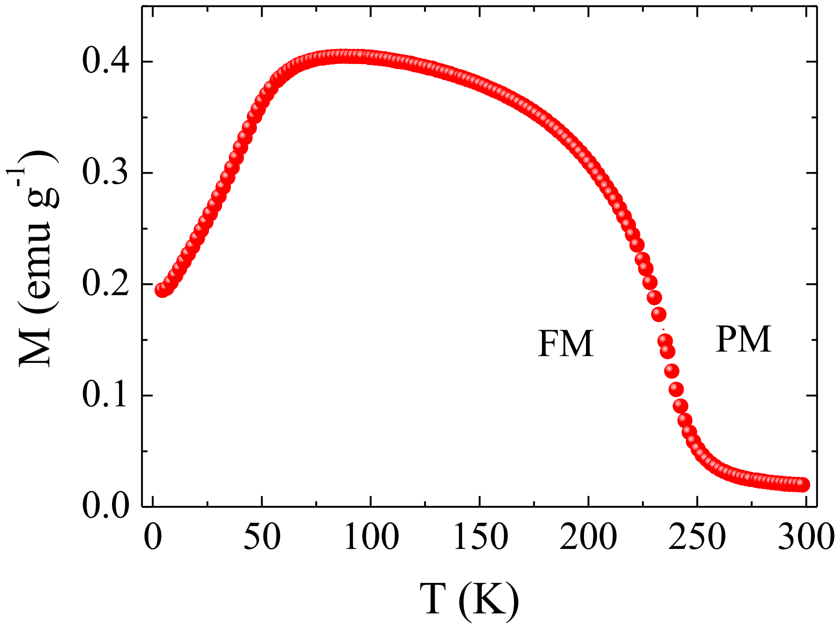
Magnetoresistance (MR) $= \dfrac{\Delta\rho}{\rho(0)} = \dfrac{\rho(H) - \rho(0)}{\rho(0)}$

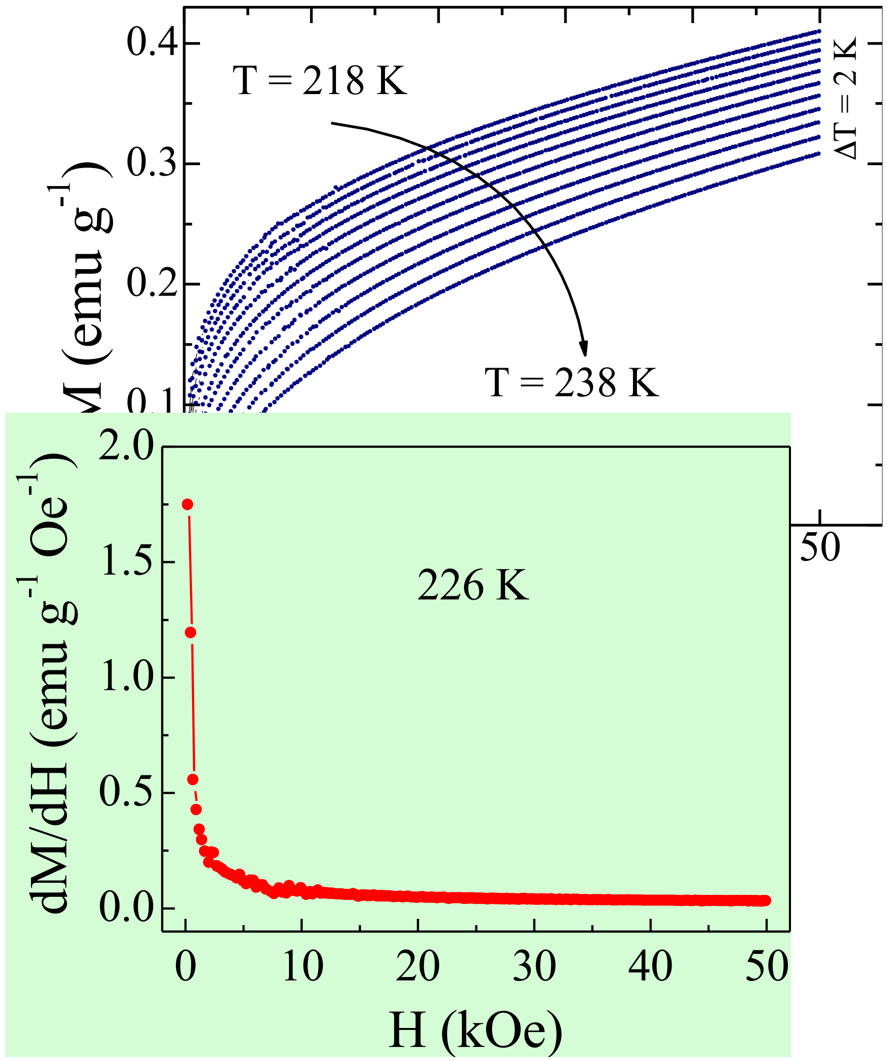
- ❑ Positive MR (weak antilocalization) in strong SOC systems, Bi_2Se_3, Bi_2Te_3, Na_2IrO_3 films.
- ❑ Negative MR at low T in VRH regime – weak localization – quantum interference effect – Quadratic field dependence.



Sr_2IrO_4 (214) : Critical Analysis

❑ Magnetic isotherms across FM transition





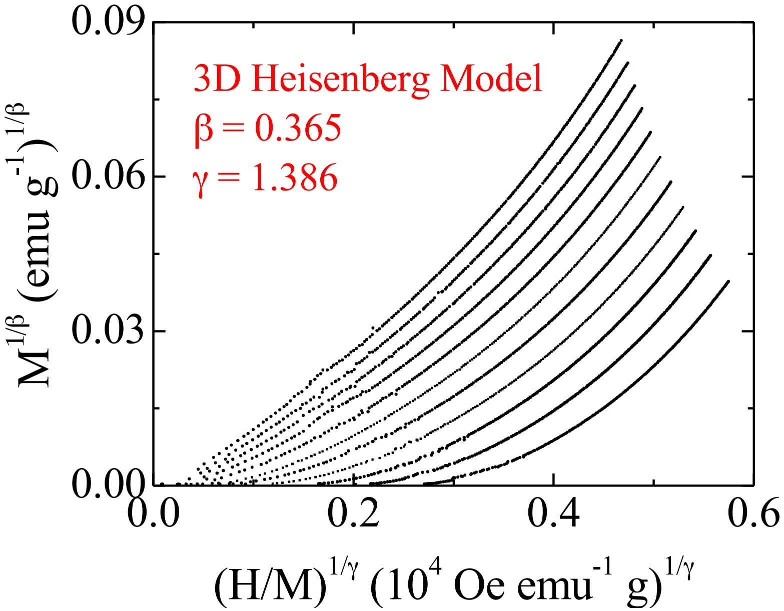
$$M_S(T) = M_0(-\epsilon)^{\beta}, \quad \epsilon < 0,$$

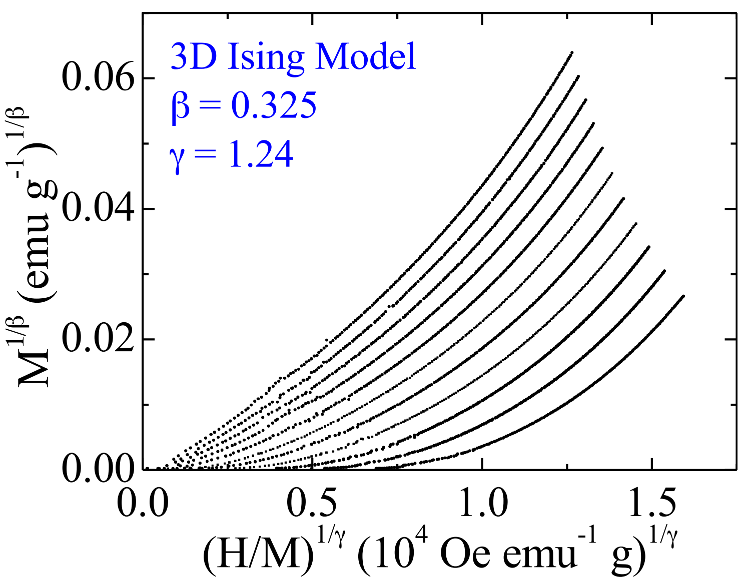
$$\chi_0^{-1}(T) = \Gamma(\epsilon)^{\gamma}, \quad \epsilon > 0,$$

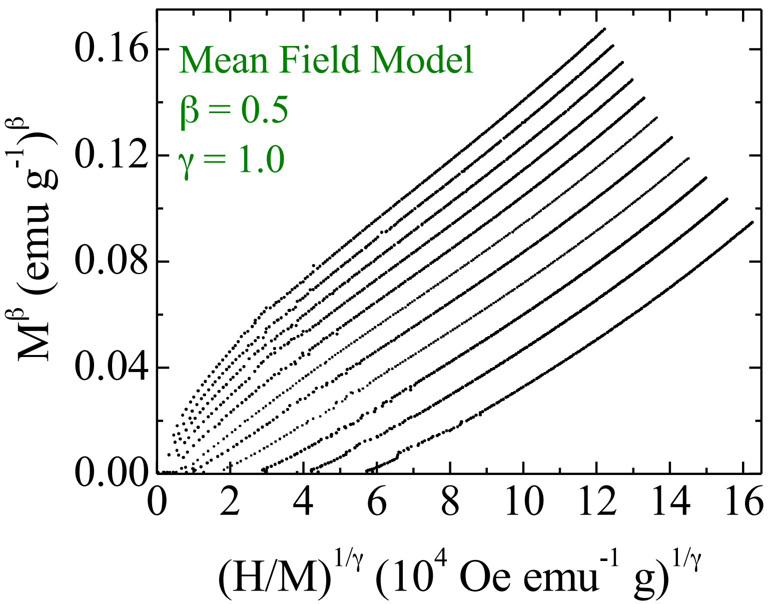
$$M = XH^{1/\delta}, \quad \epsilon = 0,$$

$$\epsilon = (T - T_C)/T_C$$

Sr_2IrO_4 (214) : Critical Analysis

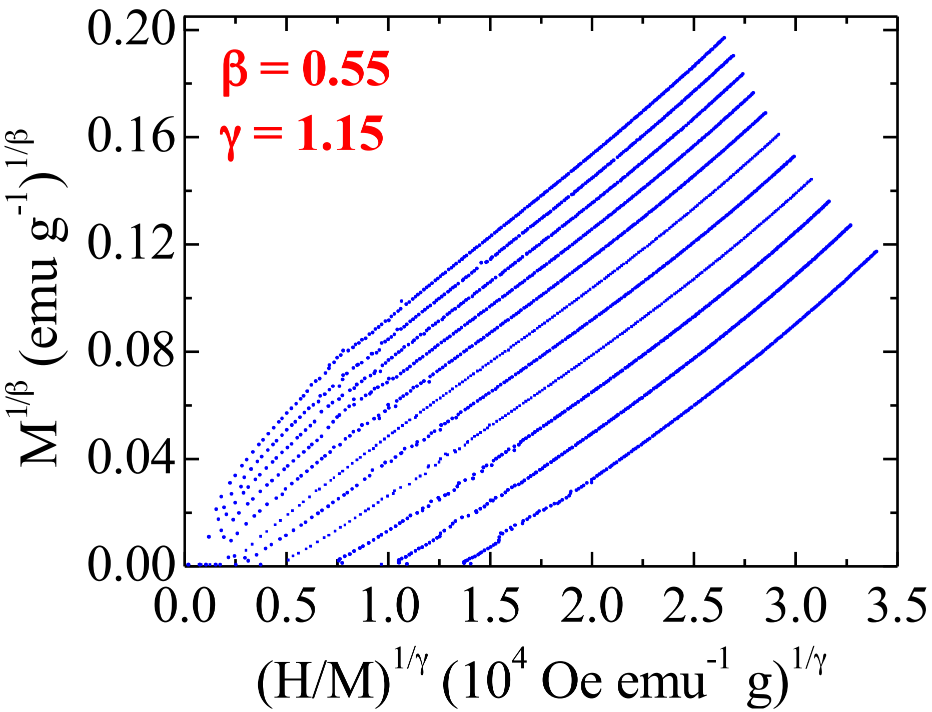






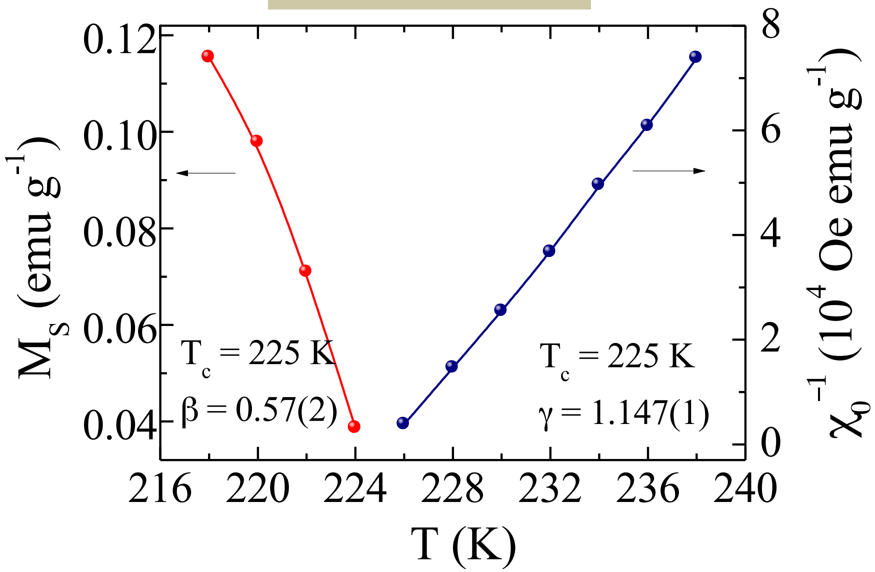
Sr_2IrO_4 (214) : Critical Analysis

Modified Arrott plot: $$\left(\frac{H}{M}\right)^{1/\gamma} = a\frac{(T - T_C)}{T} + bM^{1/\beta}$$

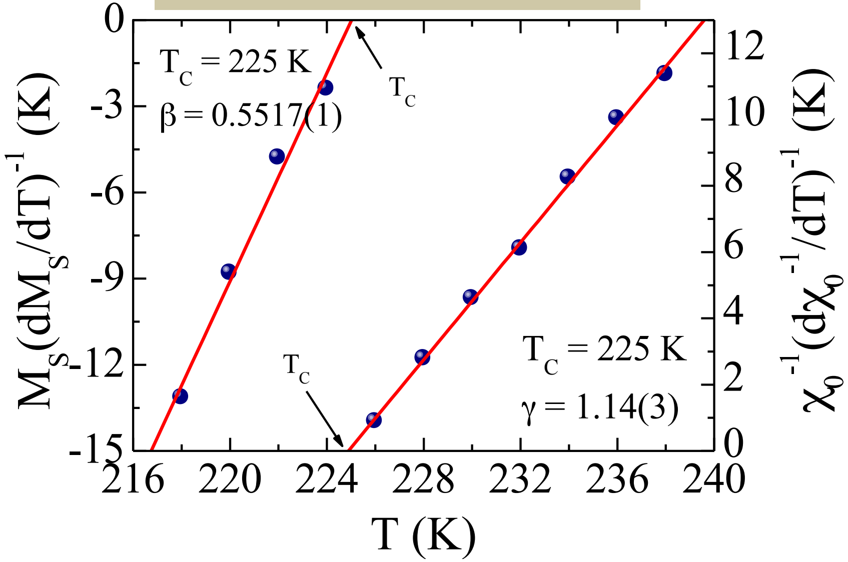


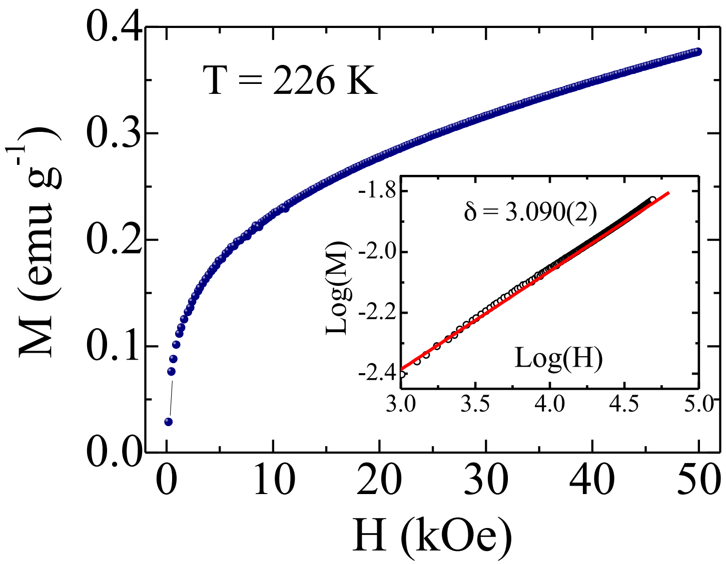
Sr_2IrO_4 (214) : Critical Analysis

Critical Plot



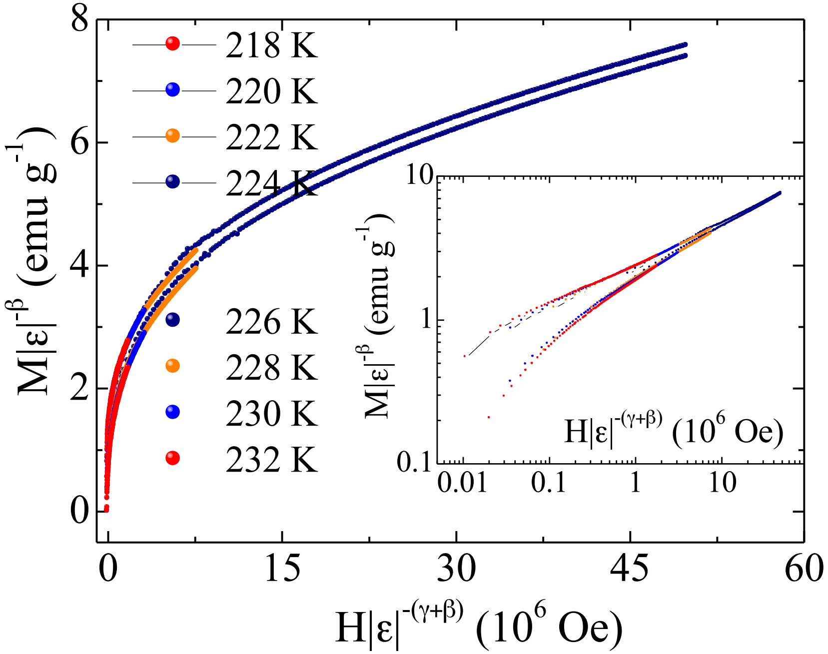
Kouvel-Fisher Plot





Critical isotherm: $M \propto H^{1/\delta}$

Sr_2IrO_4 (214) : Critical Analysis



Scaling analysis

$$M(H,\epsilon) = \epsilon^{\beta} f_{\pm}\left(\frac{H}{\epsilon^{\beta+\gamma}}\right)$$

Exponents	β	γ	δ
This Work	0.55	1.15	3.03
Mean Field	0.5	1.0	3.0
3D Heisenberg	0.365	1.386	4.8
3D Ising	0.325	1.241	4.82

Sr_2IrO_4 (214) : Thermal Demagnetization

Thermal Demagnetization ΔM :

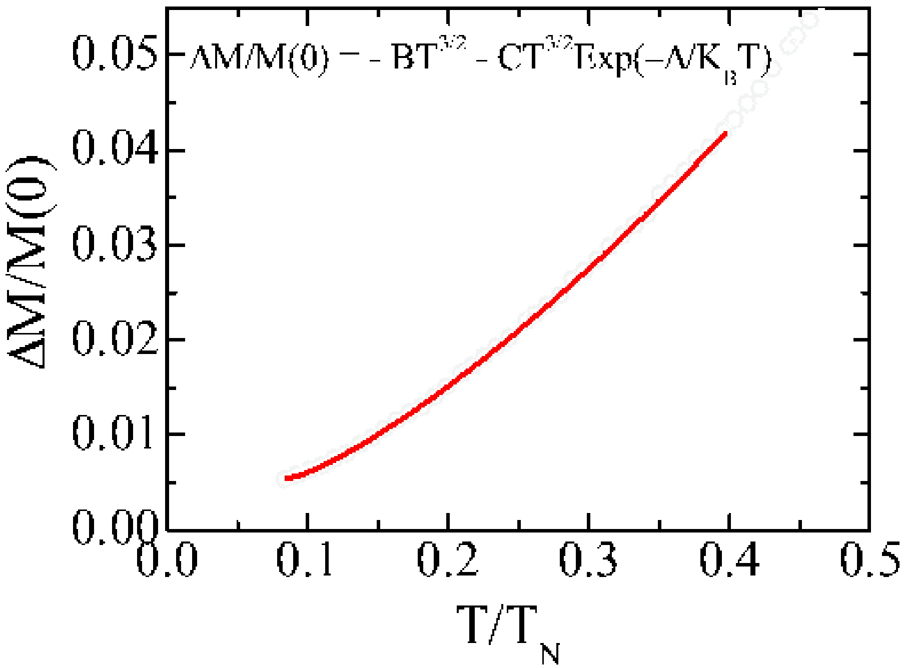
Spin-wave (SW) excitation (Bloch) :

$$\frac{\Delta M}{M(0)} = \frac{M(T) - M(0)}{M(0)} = BT^{3/2}$$

Stoner single-particle (SP) excitation:

$$\frac{\Delta M}{M(0)} = \frac{M(T) - M(0)}{M(0)} = CT^{3/2}\exp(-\frac{\Delta}{k_B T})$$

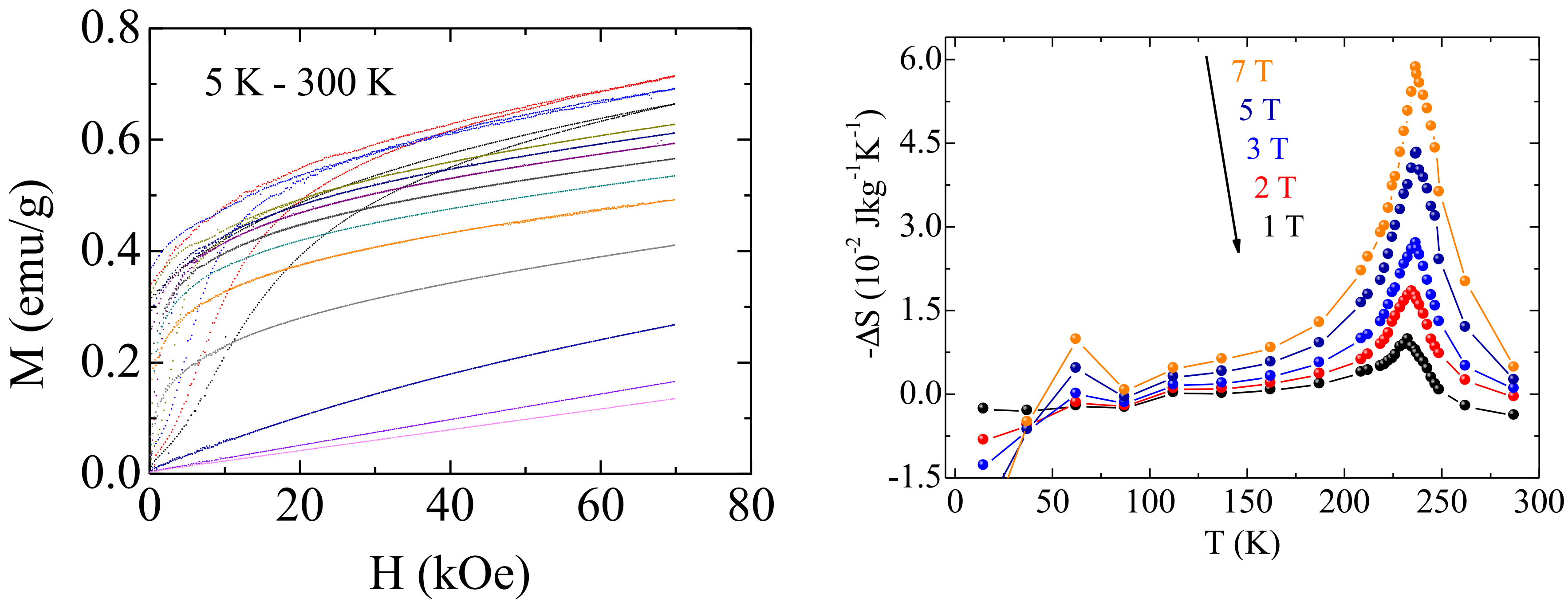
$\Delta M_{Total} = \Delta M_{SW} + \Delta M_{SP}$



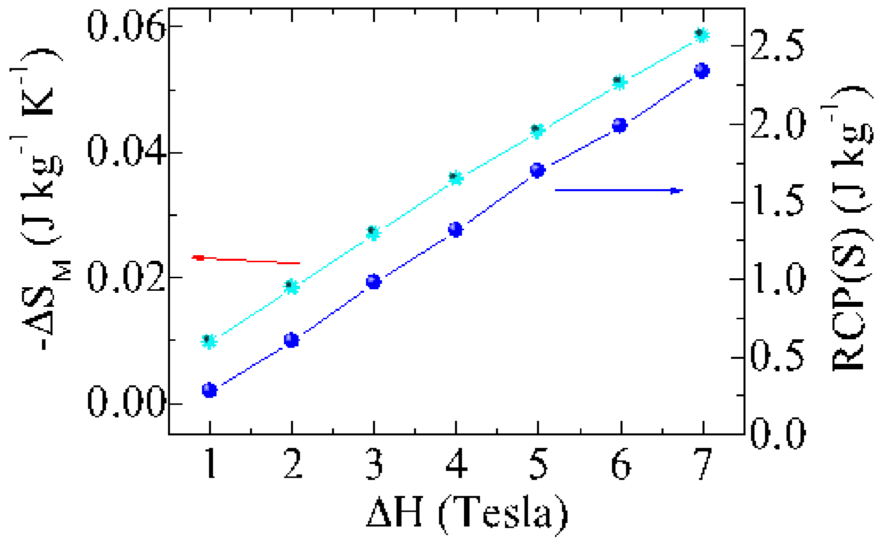
Sr_2IrO_4 (214) : Magnetocaloric Effect (MCE)

Magnetic Entropy change: $\Delta S_M(T,H) = S_M(T,H) - S_M(T,0) = \int_0^H \left(\frac{\delta M(T,H)}{\delta T} \right)_H dH$

Relative cooling power: $\Delta S_M(T,H) \times \delta T_{FWHM}$

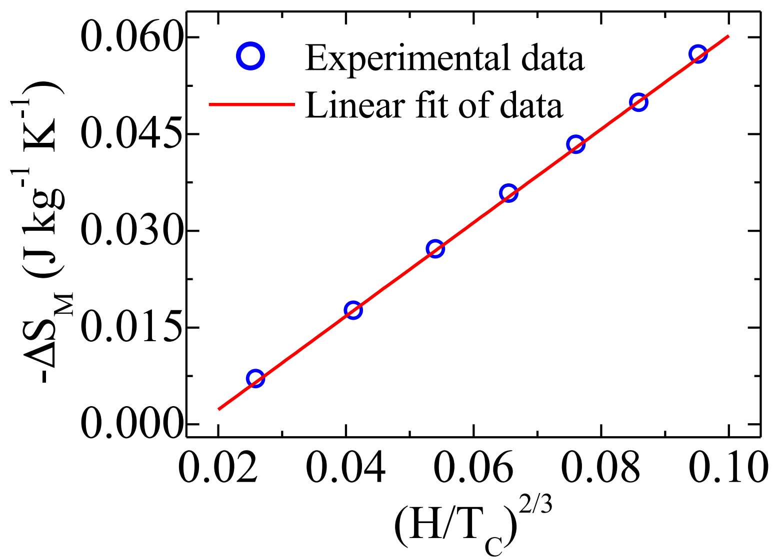


Sr_2IrO_4 (214) : Field dependence of MCE



Nice linear field dependence

For both ΔS_M and RCP.



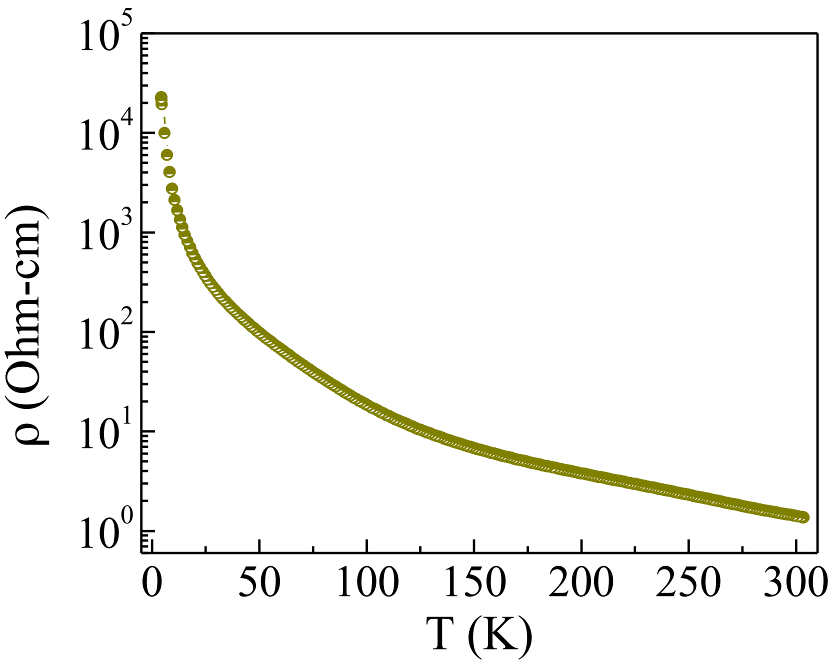
Linear dependence of

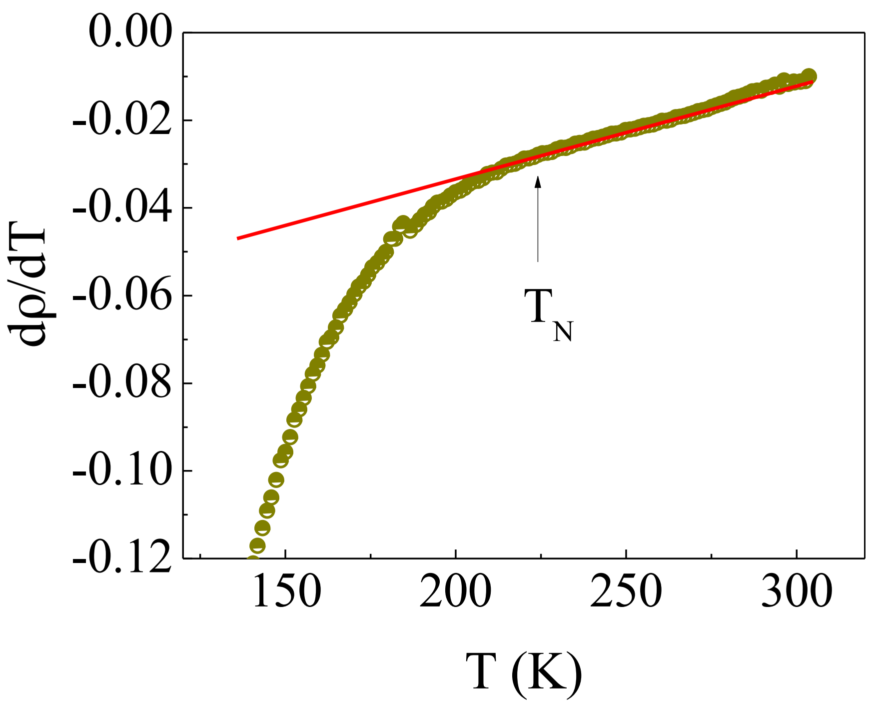
ΔS_M and $(H/T_c)^{2/3}$ shows mean

Field nature.

Sr_2IrO_4 (214) : Resistivity derivative

Mott OR Slater OR Both !!!





Acknowledgement

Institute : AIRF – JNU for low temperature XRD data.

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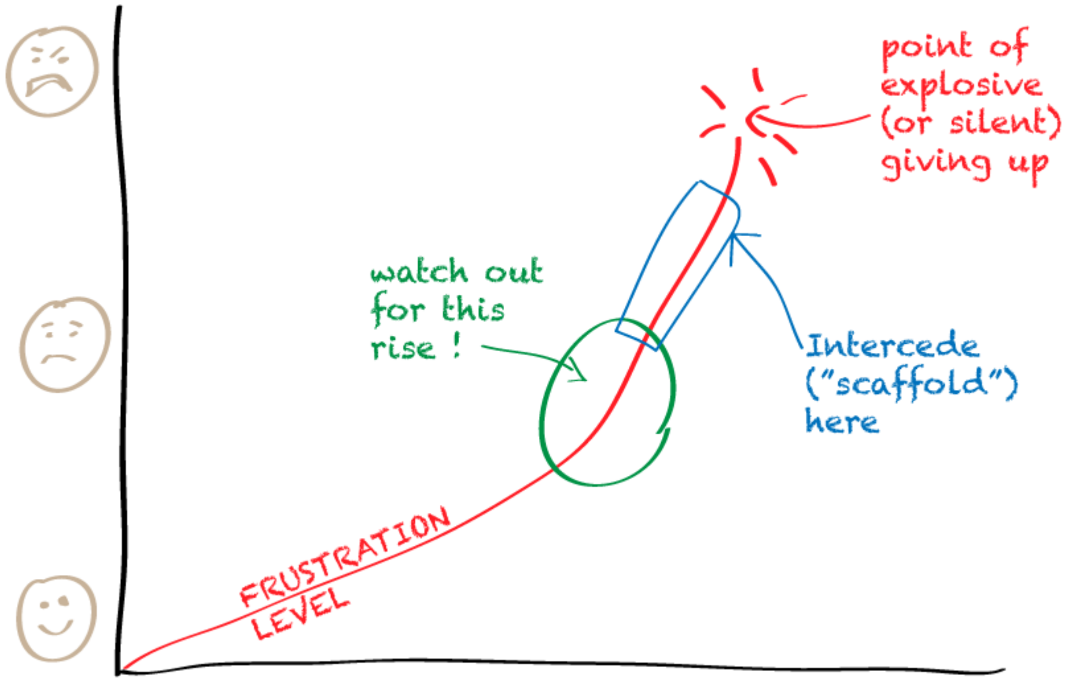
Rajeev Rawat, UGC-DAE CSR

Funding : UGC, Govt of India

DST, Govt of India

!!! Thank you !!!


point of explosive (or silent) giving up
watch out for this rise !
Intercede ("scaffold") here
FRUSTRATION LEVEL