Magnetism

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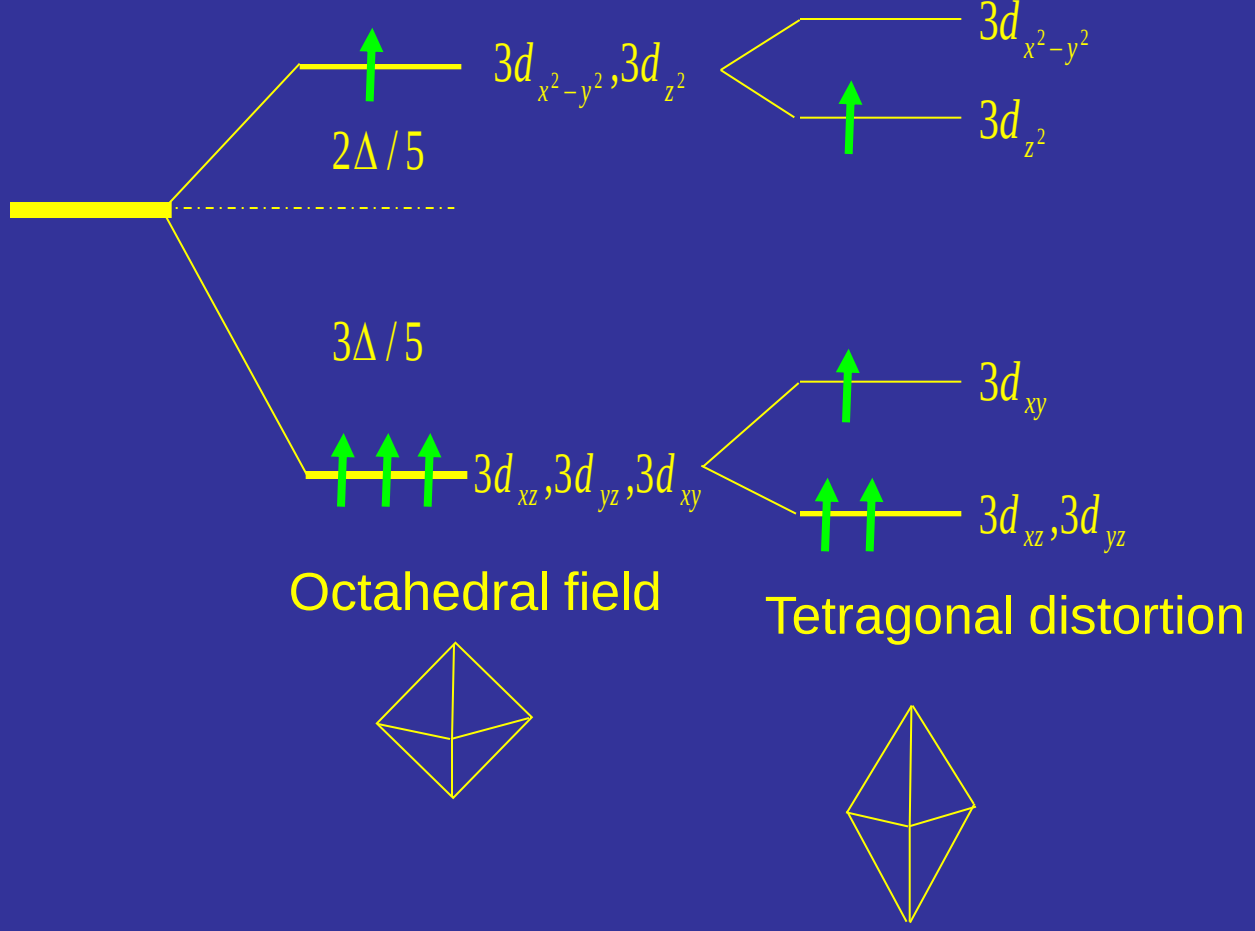
Last time

- Crystal fields
- d,f electrons
- angular momentum quenching
- p-d interactions, splitting of levels
- Spin peierls
- Jahn Teller
- Charge, orbital, spin ordering

Today

Last time	Introduction, environment	Ch.1; 2.1-2.5; 8.9; 3.1
Today	Environment, interactions	3.1; Ch.4; 7.1-7.7

Jahn Teller distortion



Mn^{3+} : $3d^4$

Energy gain due to lowering e_g orbital

Cost: elastic energy

Strong e-p coupling

Does not work for Mn^{4+}

Jahn Teller effect

- Dynamic

  Fluctuations x,y,z distortions (e.g. cubic perovskites)

- Cooperative

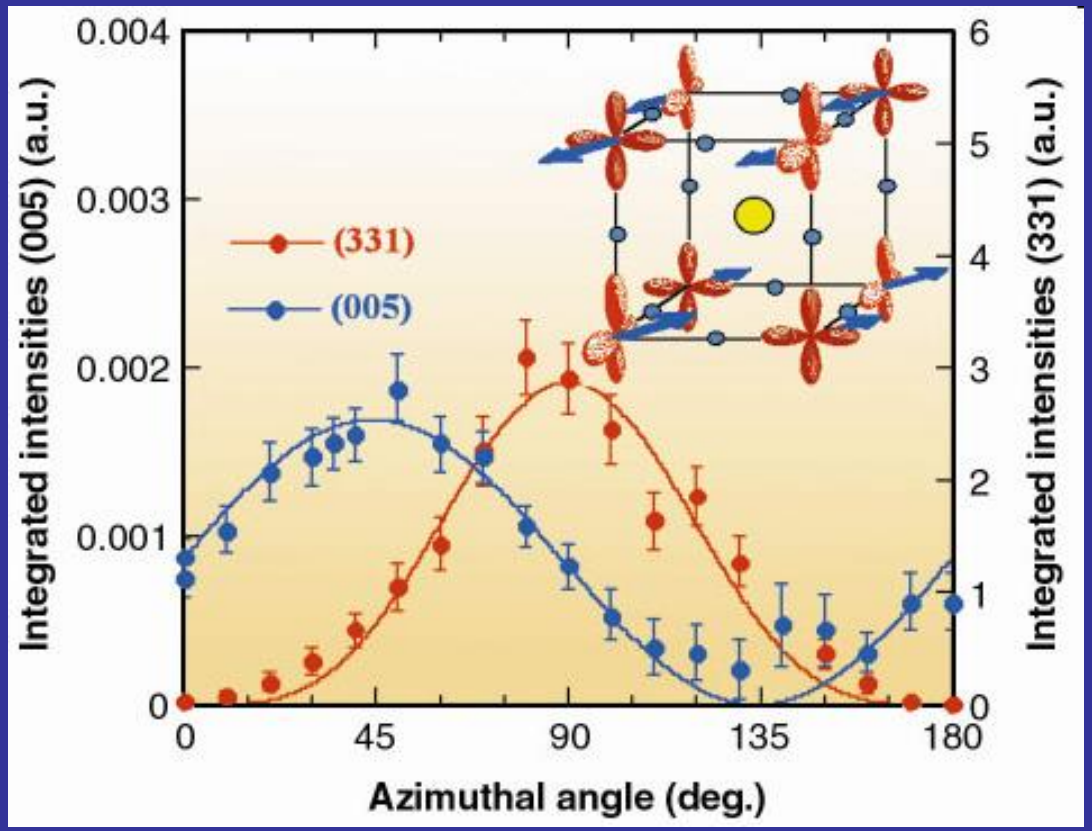
  Lattice mediated

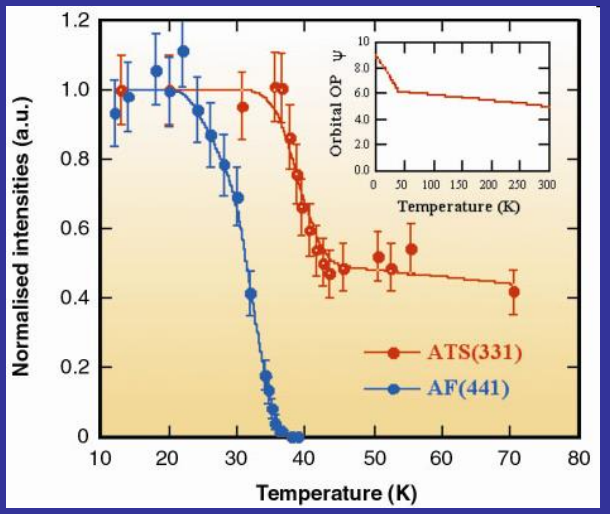
$LaMnO_3$: T > 800 K Cubic, below that tetragonal

$KCuF_3$: Orbital ordering (z^2-x^2 and z^2-y^2 orbitals)

Spin and Orbital ordering

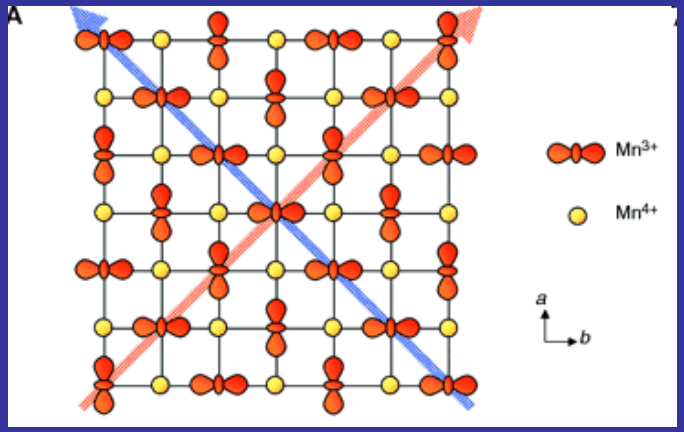
$KCuF_3$: Orbital ordering (z^2-x^2 and z^2-y^2 orbitals)





Murakami et al. PRL 1998

Charge and Orbital order



folk.uio.no/ravi

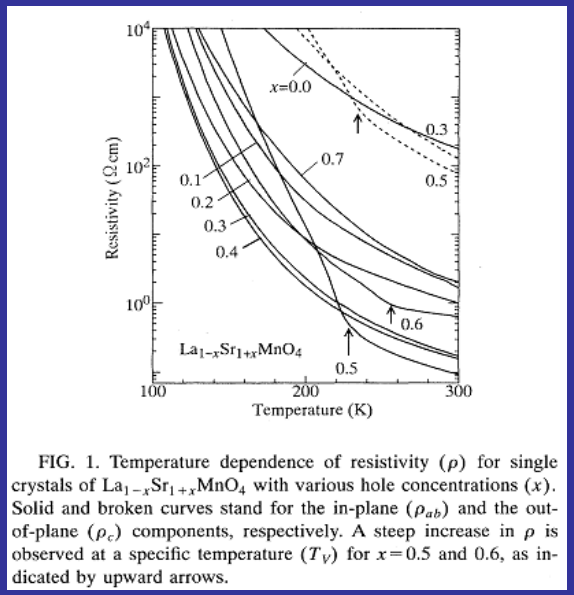


FIG. 1. Temperature dependence of resistivity (ρ) for single crystals of $La_{1-x}Sr_{1+x}MnO_4$ with various hole concentrations (x). Solid and broken curves stand for the in-plane (ρ_{ab}) and the out-of-plane (ρ_c) components, respectively. A steep increase in ρ is observed at a specific temperature (T_V) for $x=0.5$ and 0.6, as indicated by upward arrows.

Moritomo et al. PRB 1995

Charge, Orbital, Spin order in $La_{0.5}Sr_{1.5}MnO_4$

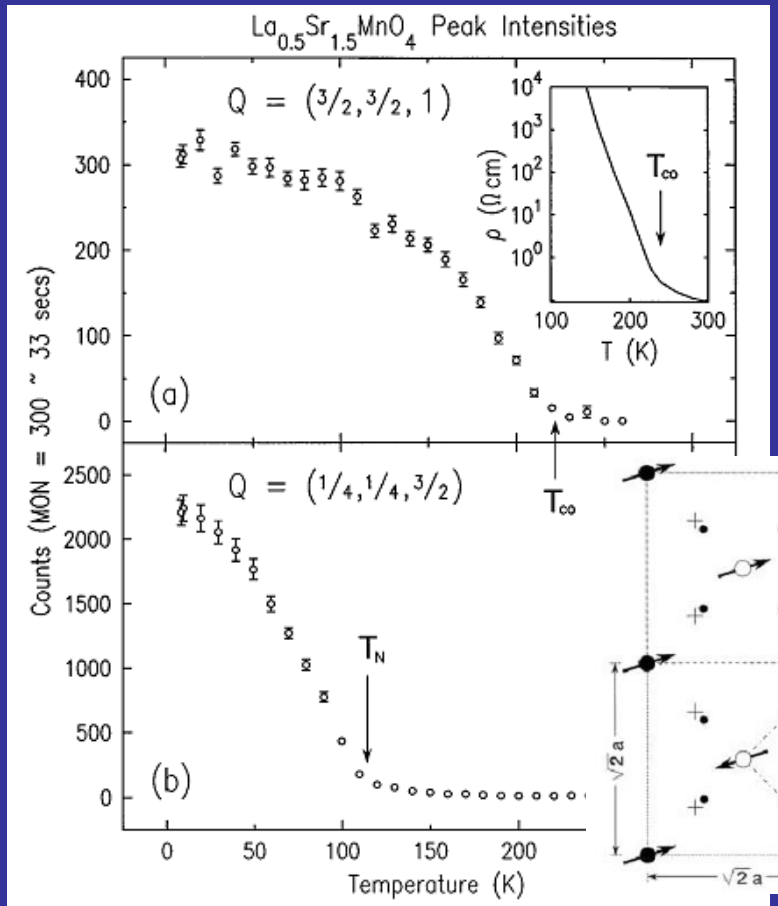


FIG. 4. Temperature dependence of the (a) charge and (b) magnetic order. Inset in (a): Resistivity vs T.

Sternlieb et al. PRL 1996

Interactions

Interactions

- Dipole – Dipole
- Direct exchange (H_2 molecule)
- Indirect exchange
- Double exchange
- Anisotropic exchange
- Rudeman Kittel Kasuya Yoshida (RKKY)
- Stoner (“spontaneous Pauli”)

- Ch. 4 & 7.2,7.3,7.7

Dipole-dipole interaction

Dipole-dipole interaction is an anisotropic interaction

$$E = \frac{\mu_0}{4\pi} \frac{\vec{\mu}_1 \cdot \vec{\mu}_2 - 3(\vec{\mu}_1 \cdot \vec{e}_{12})(\vec{\mu}_2 \cdot \vec{e}_{12})}{r_{12}^3}$$

$$E \approx 10^{-23}\ \mathrm{J} \sim 1\mathrm{K} \quad \text{for } r = 2\,\mathring{\mathrm{A}} \text{ and } \mu = \mu_B$$

In real materials: $T_c \sim 10^2 – 10^3$ K !!

→ Dipole-dipole interaction hardly ever dominates

Reminder H_2 molecule

- LCAO gives wrong solution (e.g. triplet ground state)
- Correlated picture (Heitler-London approach) is better
  - Starting point: two electron orbitals $|\phi_a(1)\phi_b(2)\rangle$ and $|\phi_a(2)\phi_b(1)\rangle$
  - Wavefunctions

$$\Psi_S = \frac{1}{\sqrt{2}}\left[\phi_a(1)\phi_b(2) + \phi_a(2)\phi_b(1)\right]\chi_S$$

$$\Psi_T = \frac{1}{\sqrt{2}}\left[\phi_a(1)\phi_b(2) - \phi_a(2)\phi_b(1)\right]\chi_T$$

  - Spin parts:

$$\chi_S = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

$$\chi_T = \begin{cases} |\uparrow\uparrow\rangle \\ \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) \\ |\downarrow\downarrow\rangle \end{cases}$$

H_2 molecule

- Singlet ground state
- Exchange energy: Pauli + Coulomb

$$H = -\frac{\eta^2}{2m}\left(\nabla_1^{\,2} + \nabla_2^{\,2}\right) + V_c(1,2)$$

$$V_c(1,2) = \frac{e^2}{|r_1 - r_2|} + \frac{e^2}{|R_1 - R_2|} - \frac{e^2}{|r_1 - R_2|} - \frac{e^2}{|r_2 - R_2|}$$

$$E_S - E_T = 2\langle \phi_a(1)\phi_b(2)|V_c|\phi_a(2)\phi_b(1)\rangle := 2J$$

$$H = -2J\$_1 \cdot S_2 = \begin{cases} -2J \cdot -\frac{3}{4} & \text{for the spin singlet} \\ -2J \cdot \frac{1}{4} & \text{for the spin tripl et} \end{cases}$$

Exchange interaction

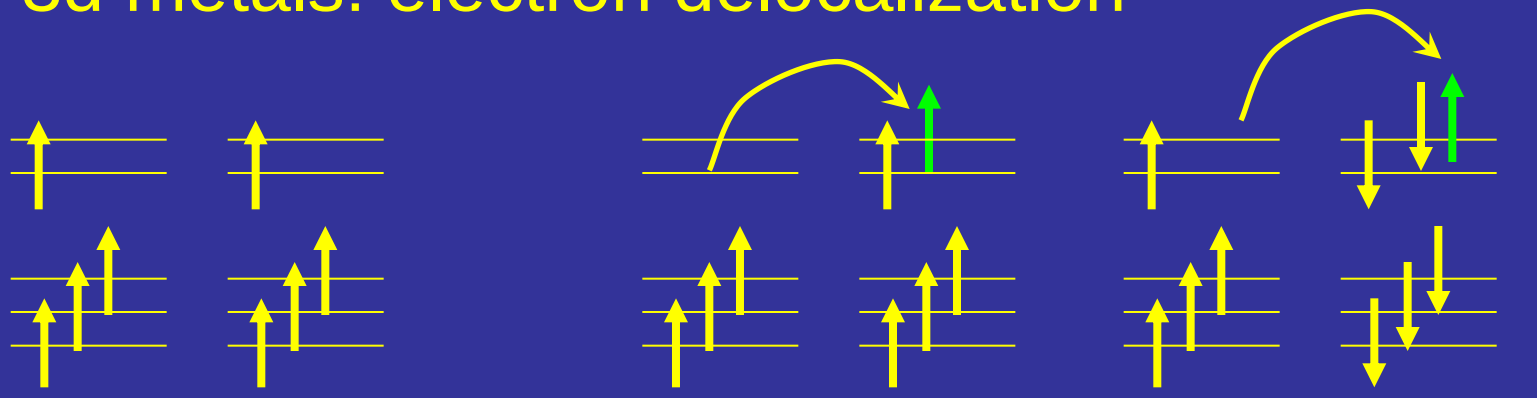
- Heisenberg Hamiltonian

$$H = -2 \cdot \Sigma'_{i,j} J_{i,j} S_i \cdot S_j$$

- J>0: Ferro
- J<0: Antiferro

Direct exchange

- Need direct wave function overlap
  - Often ferromagnetic
  - Small in 4f, 5f elements
  - Can be important in 3d oxides (but see indirect!)
  - In 3d metals: electron delocalization



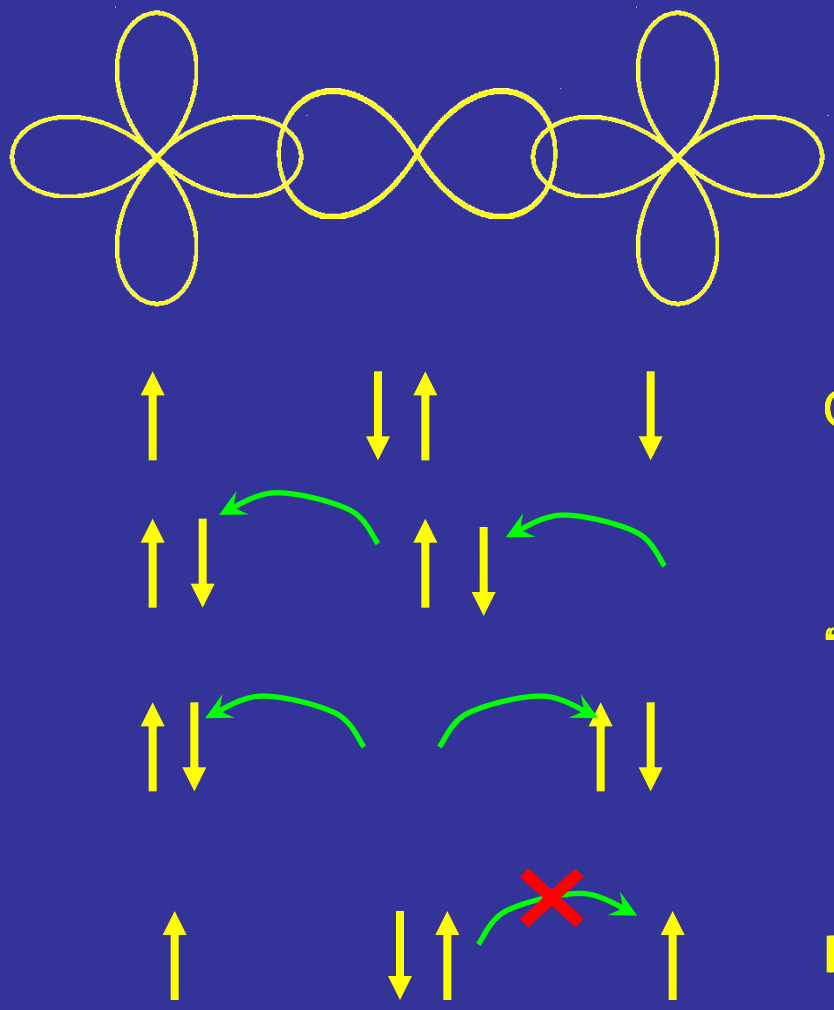
Oxide: ferro

‘hopping’: ferro

‘hopping’: antiferro

- Relatively small
- Depends on orbital occupation and geometry

Indirect exchange



Ground state antiferro

'2*hopping'

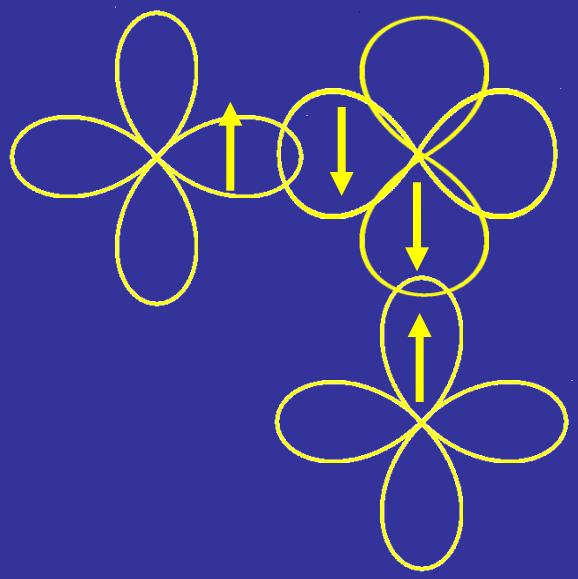
Hopping →
delocalization →
energy gain

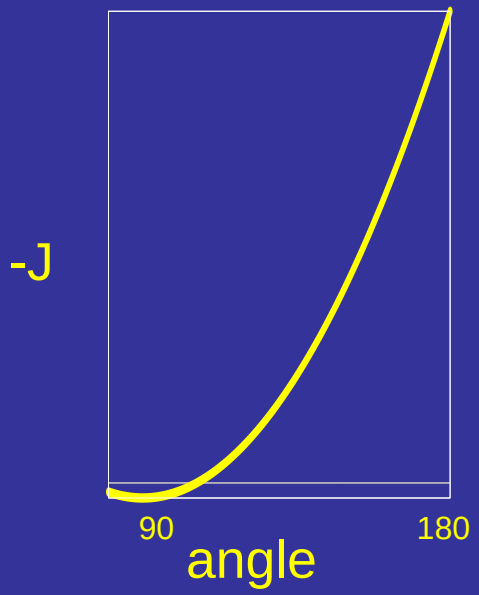
Energy: 2 hops = 2t; cost=U
→ $J \sim -t^2/U$

Pauli forbidden

Examples: High Tc's; MnO; MnF_2

Indirect exchange





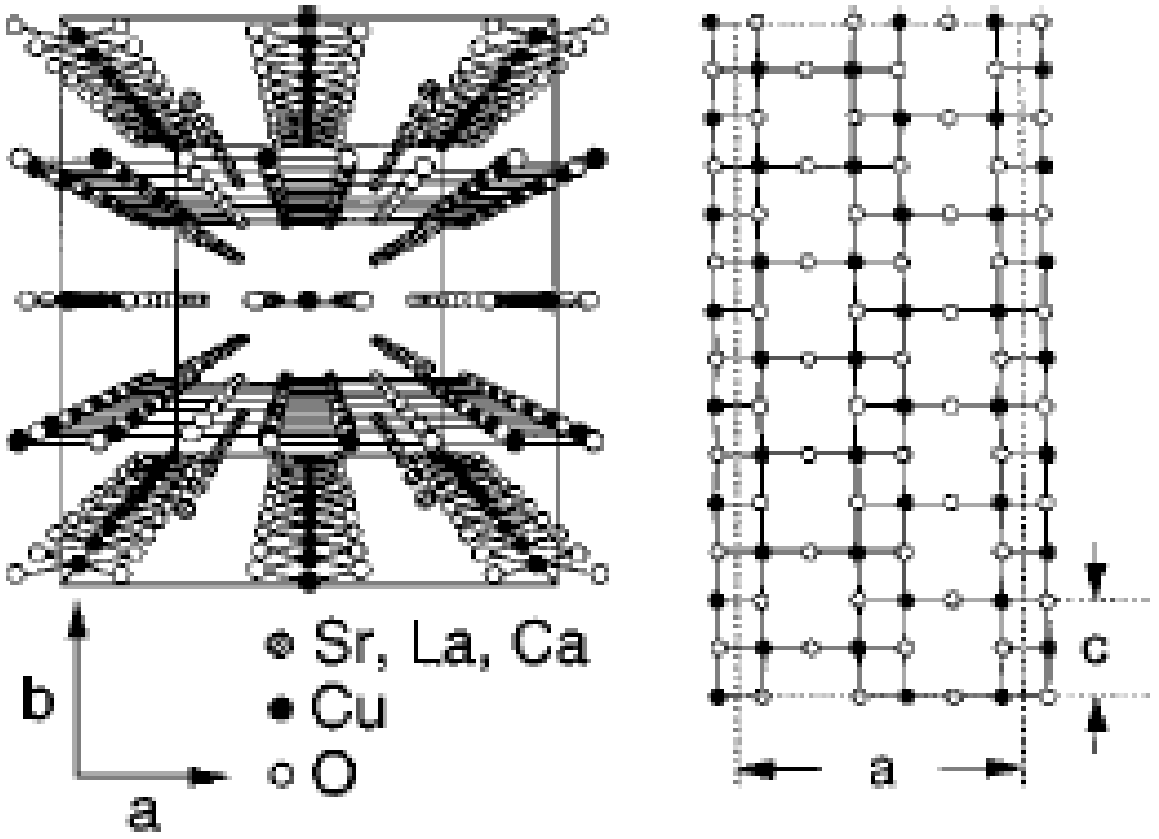
Hopping → delocalization → energy gain
Energy: 2 hops = 2t; cost=U

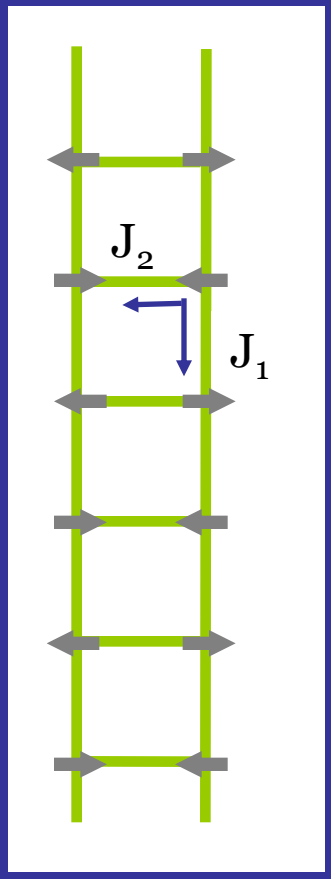
→ $J \sim -t^2/U$

Examples: High Tc's; MnO; MnF_2;
telephone number compound

Relatively strong (depends on U)
Usually AF (F when not same 3d, e.g.d^3-d^5)
Strongly dependent on angle of bonding
at 180^0 strongly AF
at zero weakly F
(goodenough kanamouri rules)

$(Sr,La,Ca)_{14}Cu_{24}O_{41}$

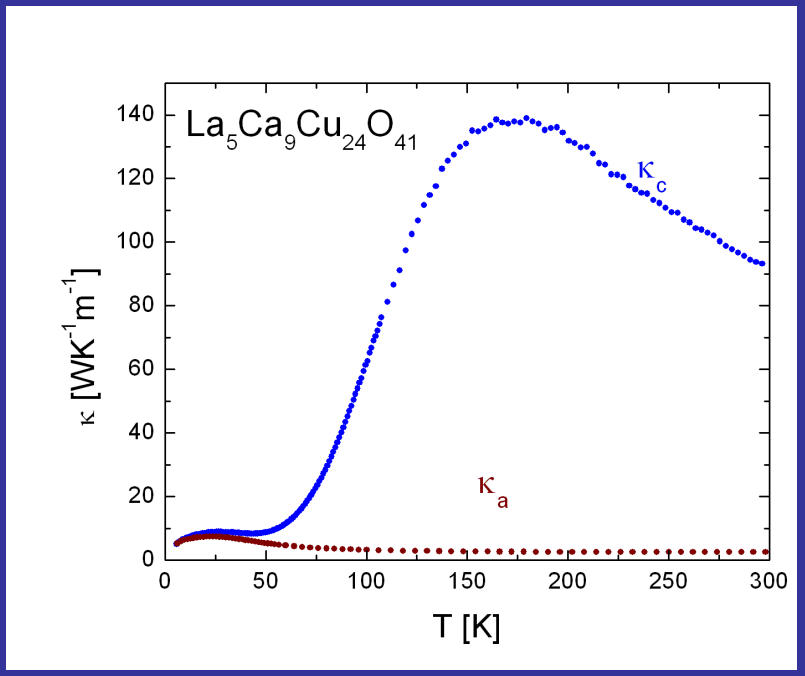


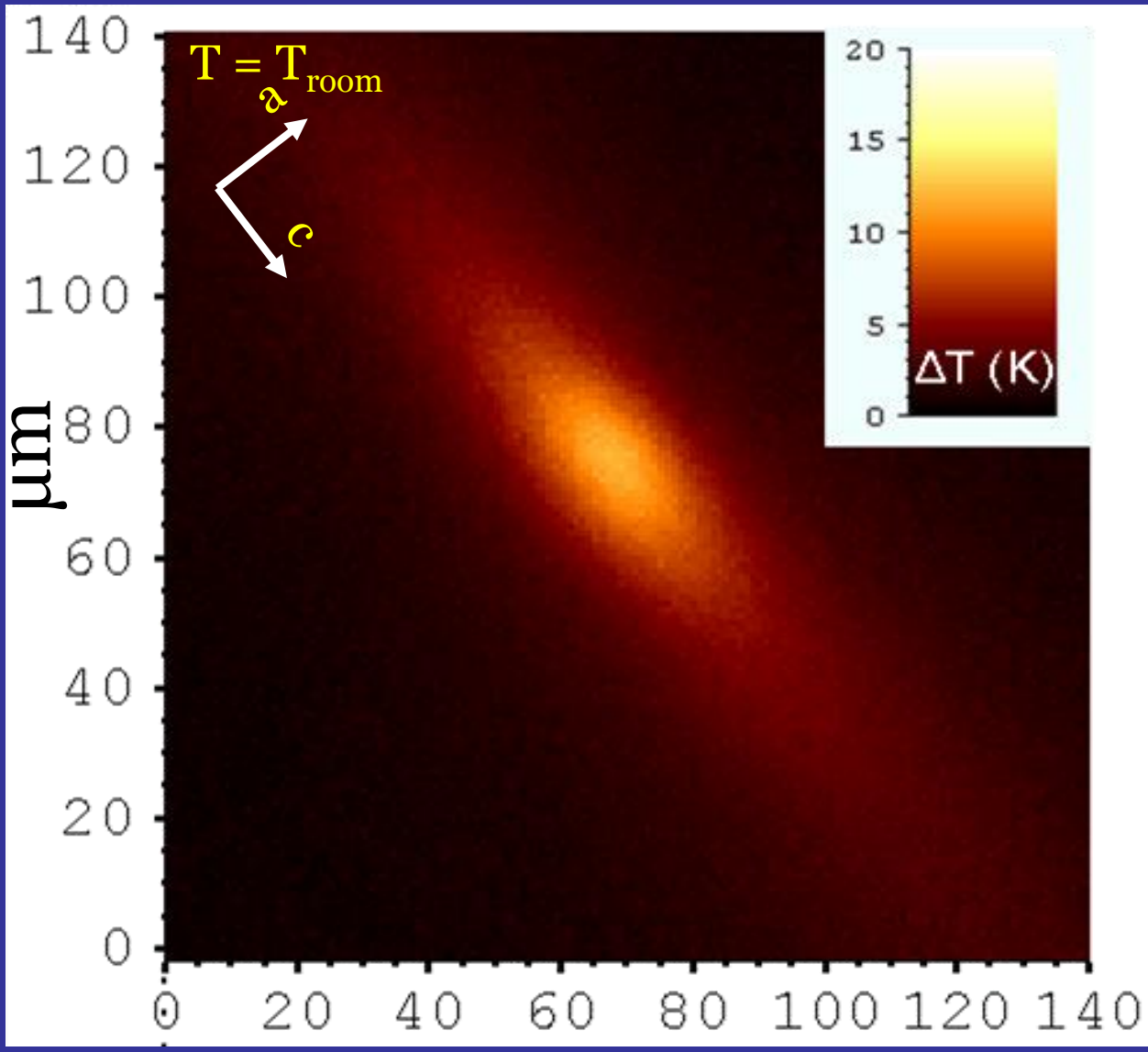


J_1=130 meV
J_2= 70 meV
Δ=32 meV

Eccleston *et al.*, PRL **81**, 1702 (1998)

$La_9Ca_5Cu_{24}O_{41}$

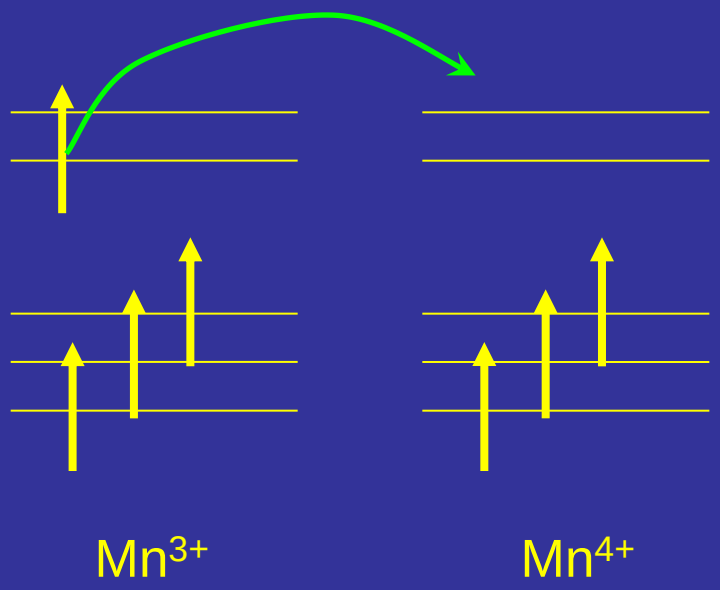


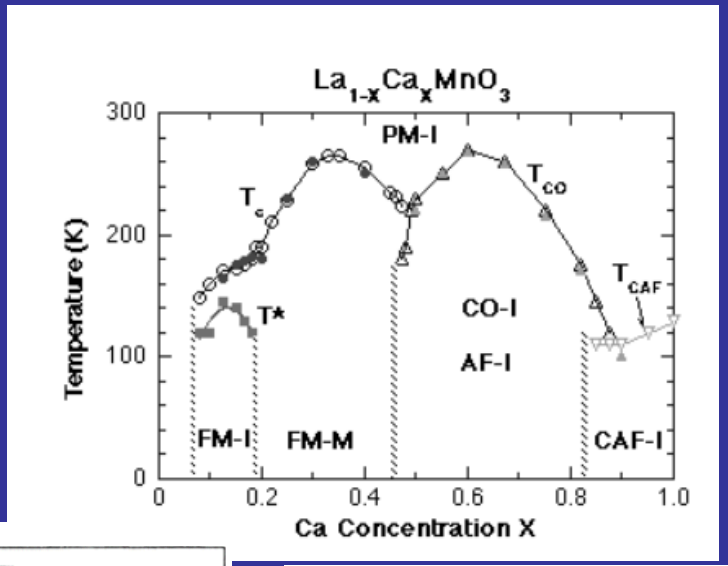


Otter et al., IJMHT 2012

Double exchange

- Mixed valence
- Usually ferro metal
- Relatively strong
- $La_{1-x}Sr_xMnO_3$ (Mn^{3+}/Mn^{4+})
  Fe_3O_4 (AB_2O_4, Fe^{2+}/Fe^{3+})





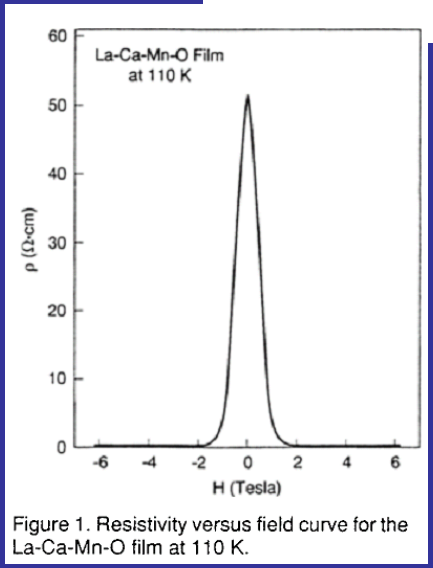


Figure 1. Resistivity versus field curve for the La-Ca-Mn-O film at 110 K.

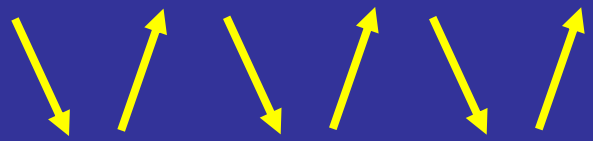
PM-I paramagnetic insulator
FM-M ferromagnetic metal
FM-I ferromagnetic insulator
CO-I charge-ordered insulator
CAF-I canted antiferromagnetic insulator

Fujishiro and co-workers

CMR in para phase close to T_{curie}

Anisotropic exchange

- Dzyaloshinsky-Moriya interaction
- Mixing in of excited d-states
- LS coupling in excited state
- If spins inversion symm. related then 0
- Form different from Heisenberg: $\vec{D} \cdot \vec{S}_i \times \vec{S}_j$
- Favors perpendicular alignment
- Examples: α-Fe_2O_3, $MnCoO_3$
- In AF's leads to net moment → weak ferro (canted AF)



nature materials | VOL 6 | JANUARY 2007 |

Multiferroics

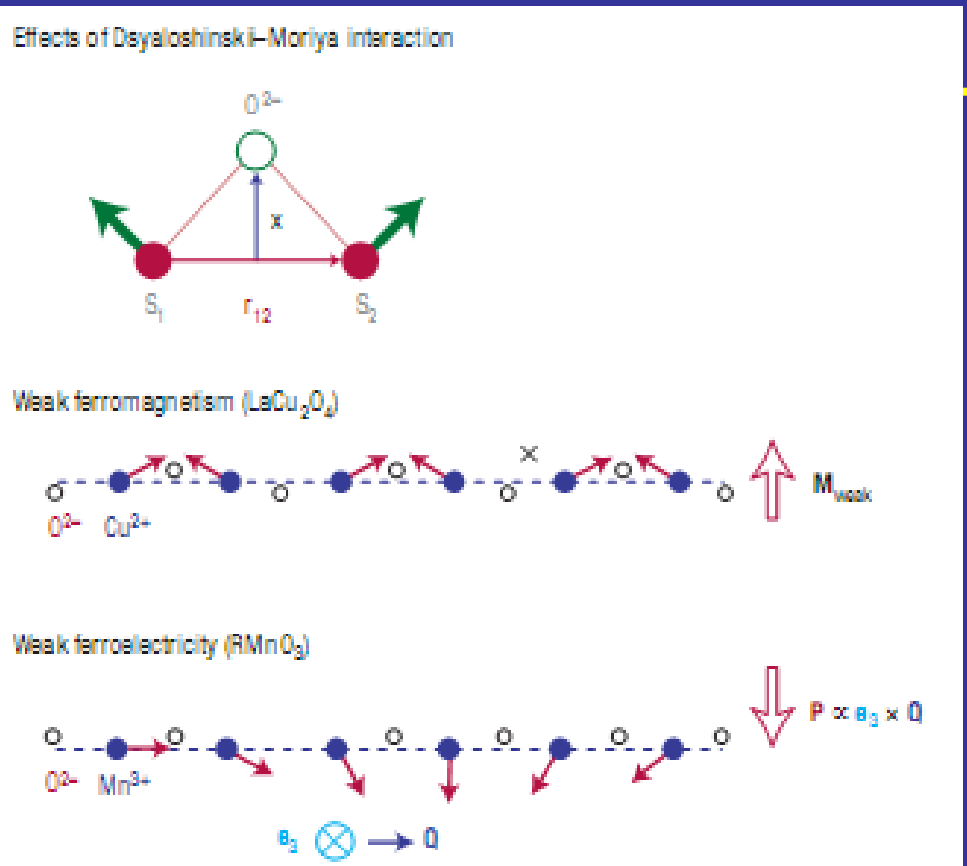
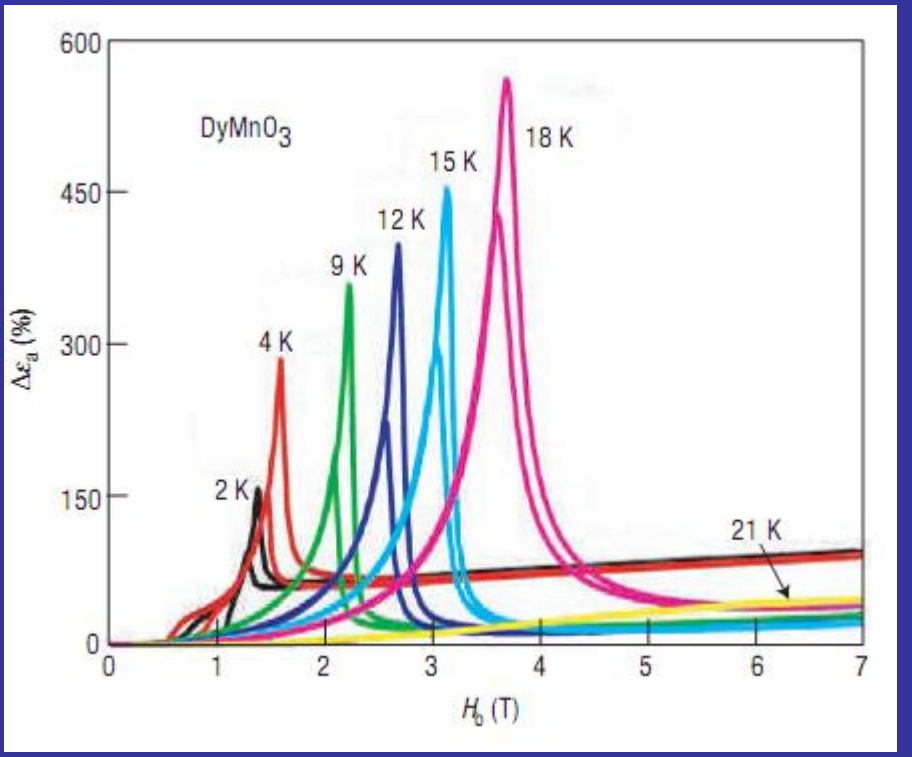


Figure 5 Effects of the antisymmetric Dzyaloshinskii–Moriya interaction. The interaction $H_{DM} = \mathbf{D}_{12} \cdot [\mathbf{S}_1 \times \mathbf{S}_2]$. The Dzyaloshinskii vector $\mathbf{D}_{12}$ is proportional to spin-orbit coupling constant λ, and depends on the position of the oxygen ion (open circle) between two magnetic transition metal ions (filled circles), $\mathbf{D}_{12} \propto \lambda \mathbf{x} \times \mathbf{r}_{12}$. Weak ferromagnetism in antiferromagnets (for example, $LaCu_2O_4$ layers) results from the alternating Dzyaloshinskii vector, whereas (weak) ferroelectricity can be induced by the exchange striction in a magnetic spiral state, which pushes negative oxygen ions in one direction transverse to the spin chain formed by positive transition metal ions.

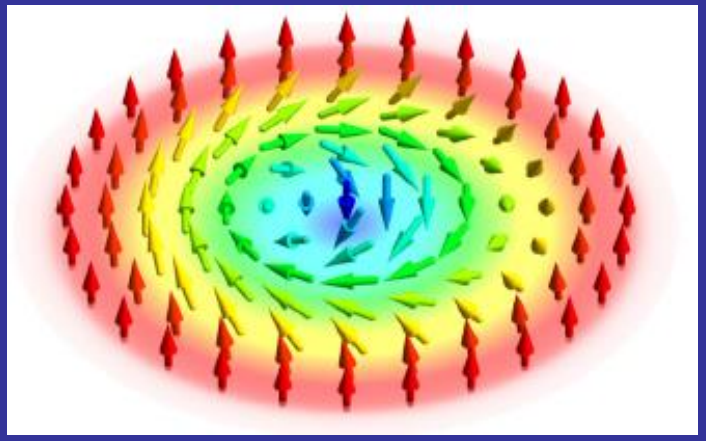


$$\mathbf{P} \propto [(\mathbf{M} \cdot \partial)\mathbf{M} - \mathbf{M}(\partial \cdot \mathbf{M})] .$$

Mostovoy & Cheong

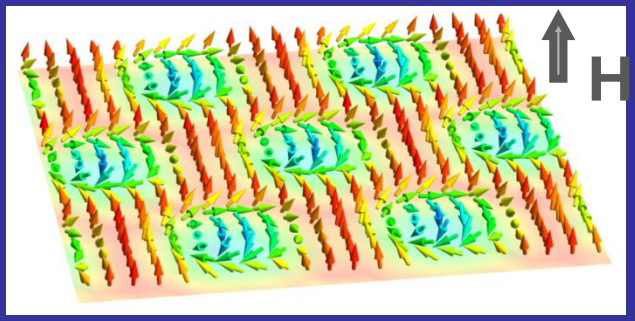
Skyrmions

Bloch skyrmion



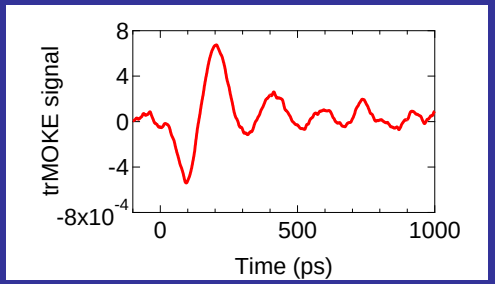
Christoph Schütte and Markus Garst
Phys. Rev. B **90**, 094423 (2014)

Skyrmion lattice



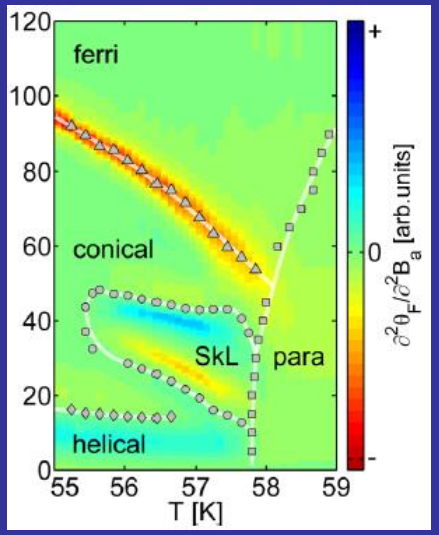
Achim Rosch, Nature Nanotechnology **8**, 160–161 (2013)

Coherent excitations



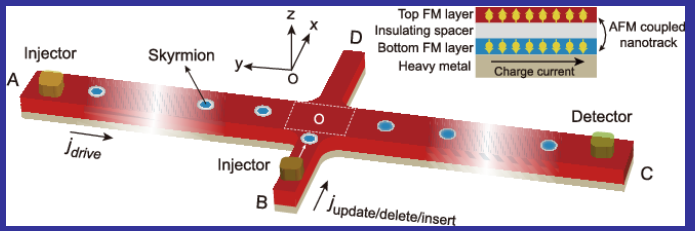
P. Padmanabham *et al.*, (2018)

Phase diagram



R. B. Versteeg *et al.*, PRB **94**, 094409 (2016)

Skyrmion racetrack



Zhu et al. (2018)