

2020/9/1 Lecture 7 (15:00-16:30)

Functional Oxide Spintronics and the material design

ISIR, Osaka University Teruo Kanki

E-mail: kanki@sanken.osaka-u.ac.jp

STO(100)

2 nm



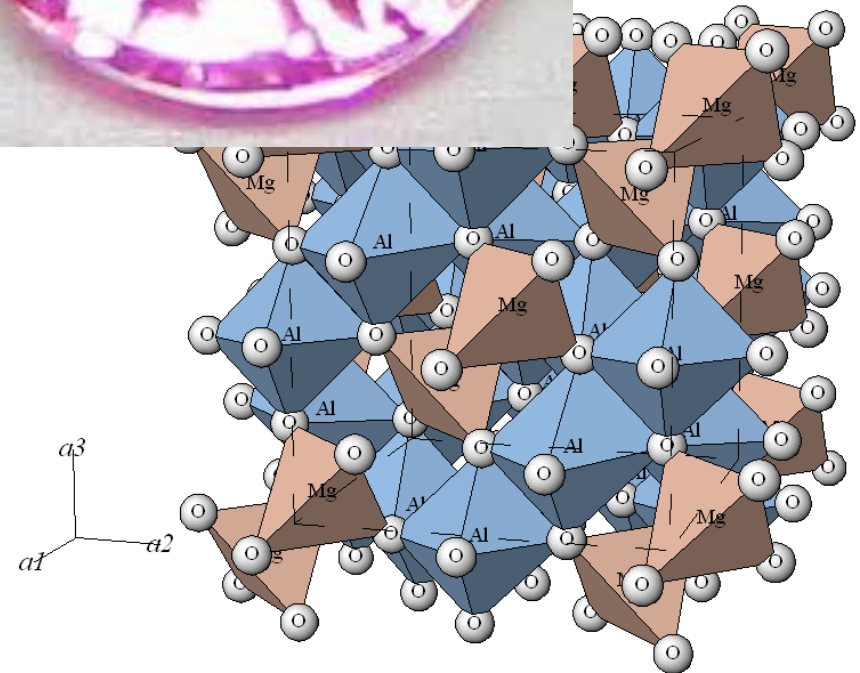


Ceramics



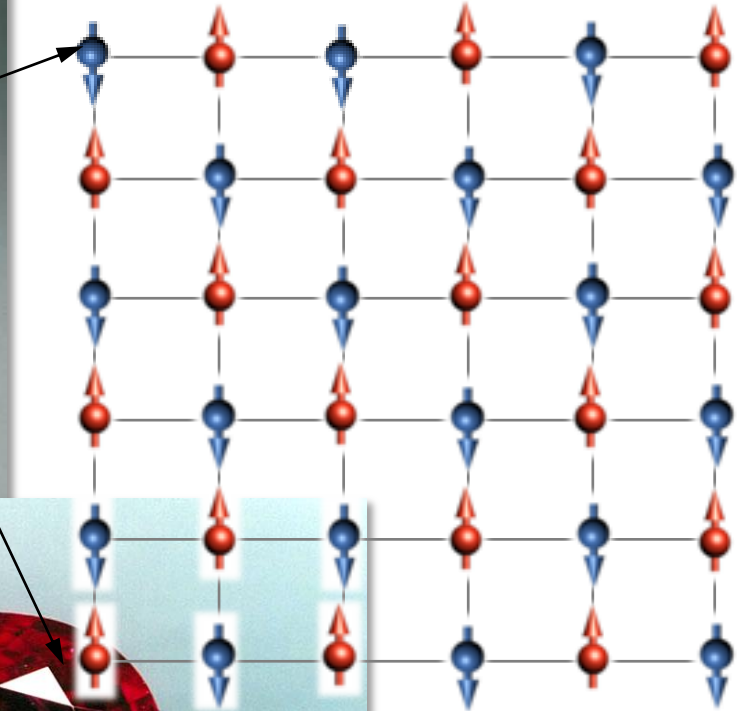


Jewelry (Spinel, Garnet)



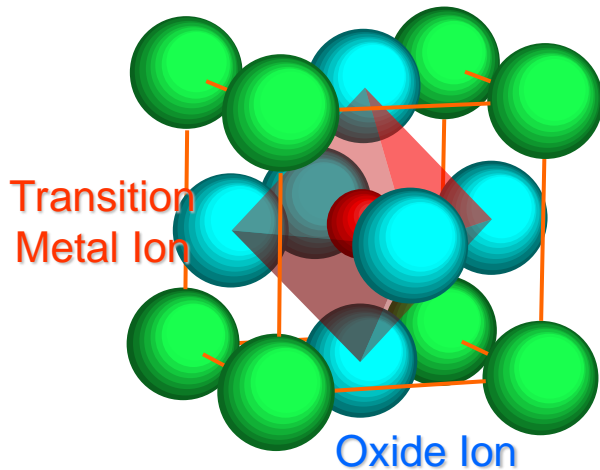


Functional Oxides





Transition Metal Oxides

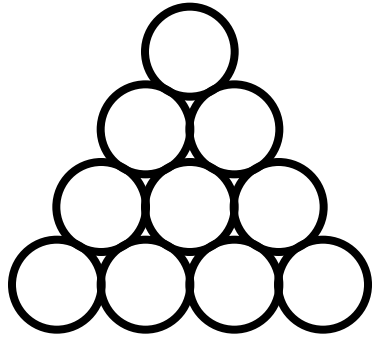


| | | | | | | | |
|---|--|---|---|---------------------------------------|--|--|---|
| 22 Ti 47.87 チタン Titanium | 23 V 50.94 バナジウム Vanadium | 24 Cr 52.00 クロム Chromium | 25 Mn 54.94 マンガン Manganese | 26 Fe 55.85 鉄 Iron | 27 Co 58.93 コバルト Cobalt | 28 Ni 58.69 ニッケル Nickel | 29 Cu 63.55 銅 Copper |
|---|--|---|---|---------------------------------------|--|--|---|

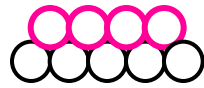
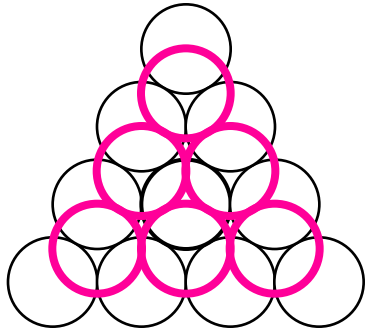
| | | |
|---------------------------|-----------------------|----------------------------------|
| Ferro dielectrics | Anti-/Ferro magnetics | High temperature superconductors |
| Piezoelectrics | Colossal MR | Conductors |
| Memory (DRAM, FRAM, RRAM) | Magnetic head | Magnetic recorder |
| | Memory (MRAM) | Josephson junction electrode |
| Piezoelectric devices | | SQUID |
| | | Bolometer |

Information processing and data storage materials related with our daily life

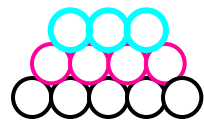
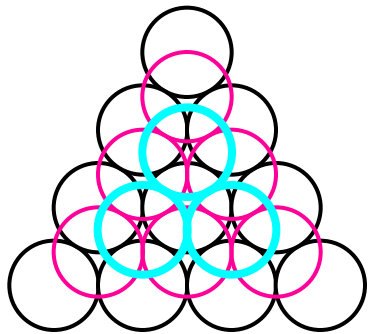
Face-centered cubic => Closed pack structure



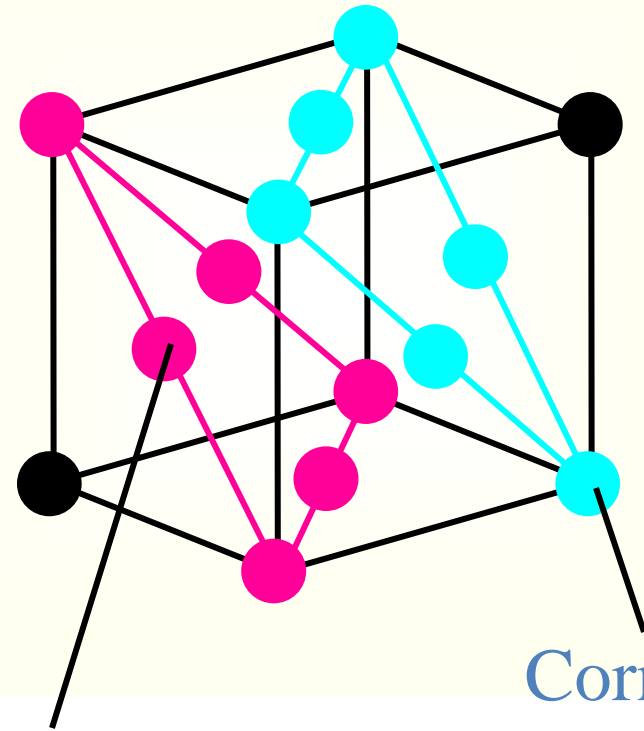
1st layer



2nd layer



3rd layer



Center face

$1/2 \times 6$ parts

Corner

$1/8 \times 8$ parts

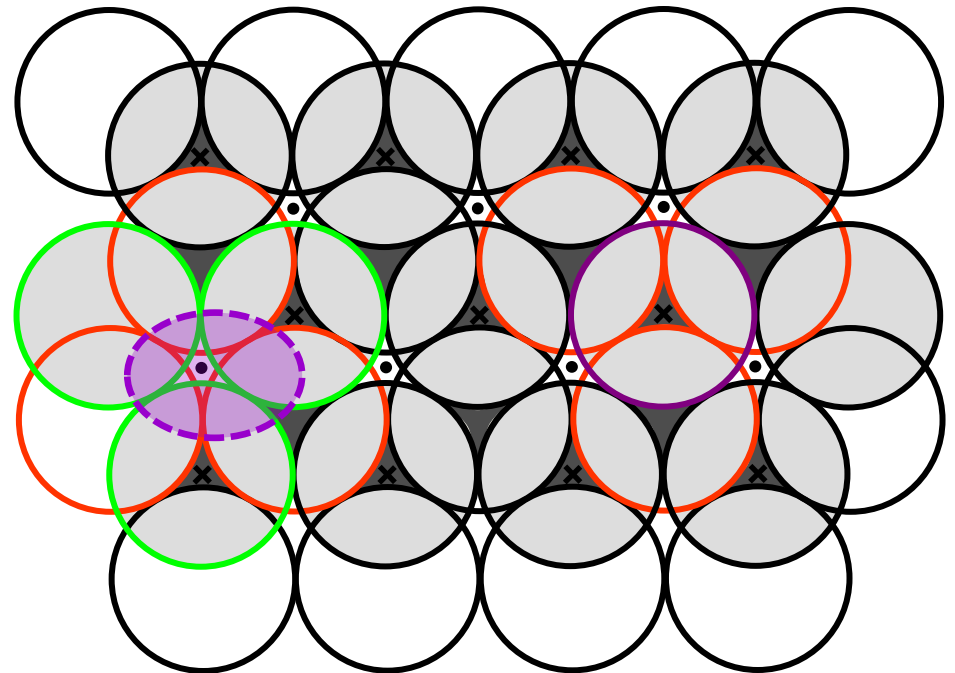
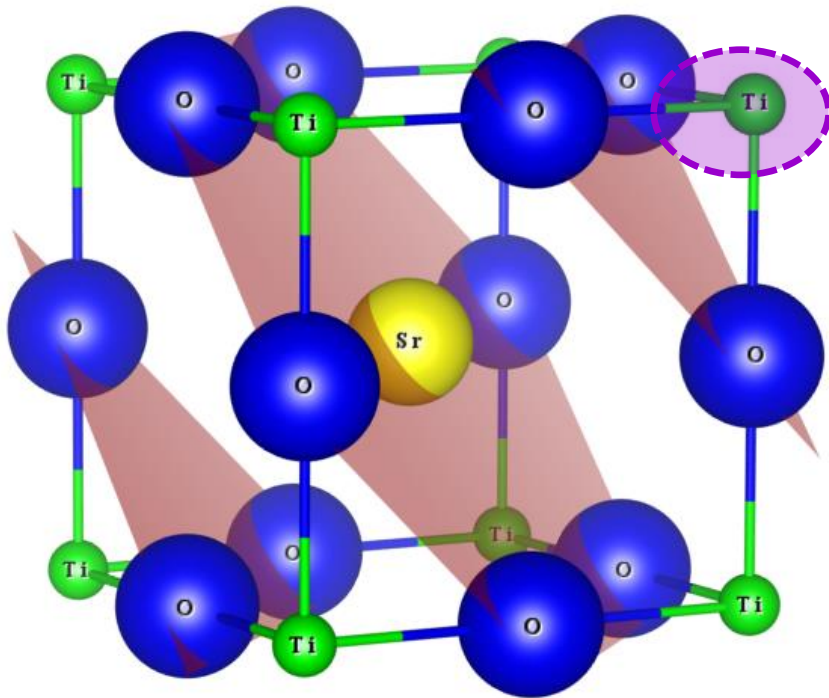
Perovskite structure: ABO_3 e.g. $SrTiO_3$

Interspace of close packed oxide ions : **Octahedral interspace**

$$O^{2-} = 1.40 \text{ \AA} ,$$

$$Sr^{2+} = 1.44 \text{ \AA} \text{ (12 coordination),}$$

$$\geq 0.414r \quad Ti^{4+} = 0.42 \text{ \AA} \text{ (6 coordination)}$$





Orbital bonding

Bonding and Antibonding states

⇒ Valence and Conduction band

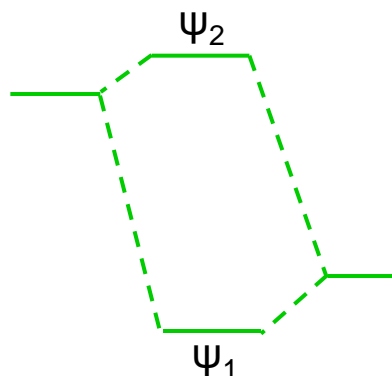
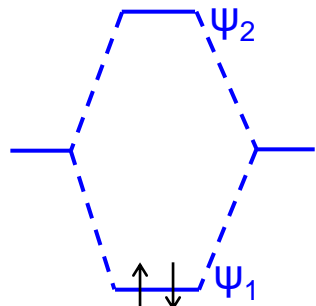
Covalent bonding H H₂ H

A A-B B

Ion bonding

$$\psi_2 = \chi_A - \chi_B$$

Energy ↑

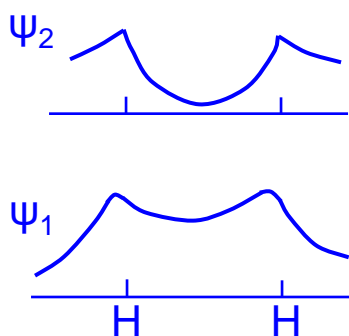


$$\psi_2 = a_2\chi_A - b_2\chi_B$$

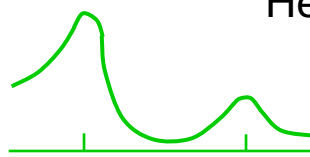
$$\psi_1 = \chi_A + \chi_B$$

$$\psi_1 = a_1\chi_A + b_1\chi_B$$

Electron density ↑



Antibonding

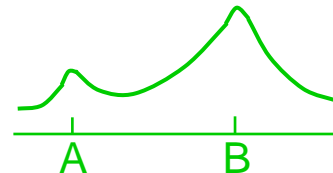


Heteronuclear diatomic molecule

(Covalent or Ionic characters)

↓
Different orbital level

Bonding



Electronegativity
Ionization potential

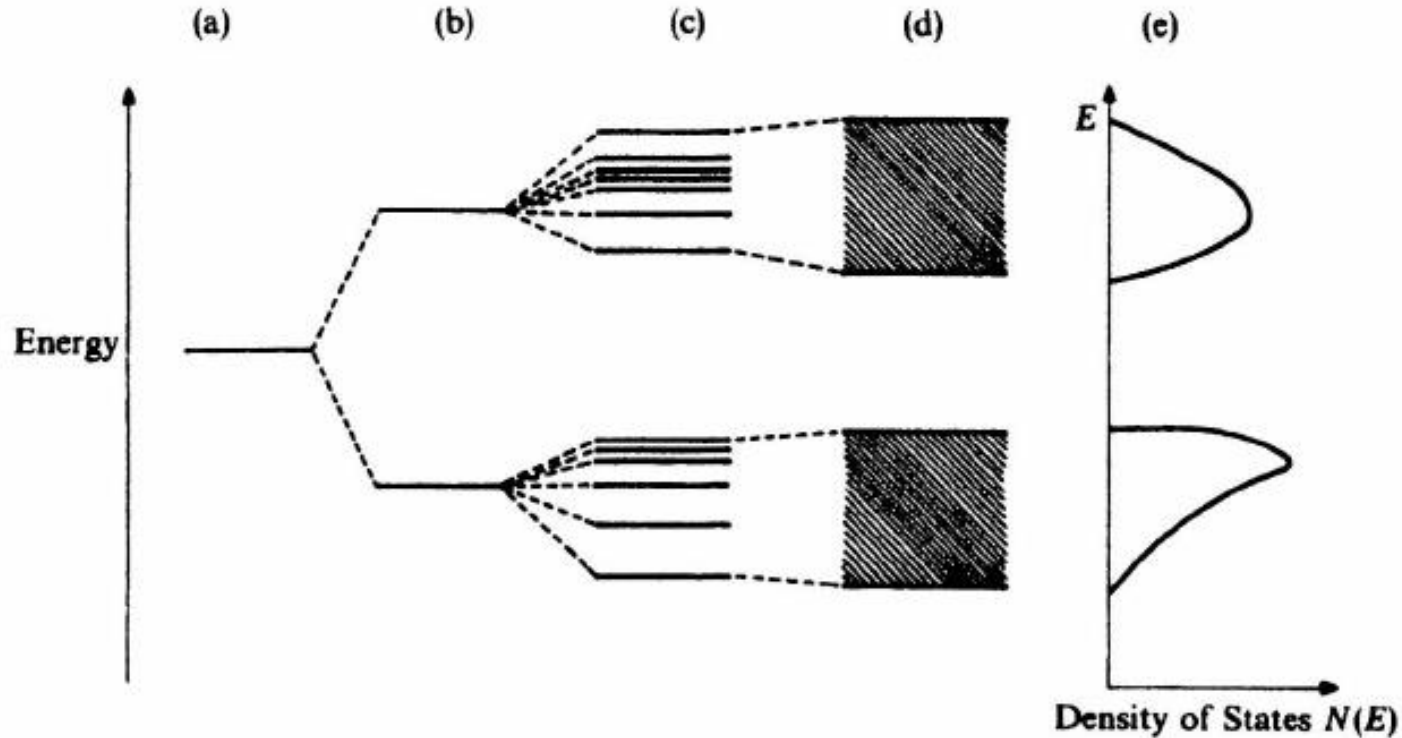
(a)

(b)

Electron distributions and energies of molecular orbitals in (a) H₂ and a heteronuclear molecule AB



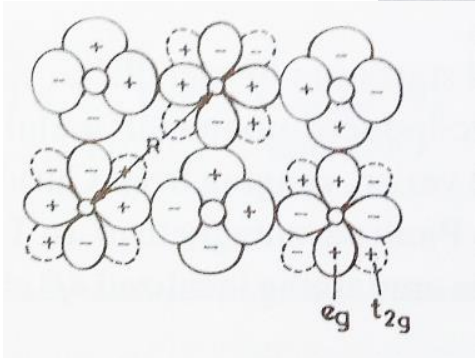
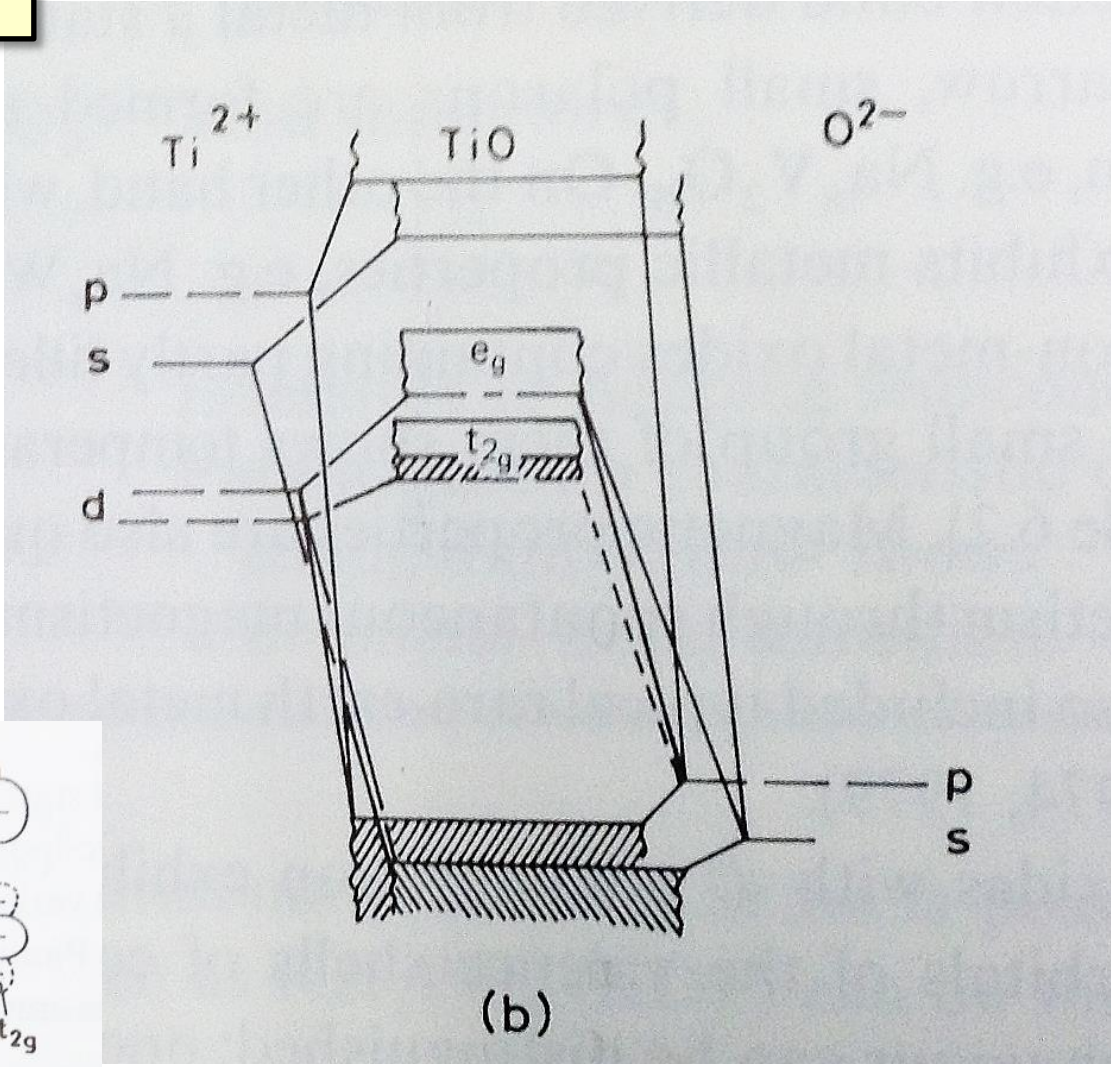
From orbital to band formation



Orbital energies of (a) atom, (b) small molecule, (c) large molecule, (d) solid, and (e) density of states corresponding to (d)

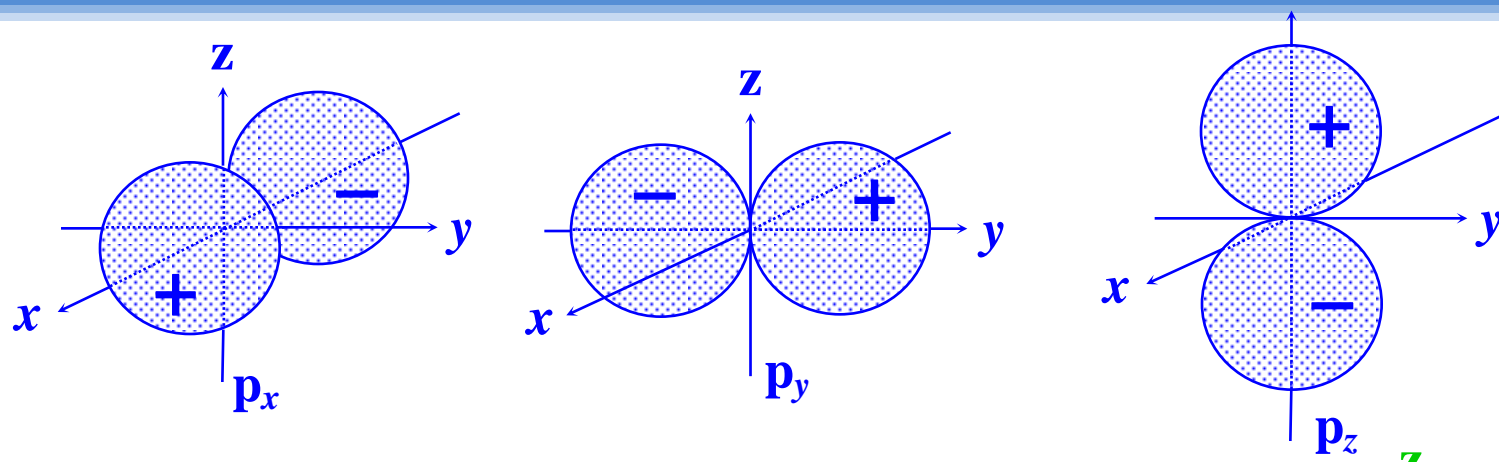


TiO

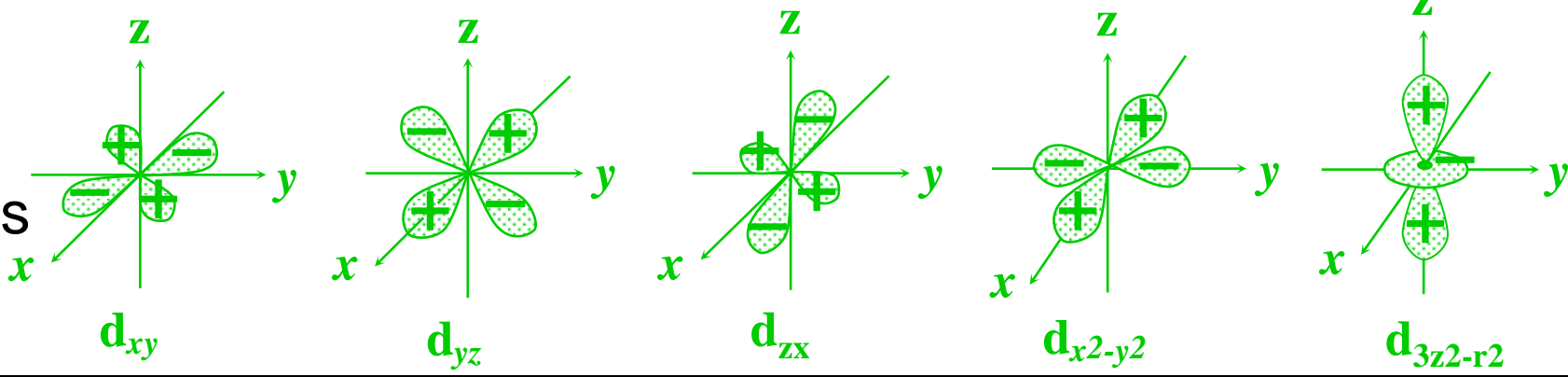


Existence of electrons - Orbital shape

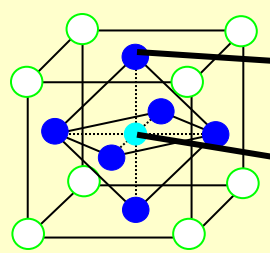
p orbitals



d orbitals

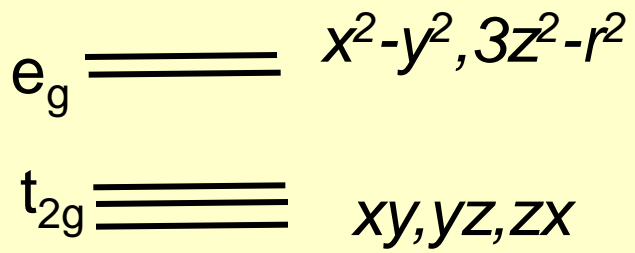


Perovskite structure



Oxygen atom
3d transition metal

Ligand field splitting
(Crystal field splitting)



Periodic Table of the Elements

| | | | | | | | | | | | | | | | | | |
|--|---|---|---|---|--|---|--|--|--|---|--|--|--|---|---|---|--|
| 1A 1 1s -1 1 1 H Hydrogen 1.008 | 2A 2 [He] 2 He Helium 4.003 | 3A 13 [Ne] 3 B Boron 10.81 | 4A 14 [Ne] 4 C Carbon 12.011 | 5A 15 [Ne] 5 N Nitrogen 14.007 | 6A 16 [Ne] 6 O Oxygen 15.999 | 7A 17 [Ne] 7 F Fluorine 18.998 | 8A 18 [Ne] 8 Ne Neon 20.180 | | | | | | | | | | |
| 11A 11 [Ar] 4 Na Sodium 22.990 | 12A 12 [Ar] 4 Mg Magnesium 24.305 | 13A 13 [Ar] 4 Al Aluminum 26.982 | 14A 14 [Ar] 4 Si Silicon 28.086 | 15A 15 [Ar] 4 P Phosphorus 30.974 | 16A 16 [Ar] 4 S Sulfur 32.06 | 17A 17 [Ar] 4 Cl Chlorine 35.45 | 18A 18 [Ar] 4 Ar Argon 39.948 | | | | | | | | | | |
| 19A 19 [Kr] 5 K Potassium 39.098 | 20A 20 [Kr] 5 Ca Calcium 40.078 | 21A 21 [Kr] 5 Sc Scandium 44.956 | 22A 22 [Kr] 5 Ti Titanium 47.88 | 23A 23 [Kr] 5 V Vanadium 50.942 | 24A 24 [Kr] 5 Cr Chromium 52.00 | 25A 25 [Kr] 5 Mn Manganese 54.938 | 26A 26 [Kr] 5 Fe Iron 55.845 | 27A 27 [Kr] 5 Co Cobalt 58.933 | 28A 28 [Kr] 5 Ni Nickel 58.69 | 29A 29 [Kr] 5 Cu Copper 63.546 | 30A 30 [Kr] 5 Zn Zinc 65.38 | 31A 31 [Kr] 5 Ga Gallium 69.723 | 32A 32 [Kr] 5 Ge Germanium 72.64 | 33A 33 [Kr] 5 As Arsenic 74.922 | 34A 34 [Kr] 5 Se Selenium 78.96 | 35A 35 [Kr] 5 Br Bromine 79.904 | 36A 36 [Kr] 5 Kr Krypton 83.80 |
| 37A 37 [Xe] 6 Rb Rubidium 85.468 | 38A 38 [Xe] 6 Sr Strontium 87.62 | 39A 39 [Xe] 6 Y Yttrium 88.906 | <p>electron configuration</p> <p>oxidation states in compounds: important, most important (for easier reading, arabic numerals are used instead of the correct roman ones)</p> <p>atomic number name (IUPAC)</p> <p>element essential to all biological species investigated essential to at least one biological species biological function suggested essential to humans suggested to be essential to humans</p> <p>atomic radius in pm (half the interatomic distance for the element; α-Fe in this example) covalent radius for single bonds in pm (after Pauling; radii for polar and multiple bonds are shorter) ionic radius in pm with oxidation number coordination number (Cr, Mn, Fe, Co: values for high-spin complexes) van der Waals radius in pm</p> <p>reduction potential E° in V with number (n) of electrons for: E° + ne⁻ ⇌ E(s) (metals) E° + ne⁻ ⇌ E⁻ EO₂ + nH⁺ + ne⁻ ⇌ E(s) + n/2 H₂O 1/2 O₂(g) + 2H⁺ + 2e⁻ ⇌ H₂O(l)</p> <p>electronegativity (Allred and Rochow)</p> <p>abundance (mass fraction in % of the element in the earth's lithosphere (upper 16 km) plus hydrosphere (oceans) plus atmosphere; mass fraction calculated from natural radioactive series or other natural nuclear reactions)</p> | | | | | | | | | | 37A 37 [Xe] 6 Br Bromine 79.904 | 38A 38 [Xe] 6 Kr Krypton 83.80 | | | |
| 39A 39 [Xe] 6 La - Lu Lanthanum - Lutetium 89 to 103 | 40A 40 [Xe] 6 Hf Hafnium 178.49 | 41A 41 [Xe] 6 Ta Tantalum 180.948 | 42A 42 [Xe] 6 W Tungsten 183.84 | 43A 43 [Xe] 6 Re Rhenium 186.207 | 44A 44 [Xe] 6 Os Osmium 190.23 | 45A 45 [Xe] 6 Ir Iridium 192.222 | 46A 46 [Xe] 6 Pt Platinum 195.084 | 47A 47 [Xe] 6 Au Gold 196.967 | 48A 48 [Xe] 6 Hg Mercury 200.59 | 49A 49 [Xe] 6 Tl Thallium 204.384 | 50A 50 [Xe] 6 Pb Lead 207.2 | 51A 51 [Xe] 6 Bi Bismuth 208.98 | 52A 52 [Xe] 6 Po Polonium 209 | 53A 53 [Xe] 6 At Astatine 210 | 54A 54 [Xe] 6 Rn Radon 222 | | |
| 57A 57 [Xe] 6 La - Lu Lanthanum - Lutetium 89 to 103 | 58A 58 [Xe] 6 Ce Cerium 140.12 | 59A 59 [Xe] 6 Pr Praseodymium 140.908 | 60A 60 [Xe] 6 Nd Neodymium 144.24 | 61A 61 [Xe] 6 Pm Promethium 145 | 62A 62 [Xe] 6 Sm Samarium 150.36 | 63A 63 [Xe] 6 Eu Europium 151.964 | 64A 64 [Xe] 6 Gd Gadolinium 157.25 | 65A 65 [Xe] 6 Tb Terbium 158.925 | 66A 66 [Xe] 6 Dy Dysprosium 162.50 | 67A 67 [Xe] 6 Ho Holmium 164.930 | 68A 68 [Xe] 6 Er Erbium 167.259 | 69A 69 [Xe] 6 Tm Thulium 168.930 | 70A 70 [Xe] 6 Yb Ytterbium 173.054 | 71A 71 [Xe] 6 Lu Lutetium 174.967 | | | |
| 71A 71 [Xe] 6 La - Lu Lanthanum - Lutetium 89 to 103 | 72A 72 [Xe] 6 Ac Actinium 227 | 73A 73 [Xe] 6 Th Thorium 232.037 | 74A 74 [Xe] 6 Pa Protactinium 231 | 75A 75 [Xe] 6 U Uranium 238.029 | 76A 76 [Xe] 6 Np Neptunium 237 | 77A 77 [Xe] 6 Pu Plutonium 244 | 78A 78 [Xe] 6 Am Americium 243 | 79A 79 [Xe] 6 Cm Curium 247 | 80A 80 [Xe] 6 Bk Berkelium 247 | 81A 81 [Xe] 6 Cf Californium 251 | 82A 82 [Xe] 6 Es Einsteinium 252 | 83A 83 [Xe] 6 Fm Fermium 257 | 84A 84 [Xe] 6 Md Mendelevium 258 | 85A 85 [Xe] 6 No Nobelium 259 | 86A 86 [Xe] 6 Lr Lawrencium 260 | | |

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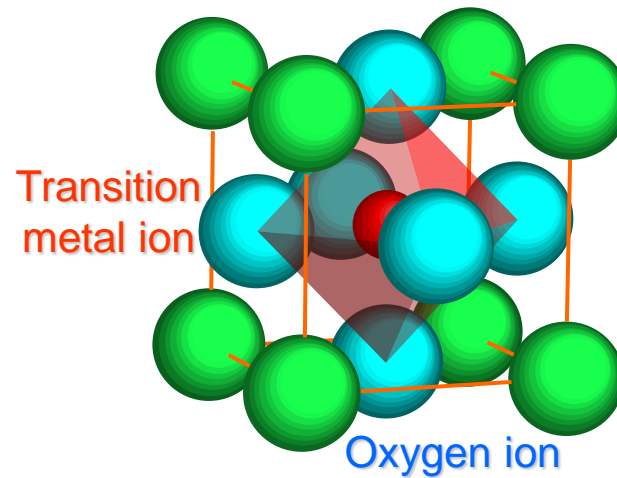
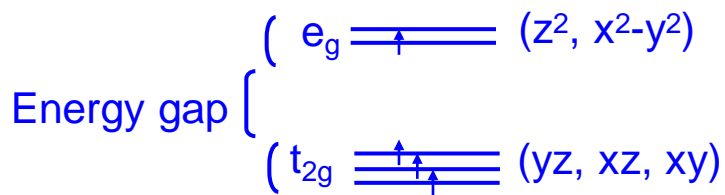
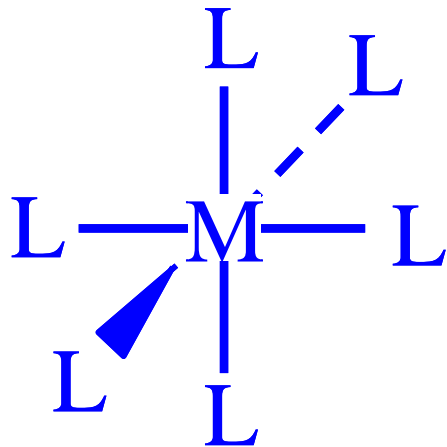
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|--|--|---|---|---|--|---|--|--|--|--|--|--|--|--|---|---|
| 57A 57 [Xe] 6 La Lanthanum 138.905 | 58A 58 [Xe] 6 Ce Cerium 140.12 | 59A 59 [Xe] 6 Pr Praseodymium 140.908 | 60A 60 [Xe] 6 Nd Neodymium 144.24 | 61A 61 [Xe] 6 Pm Promethium 145 | 62A 62 [Xe] 6 Sm Samarium 150.36 | 63A 63 [Xe] 6 Eu Europium 151.964 | 64A 64 [Xe] 6 Gd Gadolinium 157.25 | 65A 65 [Xe] 6 Tb Terbium 158.925 | 66A 66 [Xe] 6 Dy Dysprosium 162.50 | 67A 67 [Xe] 6 Ho Holmium 164.930 | 68A 68 [Xe] 6 Er Erbium 167.259 | 69A 69 [Xe] 6 Tm Thulium 168.930 | 70A 70 [Xe] 6 Yb Ytterbium 173.054 | 71A 71 [Xe] 6 Lu Lutetium 174.967 | | |
| 87A 87 [Xe] 6 Fr Francium 223 | 88A 88 [Xe] 6 Ra Radium 226 | 89A 89 [Xe] 6 Ac Actinium 227 | 90A 90 [Xe] 6 Th Thorium 232.037 | 91A 91 [Xe] 6 Pa Protactinium 231 | 92A 92 [Xe] 6 U Uranium 238.029 | 93A 93 [Xe] 6 Np Neptunium 237 | 94A 94 [Xe] 6 Pu Plutonium 244 | 95A 95 [Xe] 6 Am Americium 243 | 96A 96 [Xe] 6 Cm Curium 247 | 97A 97 [Xe] 6 Bk Berkelium 247 | 98A 98 [Xe] 6 Cf Californium 251 | 99A 99 [Xe] 6 Es Einsteinium 252 | 100A 100 [Xe] 6 Fm Fermium 257 | 101A 101 [Xe] 6 Md Mendelevium 258 | 102A 102 [Xe] 6 No Nobelium 259 | 103A 103 [Xe] 6 Lr Lawrencium 260 |

Crystal field splitting of perovskite structure

Octahedral ligands





Required interaction for material design

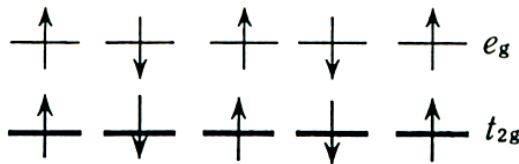
Superexchange interaction

Double exchange interaction

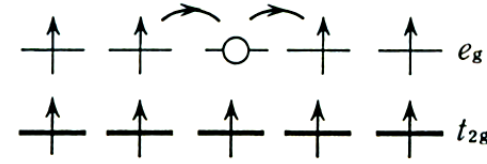
LaMnO₃

Carrier doping

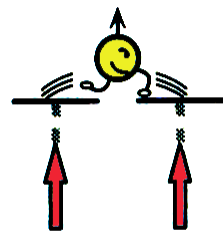
(La,Sr)MnO₃



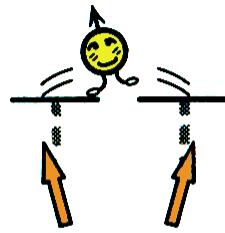
(a) LaMnO₃



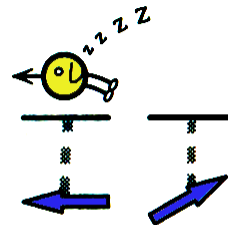
(b) La_{1-x}Sr_xMnO₃ (T ≪ T_c)



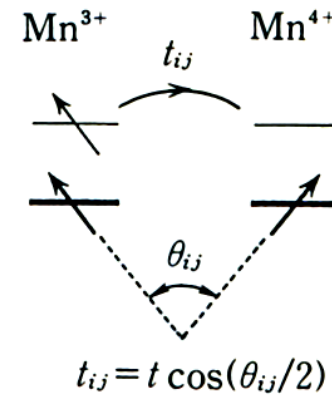
(a)



(b)



(c)



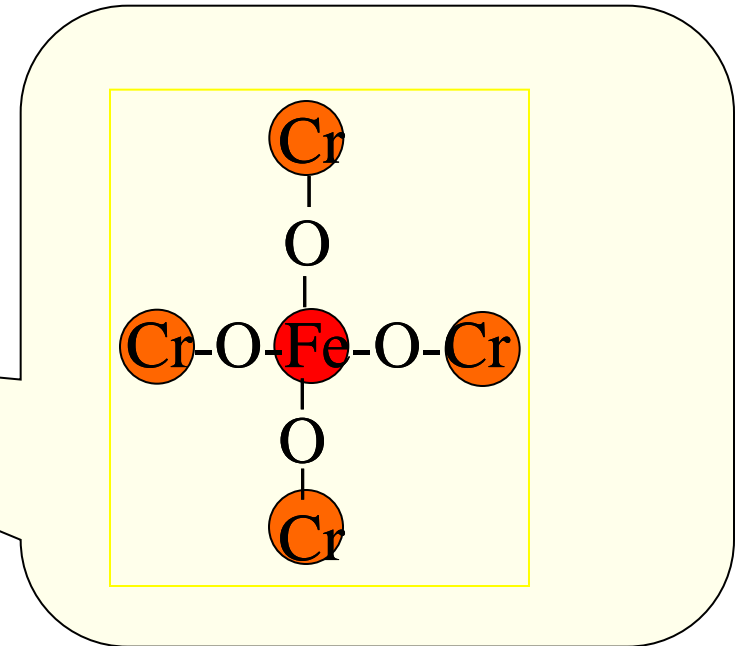
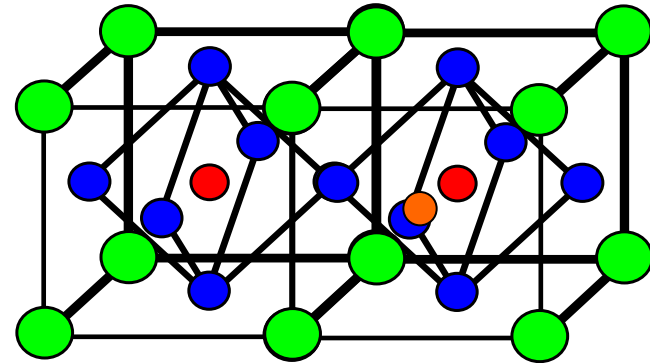
$$H = -t_{\text{Mn-Mn}} \cos\left(\frac{\theta}{2}\right) - K_{\text{Hund}} \sigma S_{\text{Mn}} - J_{t2g} \sum_{\text{LMnO}} S_{\text{Mn}}^{t2g} S_{\text{Mn}}^{t2g}$$



Kanamori-Goodenough rules

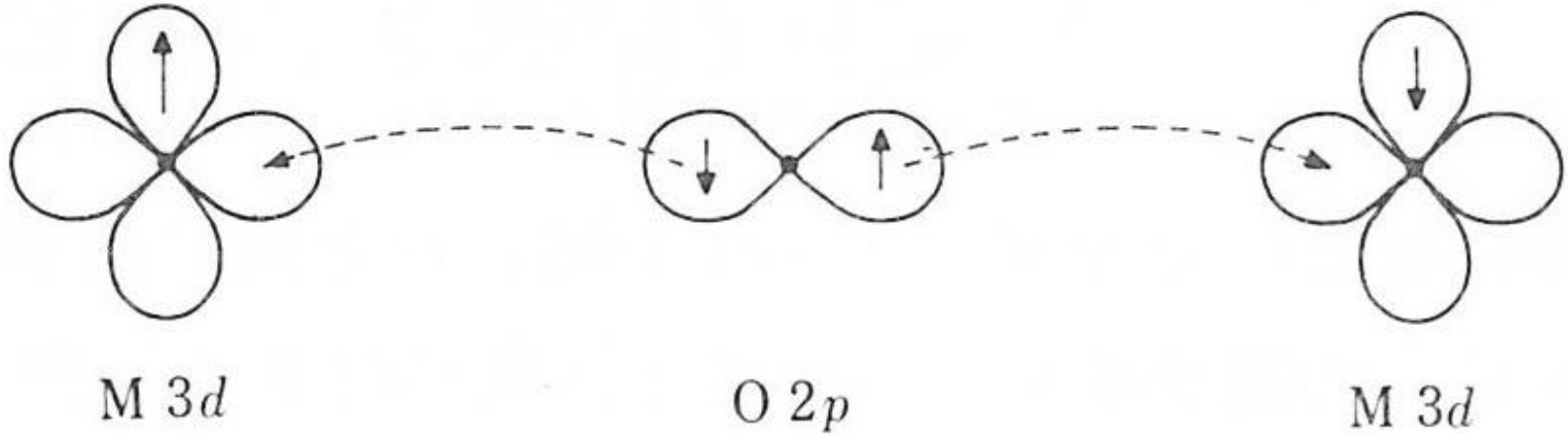
60 years ago

Kanamori former
president of Osaka Univ.





Superexchange interaction

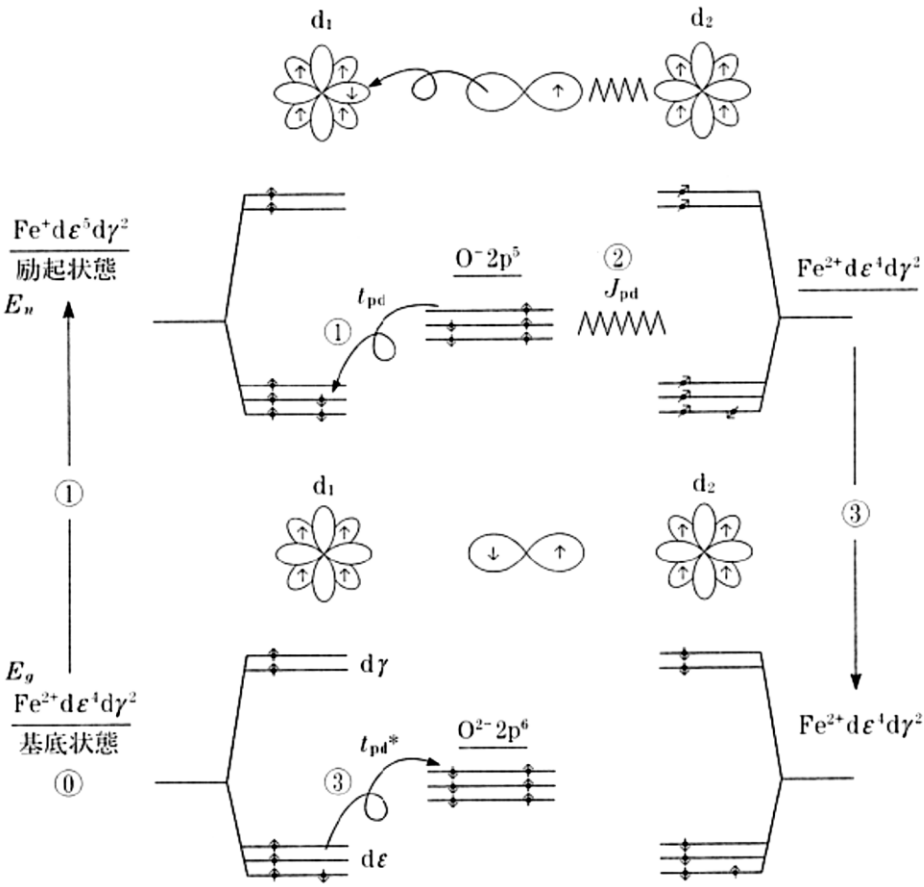


Superexchange interaction

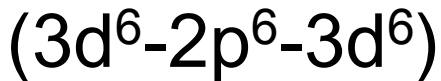
→ Indirect interaction between two magnetic atoms
through non-magnetic atom



Superexchange interaction



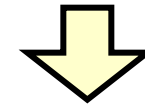
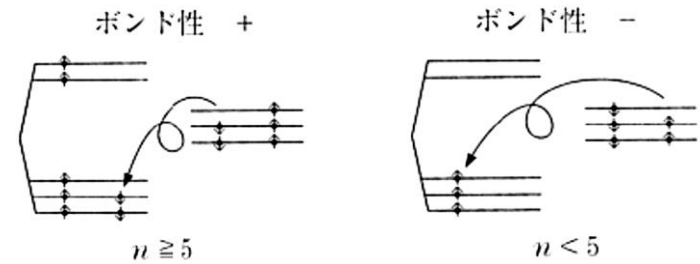
(a) Fe²⁺ - O²⁻ - Fe²⁺ 間の超交換相互作用模型



Considering an excited state in the case of electron transfer from 2p orbital to 3d orbital

(transfer integral)
$$t_{pd} = \int \phi_d^* V_{pd} \phi_p dr$$

■ bonding rule



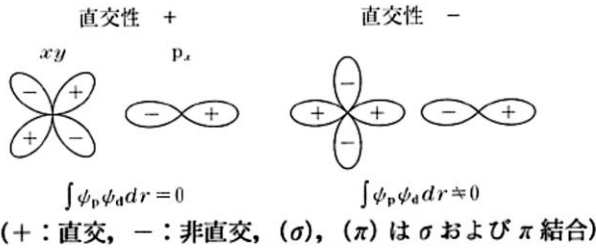
Considering a direct exchange interaction (J_{pd}) between 2p spin and 3d spin



Superexchange interaction

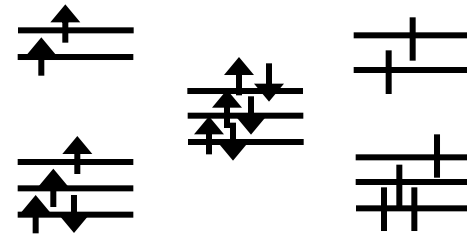
Sign of J_{pd} Ferromagnetic $J_{pd} > 0$ 、Antiferromagnetic $J_{pd} < 0$

... Orthogonal character of J_{pd}

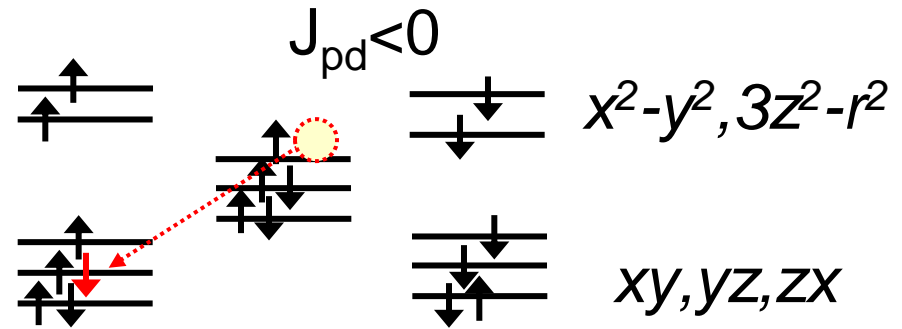


| d | | p_x | p_y | p_z | s |
|--------------|---|-------------|-------------|-------------|-------------|
| $3z^2 - r^2$ | X | $-(\sigma)$ | + | + | $-(\sigma)$ |
| | Y | + | $-(\sigma)$ | + | $-(\sigma)$ |
| | Z | + | + | $-(\sigma)$ | $-(\sigma)$ |
| $x^2 - y^2$ | X | $-(\sigma)$ | + | + | $-(\sigma)$ |
| | Y | + | $-(\sigma)$ | + | $-(\sigma)$ |
| | Z | + | + | + | + |
| xy | X | + | $-(\pi)$ | + | + |
| | Y | $-(\pi)$ | + | + | + |
| | Z | + | + | + | + |
| yz | X | + | + | + | + |
| | Y | + | + | $-(\pi)$ | + |
| | Z | + | $-(\pi)$ | + | + |
| zx | X | + | + | $-(\pi)$ | + |
| | Y | + | + | + | + |
| | Z | $-(\pi)$ | + | + | + |

Fe^{2+} O^{2-} Fe^{2+}



$3d^6$ $2p^6$ $3d^6$



Orthogonal character table in case that d orbital function locates the origin and

s and p orbitals arrange Orthogonal coordinates of X, Y and Z axes

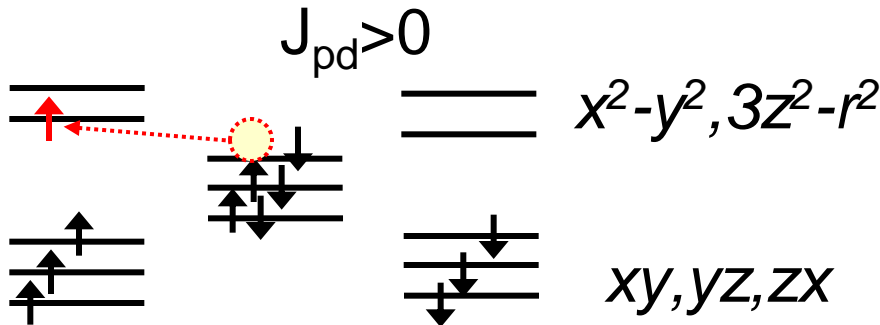
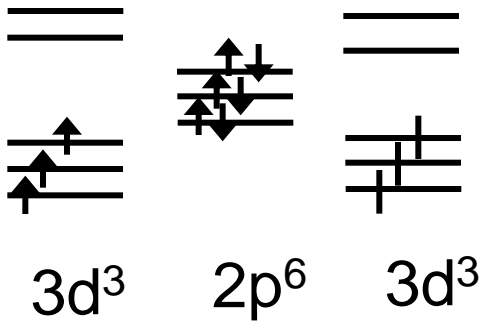
FeO is an antiferromagnetic material



Superexchange interaction

Ex.) $Mn^{4+} - Mn^{4+}$: Antiferromagnetic

Mn^{4+} O^{2-} Mn^{4+}



(+ : 直交, - : 非直交, (σ), (π) は σ および π 結合)

| | d | p_x | p_y | p_z | s |
|--------------|---|-------------|-------------|-------------|-------------|
| $3z^2 - r^2$ | X | $-(\sigma)$ | + | + | $-(\sigma)$ |
| | Y | + | $-(\sigma)$ | + | $-(\sigma)$ |
| | Z | + | + | $-(\sigma)$ | $-(\sigma)$ |
| $x^2 - y^2$ | X | $-(\sigma)$ | + | + | $-(\sigma)$ |
| | Y | + | $-(\sigma)$ | + | $-(\sigma)$ |
| | Z | + | + | + | + |
| xy | X | + | $-(\pi)$ | + | + |
| | Y | $-(\pi)$ | + | + | + |
| | Z | + | + | + | + |
| yz | X | + | + | + | + |
| | Y | + | + | $-(\pi)$ | + |
| | Z | + | $-(\pi)$ | + | + |
| zx | X | + | + | $-(\pi)$ | + |
| | Y | + | + | + | + |
| | Z | $-(\pi)$ | + | + | + |



Double exchange interaction

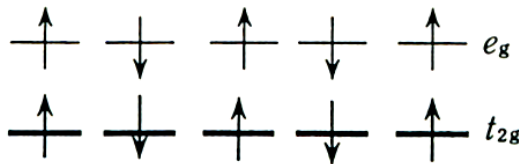
Superexchange interaction

Double exchange interaction

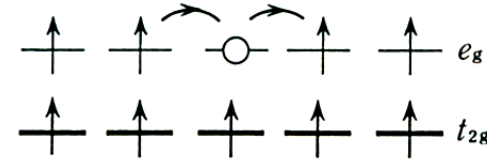
LaMnO₃

Carrier doping

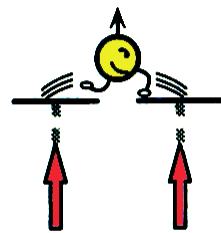
(La,Sr)MnO₃



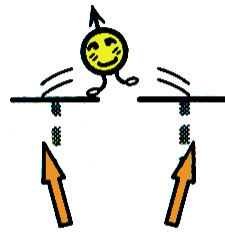
(a) LaMnO₃



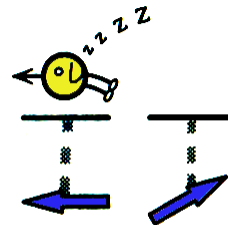
(b) La_{1-x}Sr_xMnO₃ ($T \ll T_C$)



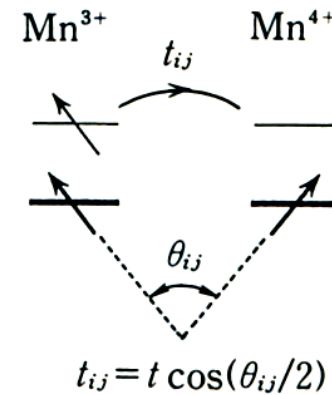
(a)



(b)



(c)

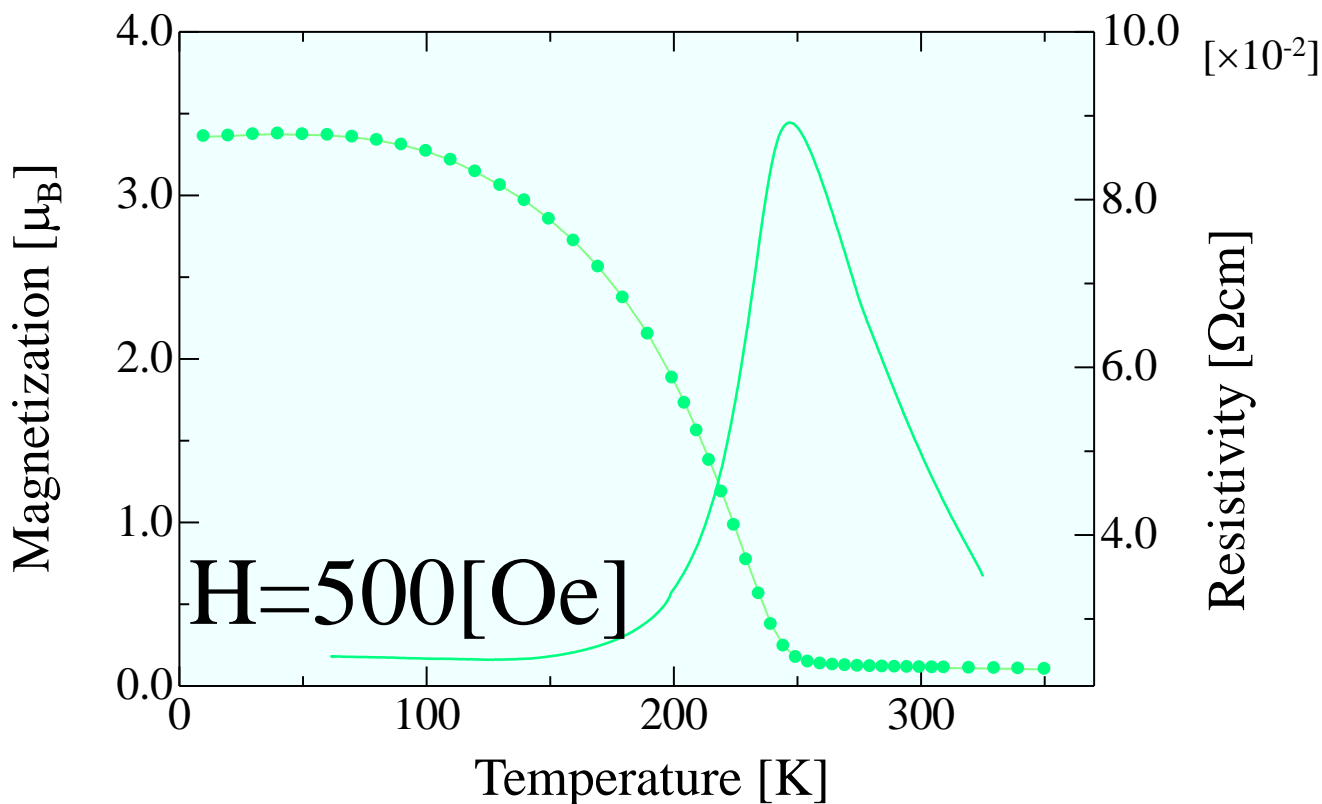


$$H = -t_{\text{Mn-Mn}} \cos\left(\frac{\theta}{2}\right) - K_{\text{Hund}} \sigma S_{\text{Mn}} - J_{t_{2g}} \sum_{\text{LMnO}} S_{\text{Mn}}^{t_{2g}} S_{\text{Mn}}^{t_{2g}}$$

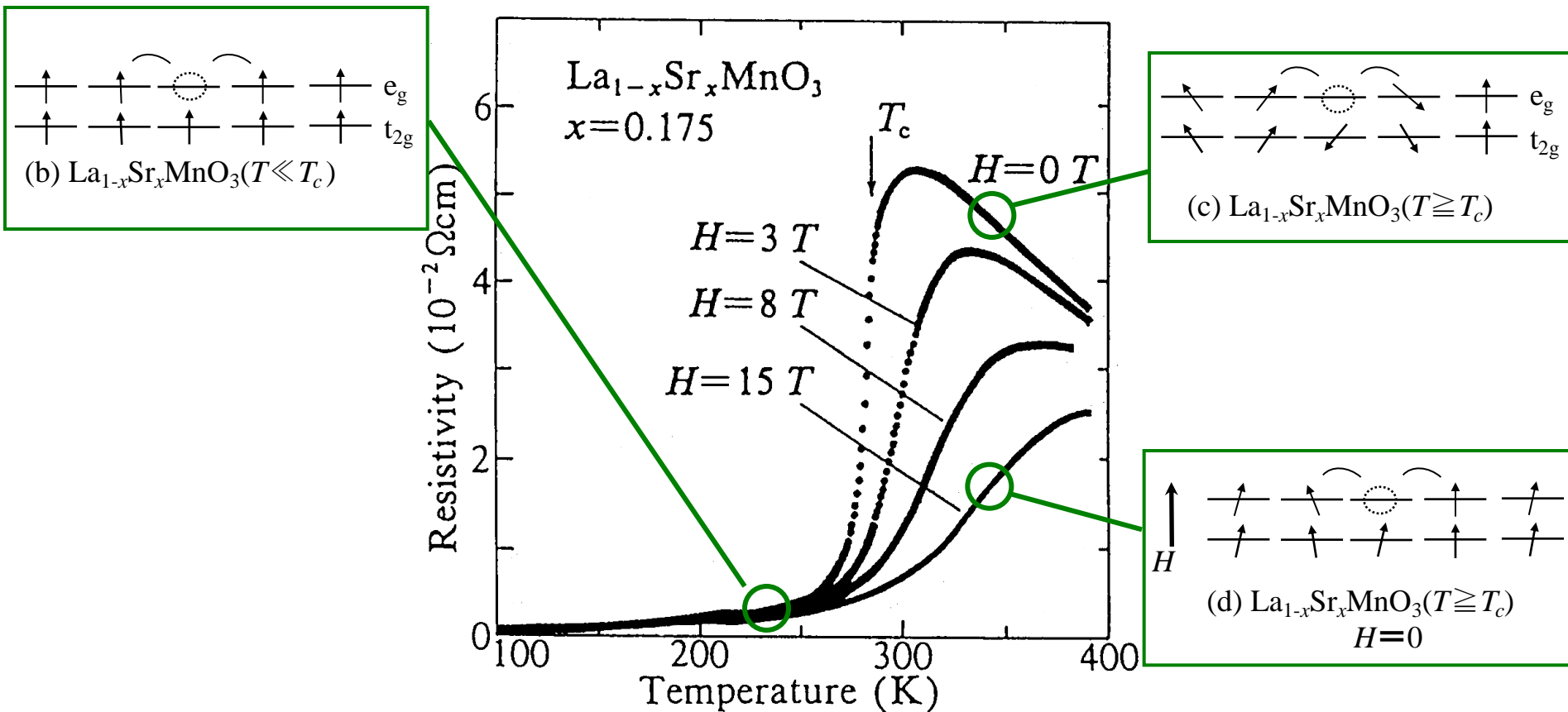


Magnetism modulation due to change of electron transfer integral

$$H = -t_{\text{Mn-Mn}} \cos\left(\frac{\theta}{2}\right) - K_{\text{Hund}} \sigma S_{\text{Mn}} - J_{t2g} \sum_{\text{LMnO}} S_{\text{Mn}}^{t2g} S_{\text{Mn}}^{t2g}$$

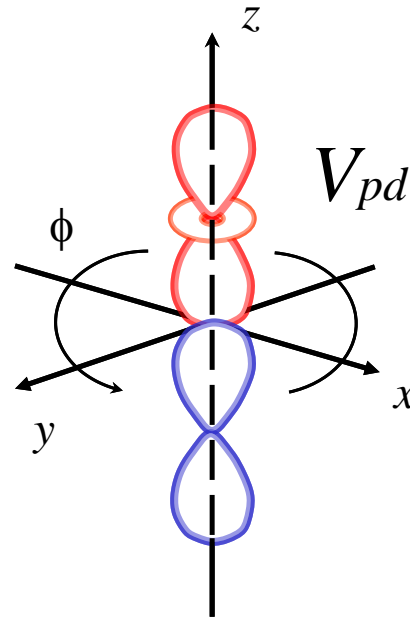
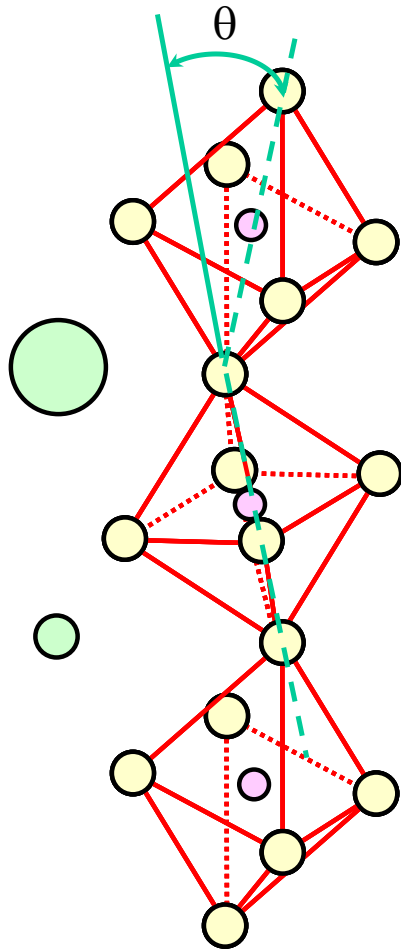


Colossal magneto resistance (CMR)



Temperature dependence of resistivity with a variety of magnetic fields in $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ crystal (negative CMR) .
 T_c indicates the Curie temperature at $H=0\text{ T}$.

Main parameters of transfer integral changes



Harrison's equation

$$V_{pd\sigma} = \langle \varphi_d | H | \varphi_p \rangle \sim d^{-7/2}$$

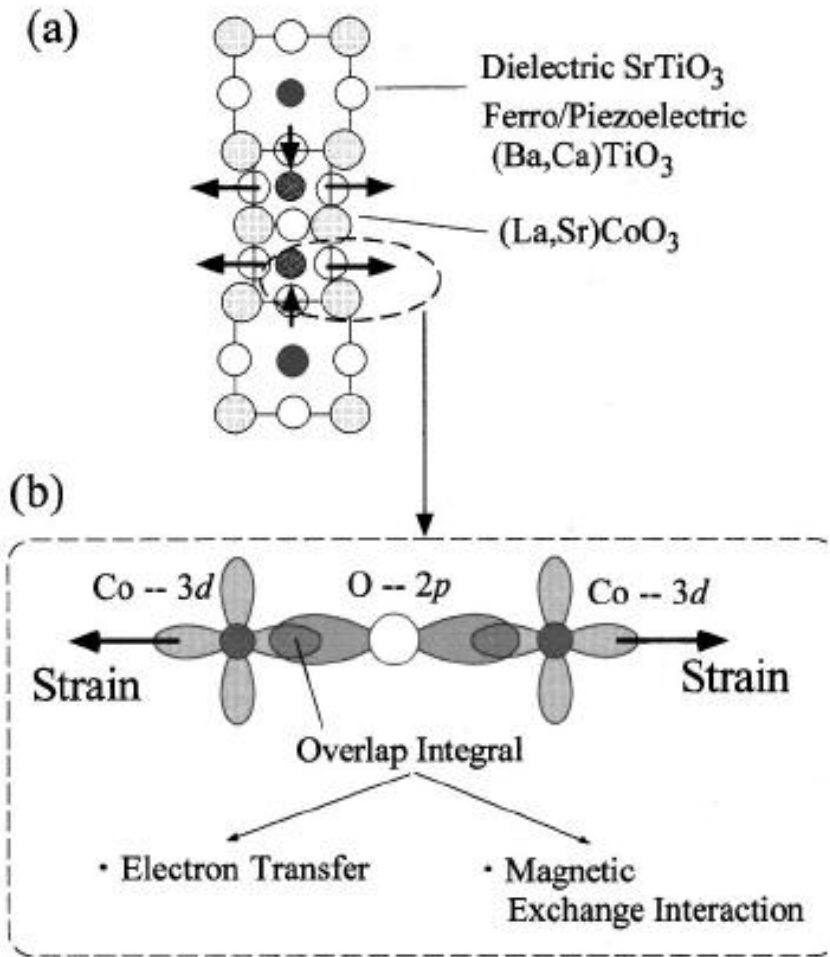
d : the distance between orbitals

ϕ : the bond angle

$$E_{3z^2-r^2, 3z^2-r^2} = \left[n^2 - \frac{1}{2}(l^2 + m^2) \right]^2 V_{dd\sigma} + 3n^2(l^2 + m^2)V_{dd\pi} + \frac{3}{4}(l^2 + m^2)^2 V_{dd\delta}$$

$$\approx \cos \phi$$

Main parameters of transfer integral changes



Tensile strain

↑

$$V_{pd\sigma} \sim d^{-7/2}$$

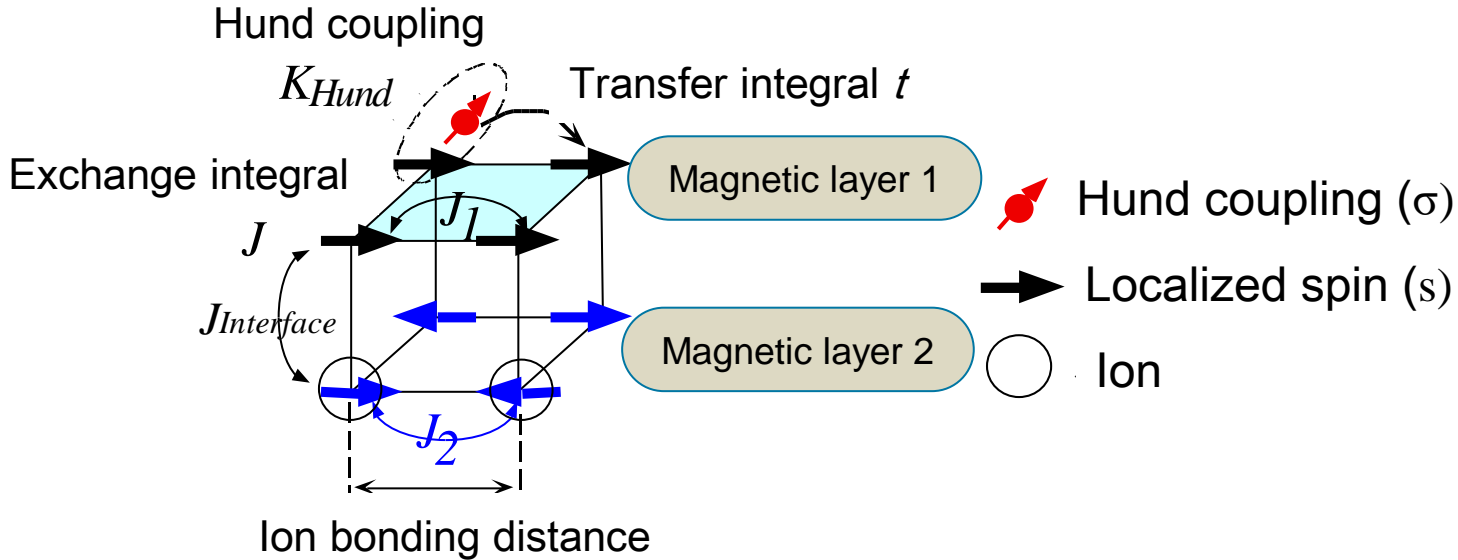
↓

Compressive strain

Band width $W = 2zV$
 z : Coordination number



Material design for oxide spintronics



$$\begin{aligned}
 H_{electron} = & \sum E_d + \frac{1}{2} \sum U + K_{Hund} \sum_i \sigma S_i + \sum_{i,j} J_{ij} S_i S_j \\
 & + \sum E_p + \sum t + A \sum_i d Q d
 \end{aligned}$$

d electron energy
Coulomb integral
Hund coupling
Exchange integral

E_p
Transfer integral



Material design for oxide spintronics

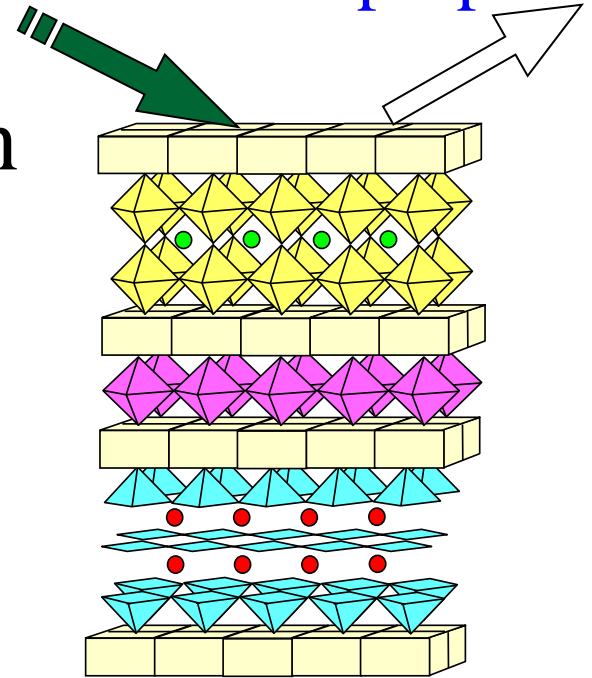
(1) Introduce strain effect

(2) Introduce magnetic interaction between different layers

(3) Integrate different functional materials

$h\nu$, H , E

Nobel
physical
properties

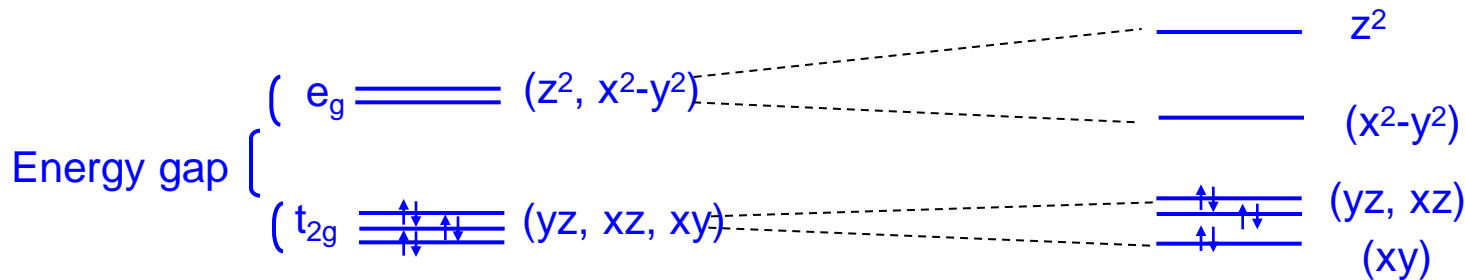
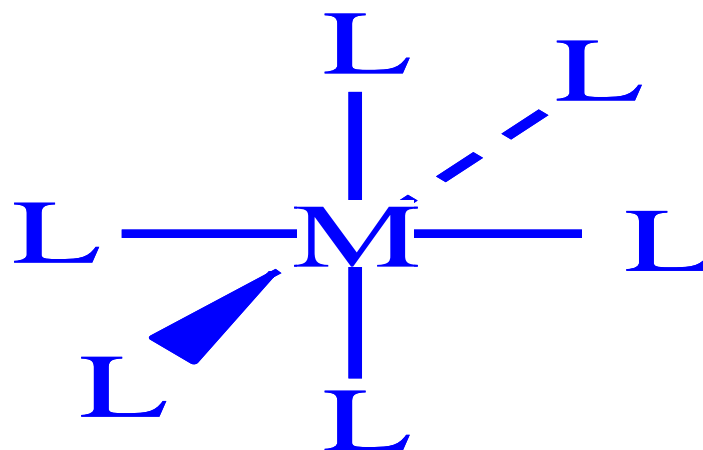
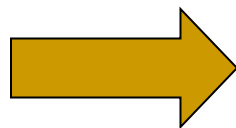
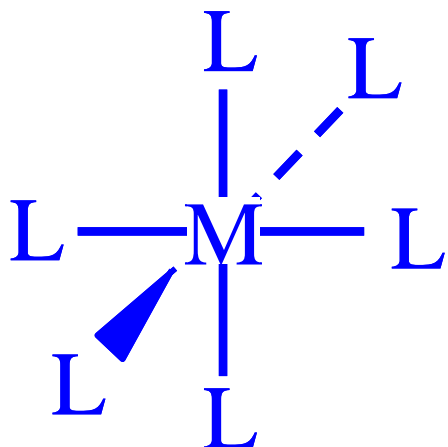




Control of crystal field splitting due to strain effect

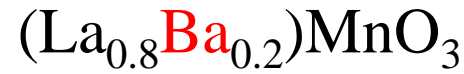
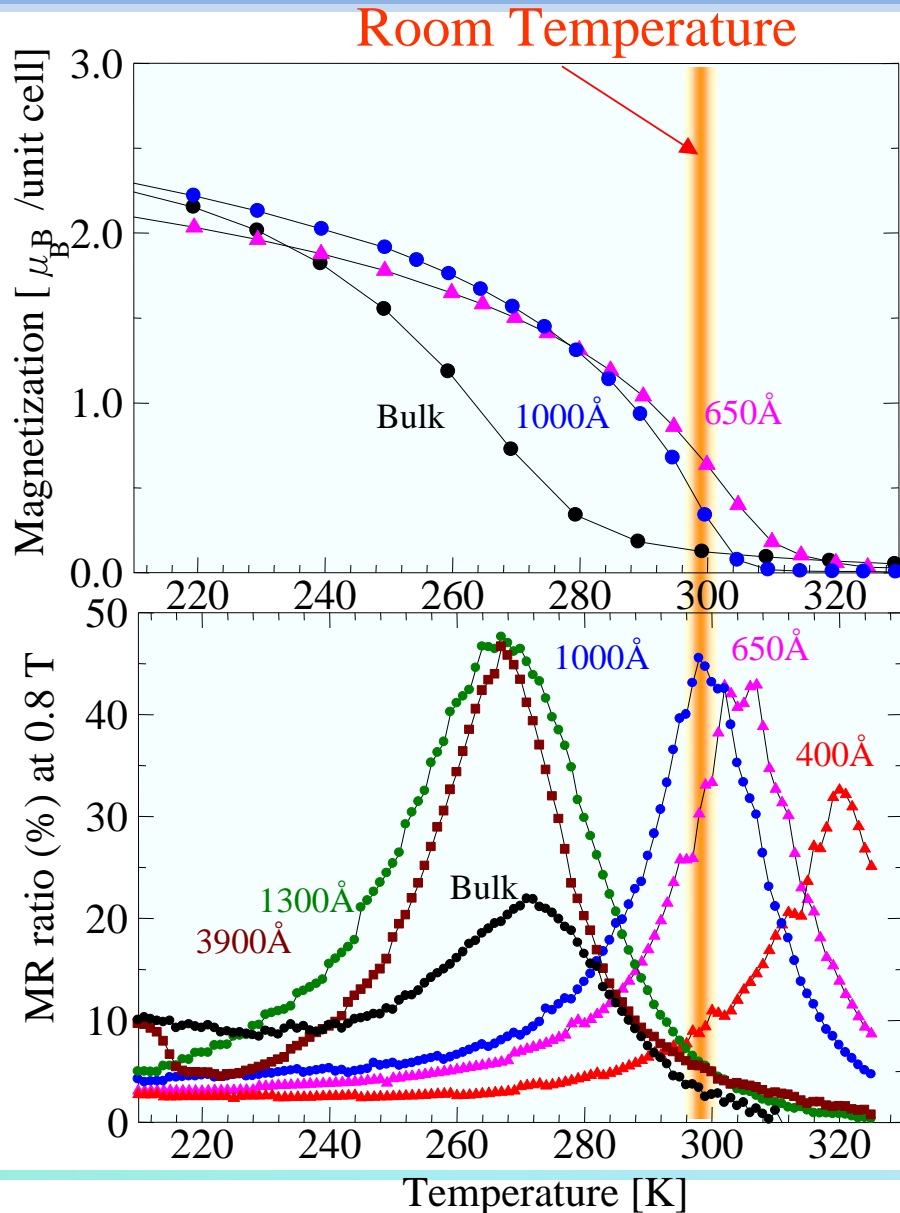
Octahedral coordination

In-plane tensile strain

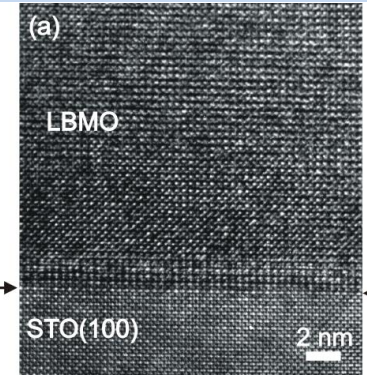




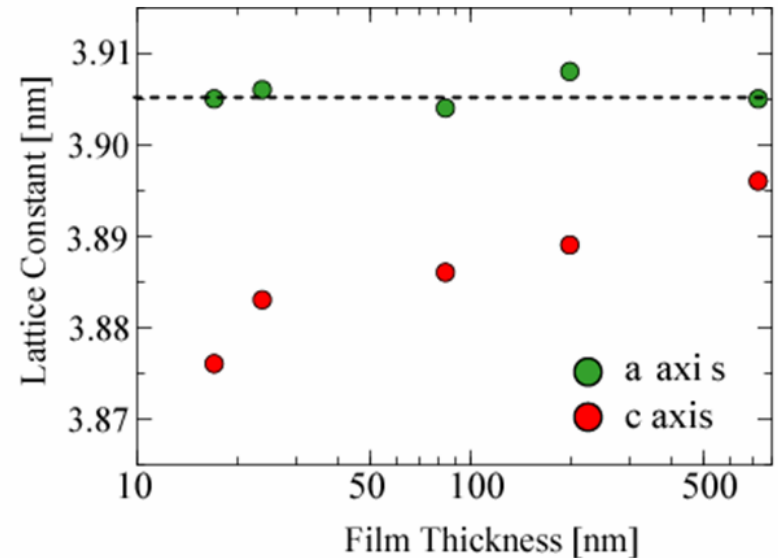
Design of room temperature CMR materials



SrTiO₃ substrate



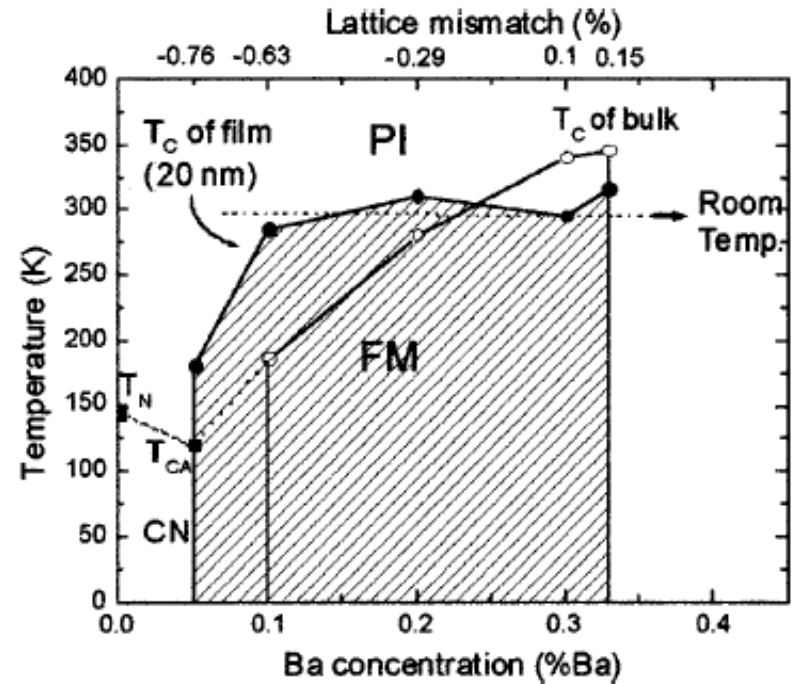
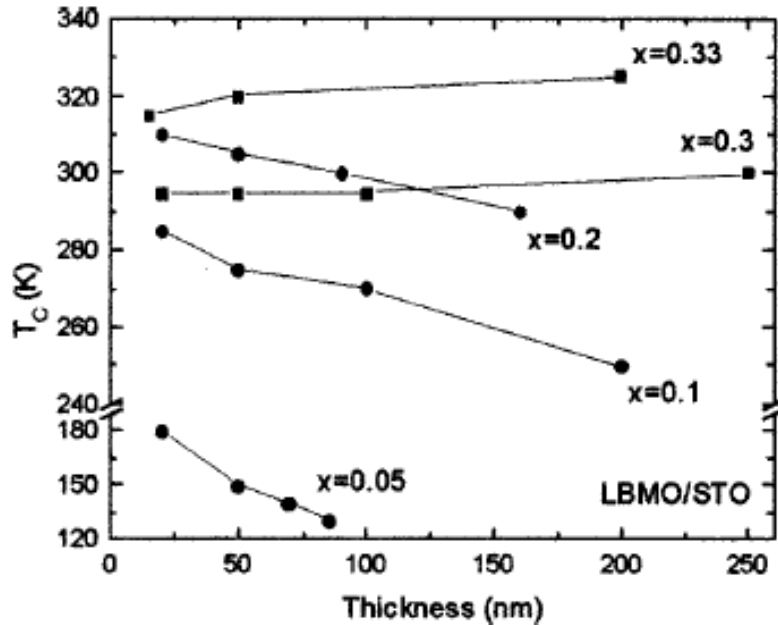
Tensile strain
(0.3%)



Phys. Rev. B **64**, 224418(2001)

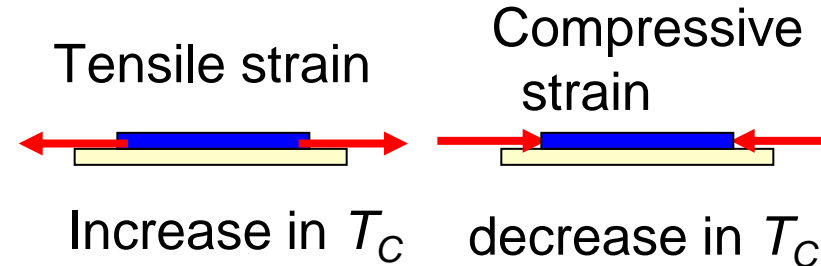


Strain effect vs T_C in LBMO films



Tensile strain \leftarrow \rightarrow Compressive strain

| x | 0.05 | 0.1 | 0.2 | 0.3 | 0.33 |
|---------------------------|------------------|-------|-------|-----|------|
| Lattice mismatch (%) | -0.76 | -0.63 | -0.29 | 0.1 | 0.15 |
| Strain type | T | T | T | C | C |
| T_C of bulk (K) | 120 ^a | 185 | 280 | 340 | 345 |
| T_C of film (20 nm) (K) | 180 | 285 | 310 | 290 | 315 |



Phys. Rev. B **64**, 184404(2001)

^aFor $x=0.05$, spin canting transition temperature $T_{CA}=120$ K.



Stability of double exchange magnetism

Stability of magnetism induced by double exchange interaction

$$\Delta\varepsilon_{ex}^D = zxt_{ij} = zxb_{\sigma} \langle \cos(\theta_{ij} / 2) \rangle$$

C. Zener: Phys. Rev. **82** (1951) 403

P. W. Anderson and H. Hasegawa: Phys. Rev. **100** (1955) 675

P. G. de Gennes: Phys. Rev. **118** (1960) 141

Z: the coordination number of nearest neighbor atoms ; Z=6

t_{ij} : the transfer energy

θ_{ij} : the spin angle between Mn_i and Mn_j

Main parameters indicating the stability of double exchange magnetism

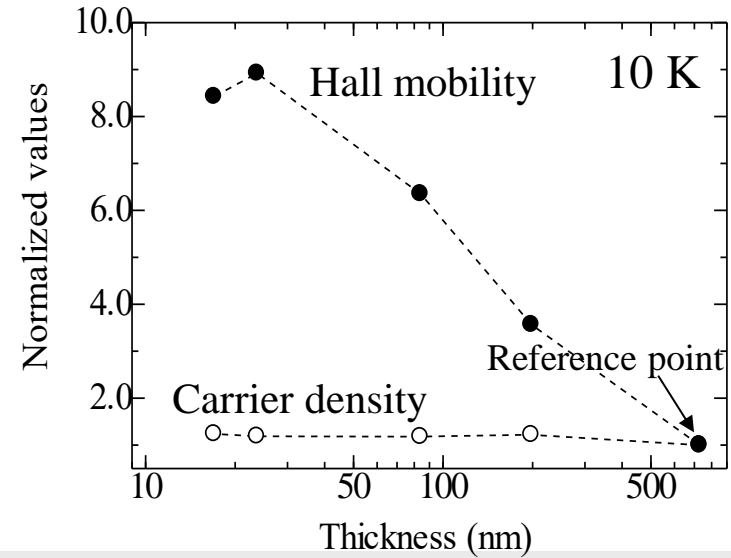
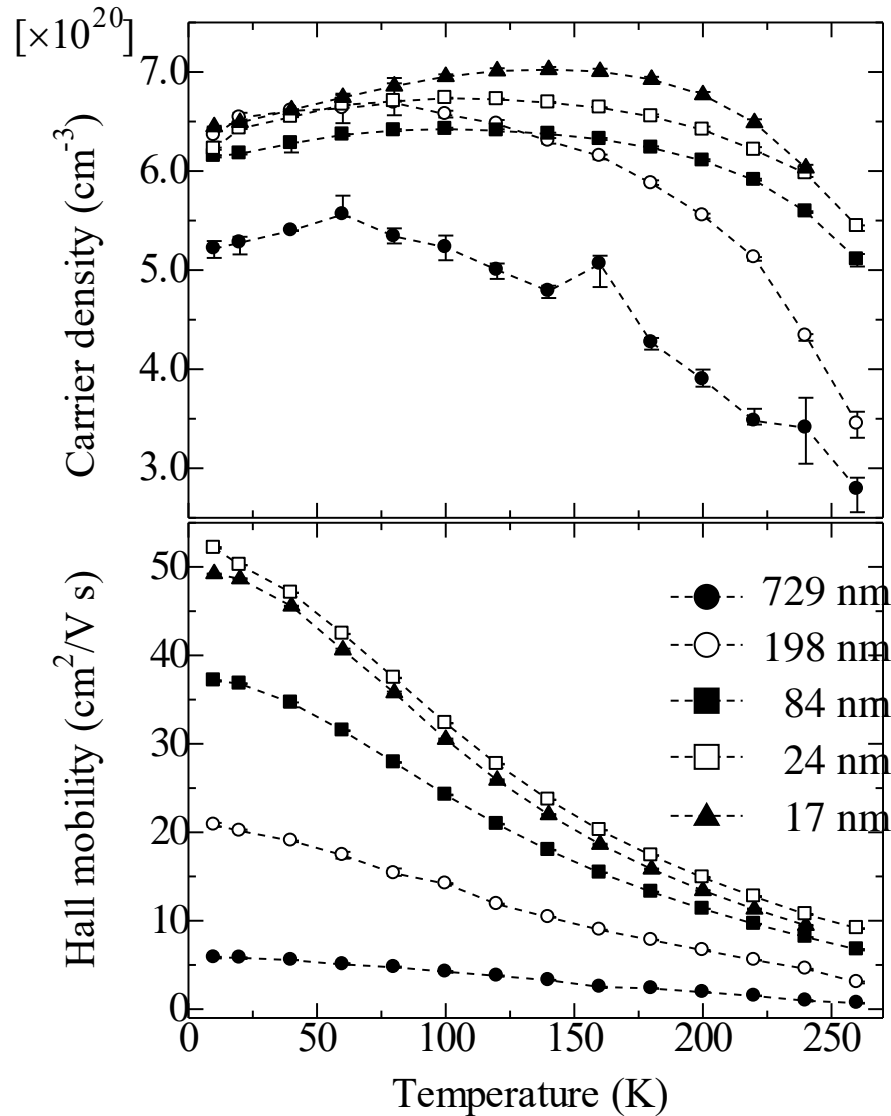
x : the number of carriers per a Mn site

b_{σ} : Spin-independent components

(dependence of orbital overlap and bond angle of Mn-O-Mn)



Carrier density and Hall mobility



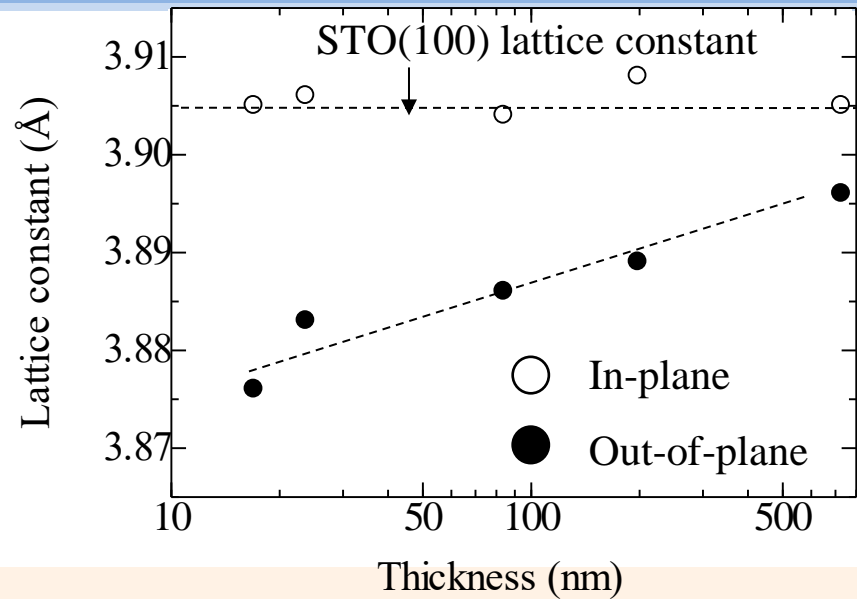
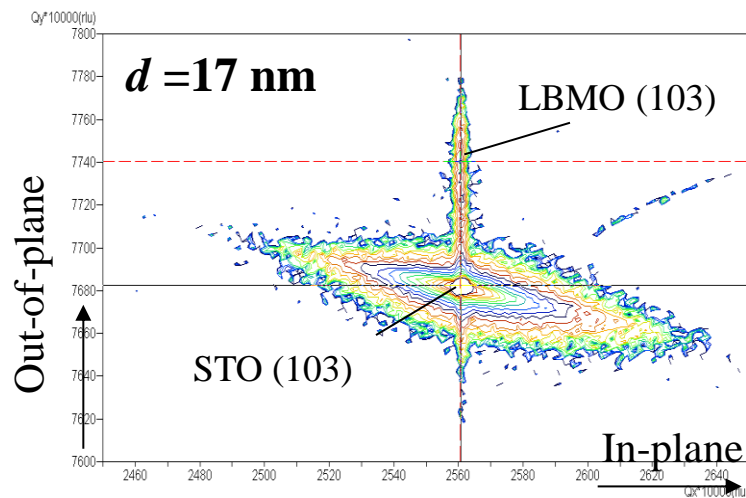
Carrier density: Constant

- ➡ the number of carrier x : constant
- ➡ **Not generating cation deficiency**

Hall mobility: Increase

- ➡ Increase in transfer integral
- ➡ **change in orbital overlap state due to lattice strain effect**

Stability of transfer integral due to lattice strain effect



Calculation of stability in double exchange interaction every thickness

◆ stability of double exchange interaction

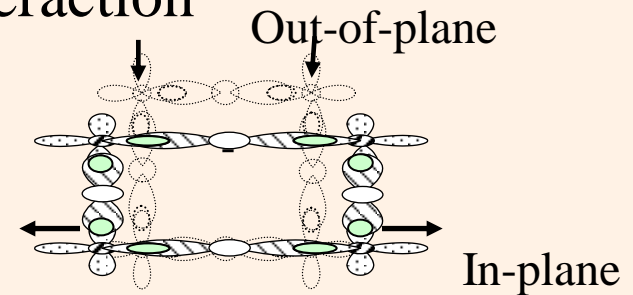
$$\Delta \varepsilon_{ex}^D = z \Delta x \Delta t_{ij} \propto \Delta x \Delta b_{\sigma} \propto \Delta b_{\sigma}$$

x : the number of carriers per a Mn site

b_{σ} : Spin-independent components

(dependence of orbital overlap and bond angle of Mn-O-Mn)

Z : the coordination number of nearest neighbor atoms ; $Z=6$





Contribution elements of stability in double exchange interaction

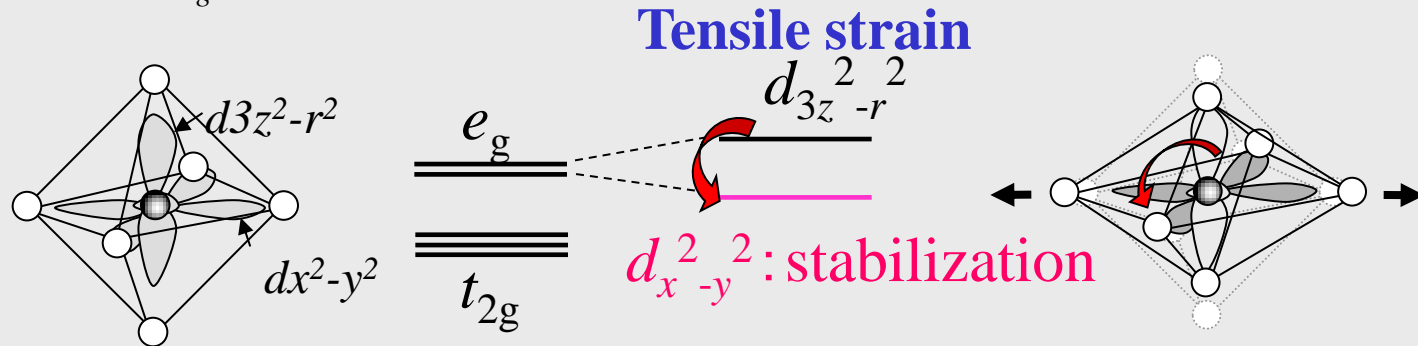
1. In-plane and Out-of-plane orbital overlap

→ determination from lattice constants obtained by experiments

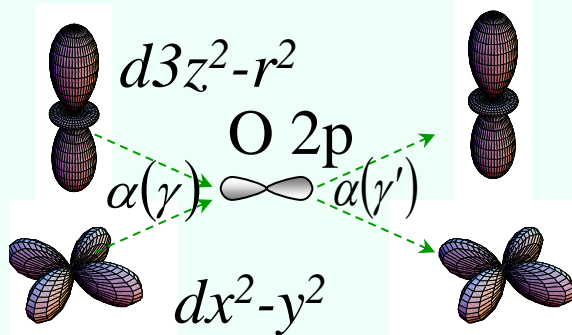
matrix element between p and d orbitals: $V_{pd} = d_{\text{Mn-O}}^{-7/2}$

Mn-O-Mn bond angle: 180°

2. Redistribution of e_g electrons due to lattice strain effect → calculation by the DV- $X\alpha$ method



3. Anisotropy of d orbital



| Transfer strength $\gamma \setminus \gamma'$ | Out-of-plane | | In-plane | |
|---|---------------------|----------------------|---------------------|----------------------|
| | $ x^2 - y^2\rangle$ | $ 3z^2 - r^2\rangle$ | $ x^2 - y^2\rangle$ | $ 3z^2 - r^2\rangle$ |
| $ x^2 - y^2\rangle$ | 0 | 0 | 3/4 | $\sqrt{3}/4$ |
| $ 3z^2 - r^2\rangle$ | 0 | 1 | $\sqrt{3}/4$ | 1/4 |

Phys. Rev. B **64**, 224418(2001)



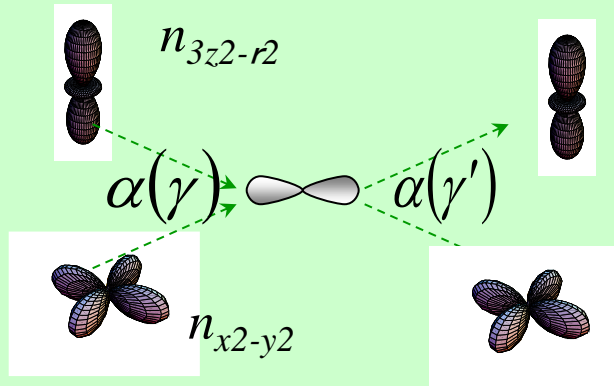
Contribution elements of stability in double exchange interaction

Stability of averaged double exchange interaction

$$\Delta \varepsilon_{ex}^D \propto \sum_{\langle i, j \rangle} (n_{x^2-y^2}, n_{3z^2-r^2}, \alpha(\gamma_i)\alpha(\gamma'_j), d_{in}^{-7}, d_{out}^{-7})$$

Transfer strength from Mn3d orbital to O2p orbital $\alpha(\gamma)$

Transfer strength from O2p orbital to Mn3d orbital $\alpha(\gamma')$



d_{in} : the in-plane Mn-O length
 d_{out} : the out-of-plane Mn-O length
 → derived by XRD measurement

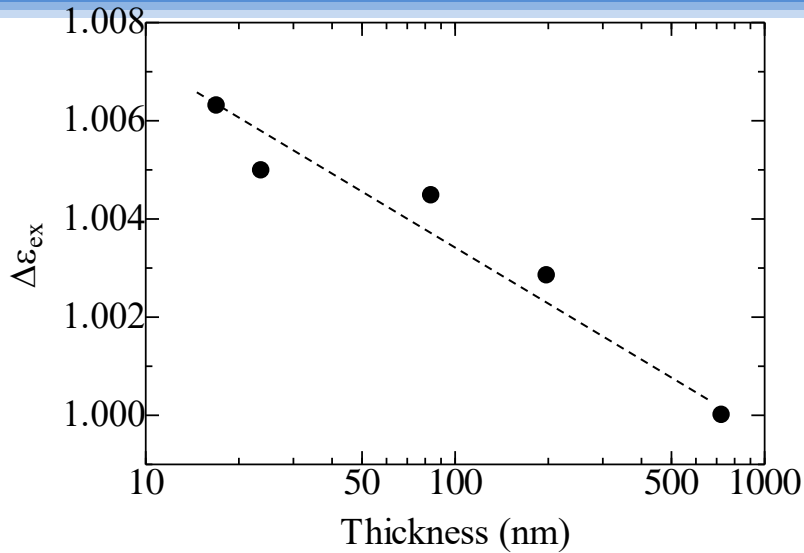
$n_{x^2-y^2}$: the ration of occupied electrons in $d_{x^2-y^2}$ orbital
 $n_{3z^2-r^2}$: the ration of occupied electrons in $d_{3z^2-r^2}$ orbital
 → calculation by the DV- $X\alpha$ method using experimental lattice constants

In-plane: 4 directions

Out-of-plane : 2 directions

$$\Delta \varepsilon_{ex}^D \propto \left((3 + \sqrt{3})n_{x^2-y^2} + (1 + \sqrt{3})n_{3z^2-r^2} \right) d_{in}^{-7} + 2n_{3z^2-r^2} d_{out}^{-7}$$

Stability of double exchange magnetism

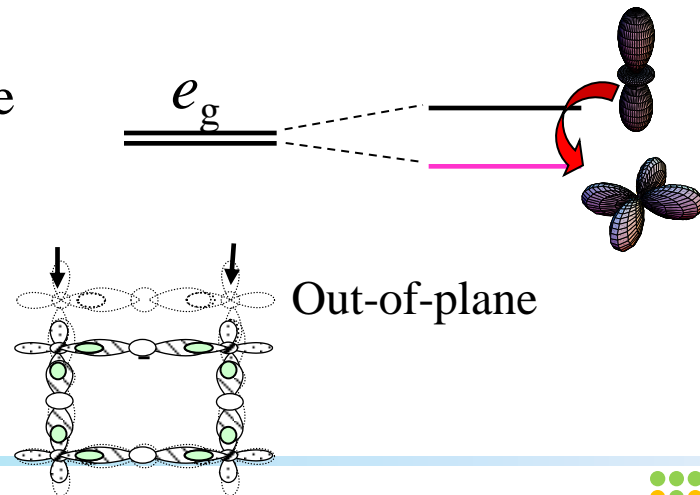


Stabilization of double exchange interaction with decreasing film thickness

What is main factors of T_C increase in strained (La,Ba)MnO₃ thin films

◆ redistribution effect by e_g electrons due to anisotropy d orbital.

◆ Orbital overlap of in-plane and out-of-plane





Function of interface

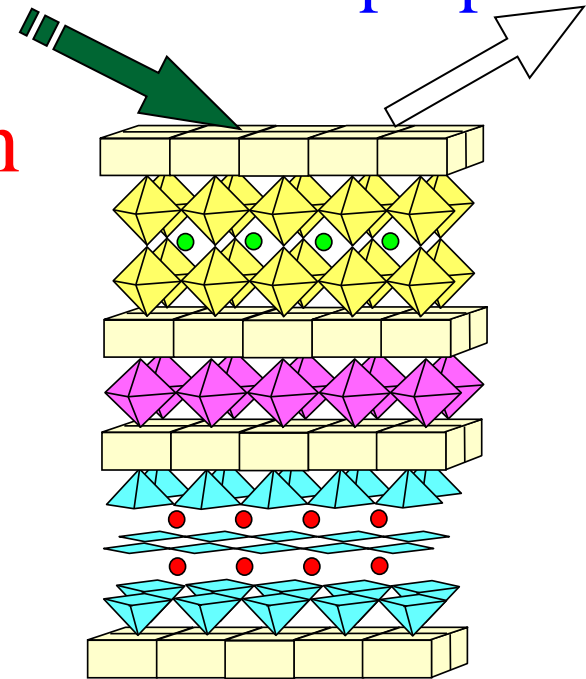
(1) Introduce strain effect

(2) Introduce magnetic interaction
between different layers

(3) Integrate different functional
materials

$h\nu$, H , E

Nobel
physical
properties



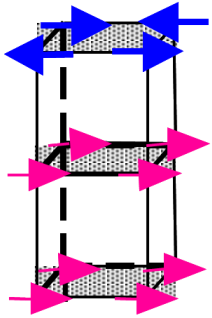
Control of interface magnetic interaction

Conductive electron

Localized spin

$$H = -t_{\text{Mn-Mn}} \cos\left(\frac{\theta}{2}\right) - K_{\text{Hund}} \sigma S_{\text{Mn}} - J_{\text{t2g}} \sum_{\text{LMnO}} S_{\text{Mn}}^{t2g} S_{\text{Mn}}^{t2g} - J_{\text{Fe-Mn}} S_{\text{Mn}}^{t2g} S_{\text{Fe}} - \sum_{\text{LFeO}} J_{\text{Fe-Fe}} S_{\text{Fe}} S_{\text{Fe}}$$

Antiferromagnet LaFeO_3 Interface magnetic interaction

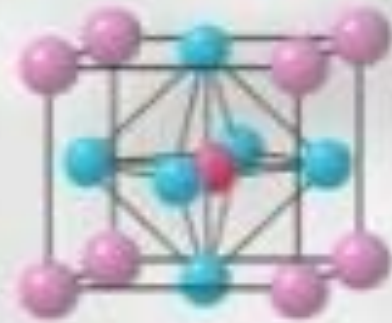


Combined with two materials

Ferromagnet $(\text{La,Sr})\text{MnO}_3$



Spin frustration superlattice

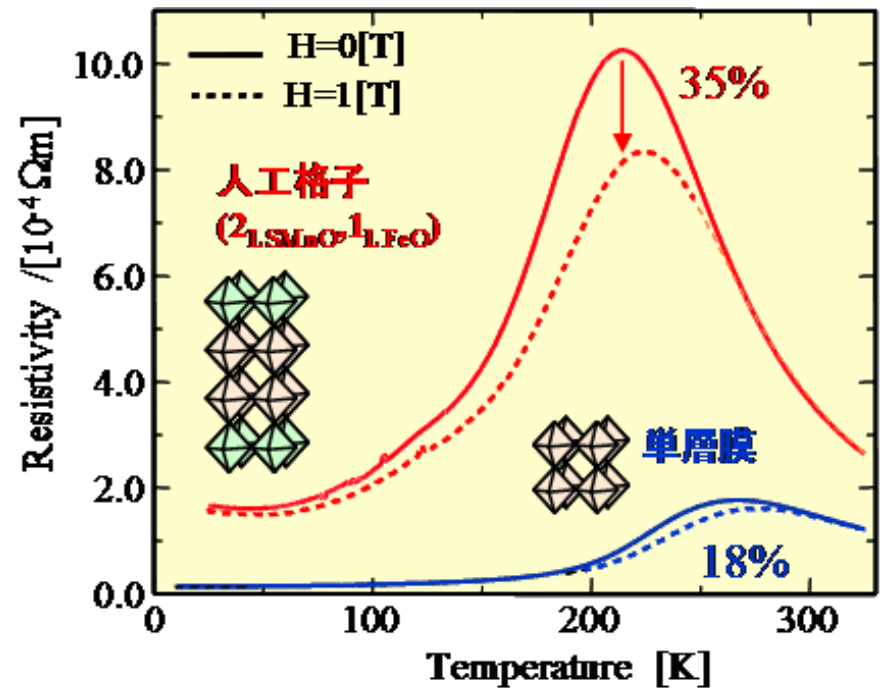
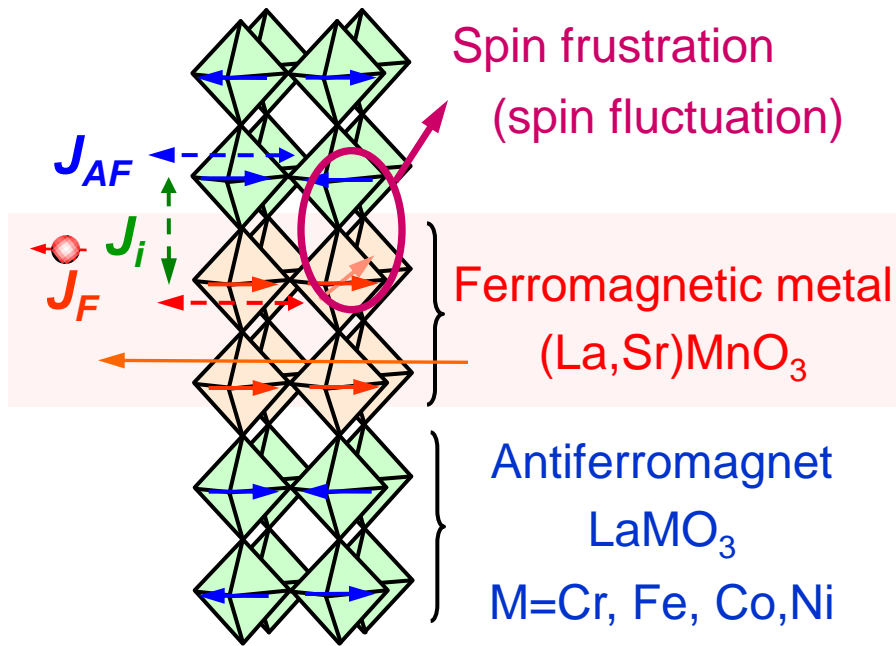


(2006)



High sensitive response by magnetic field

Spin frustration superlattice

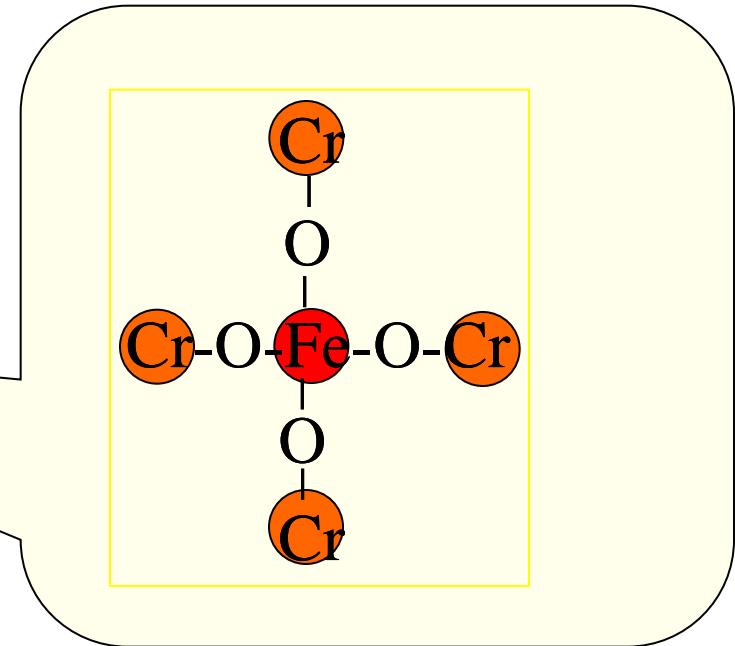
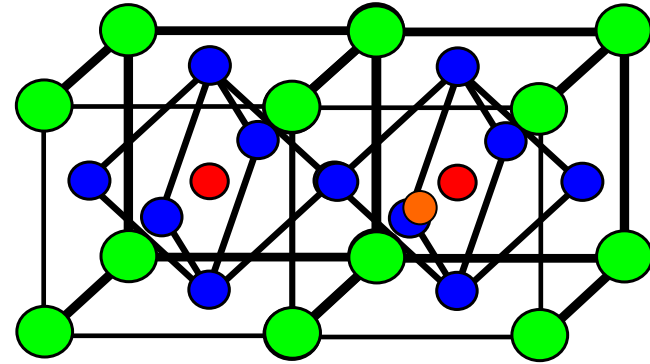




Theoretical prediction : New ferromagnet

60 years ago

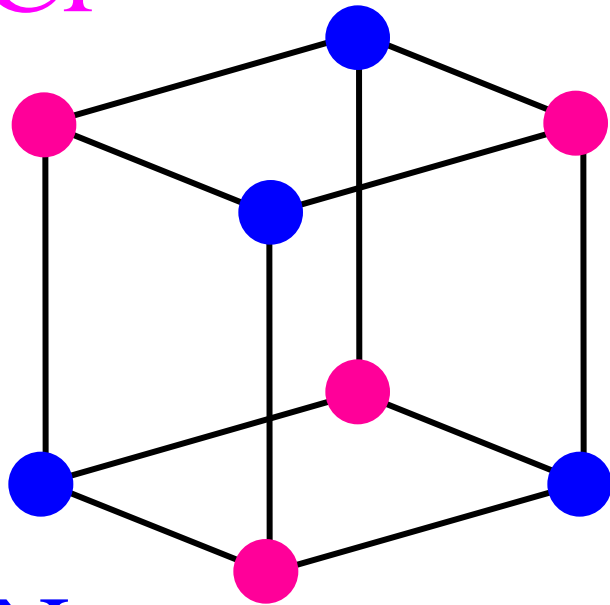
Kanamori former
president of Osaka Univ.





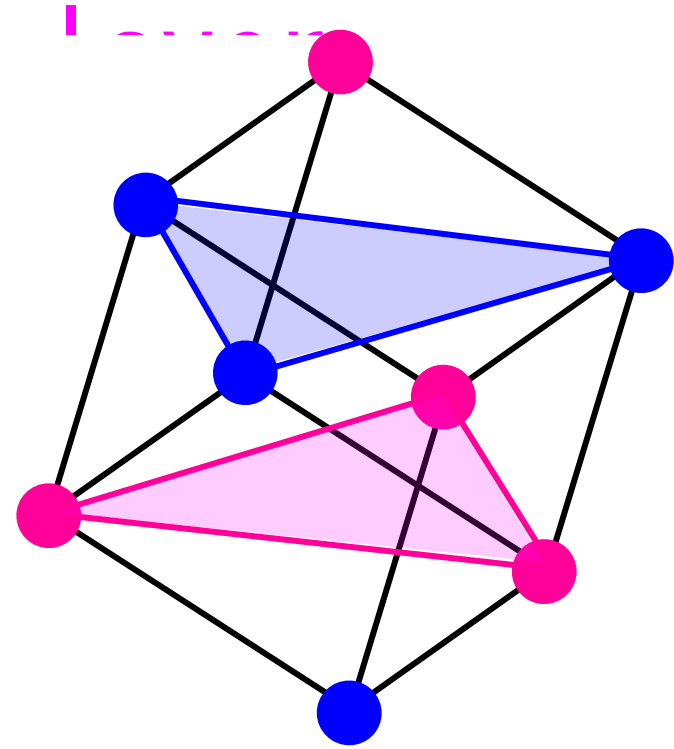
NaCl structure

Cl



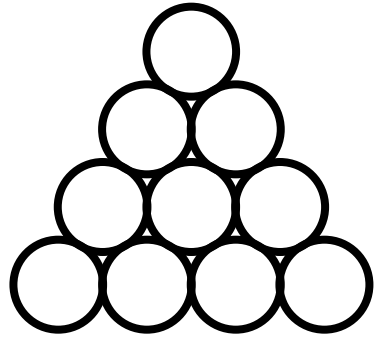
Na

Cl⁻

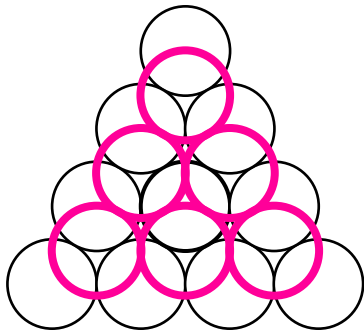


Na layer

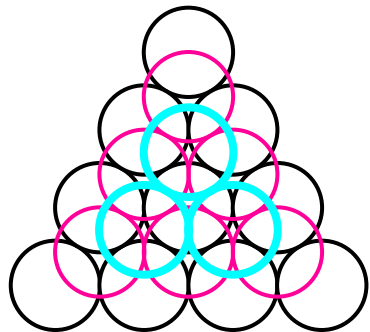
Lattice-direction control superlattice



○○○○○
1st layer

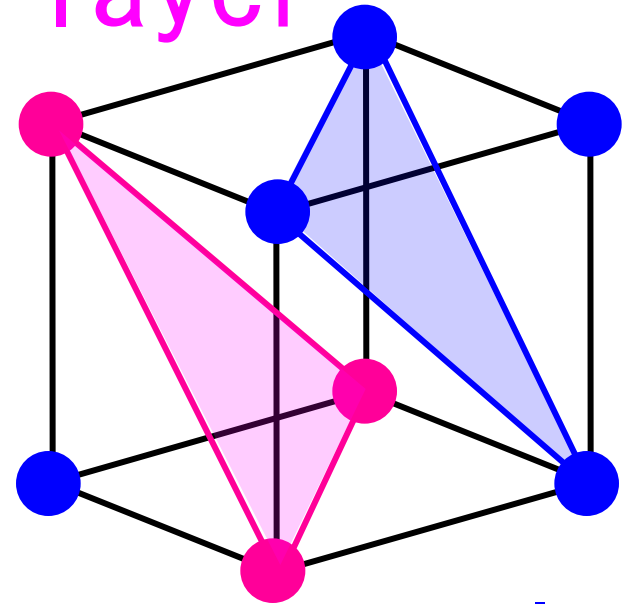


○○○○○
○○○○○
2nd layer



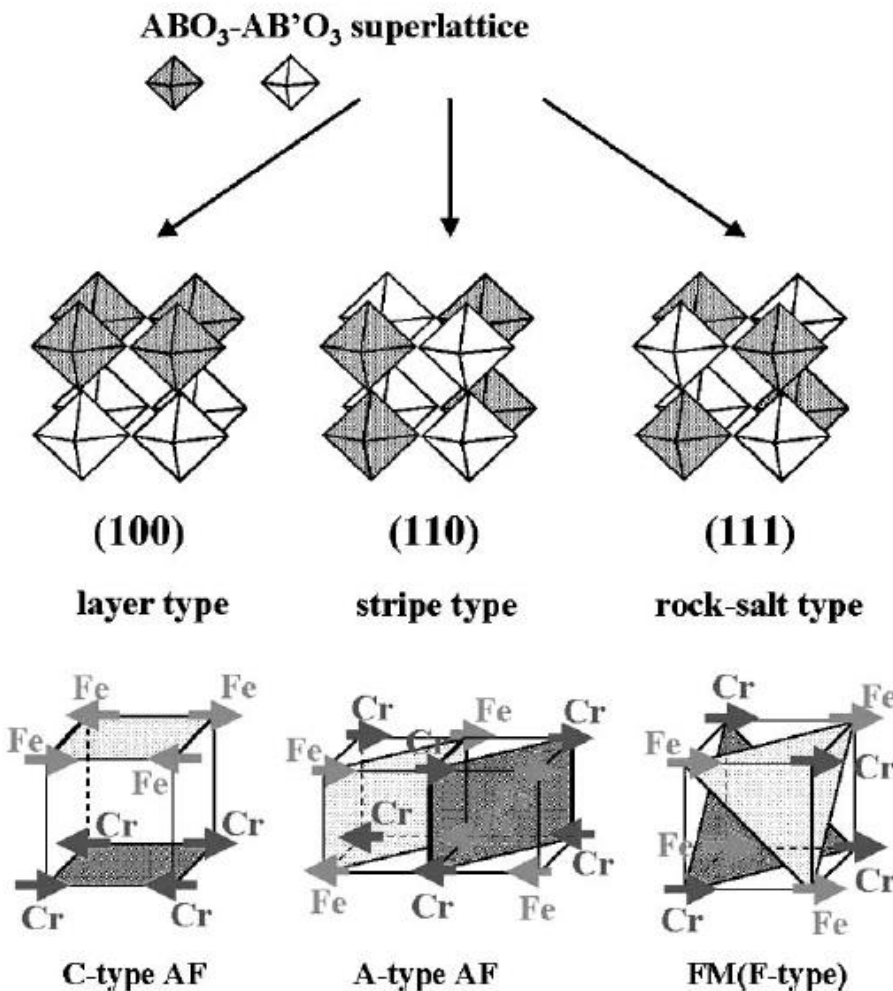
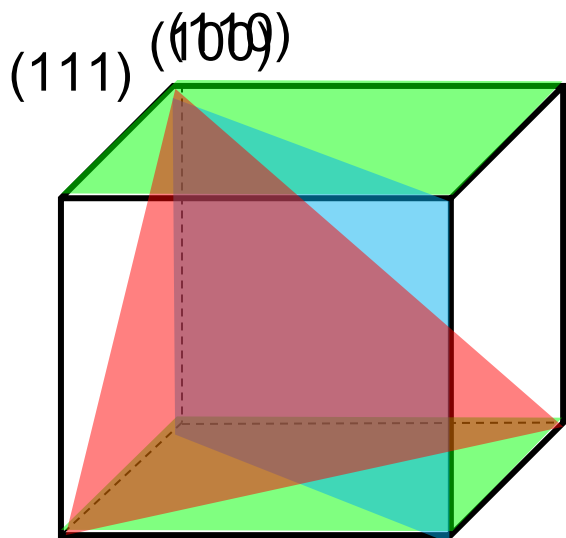
○○○○○
○○○○○
○○○○○
3rd layer

Cl layer



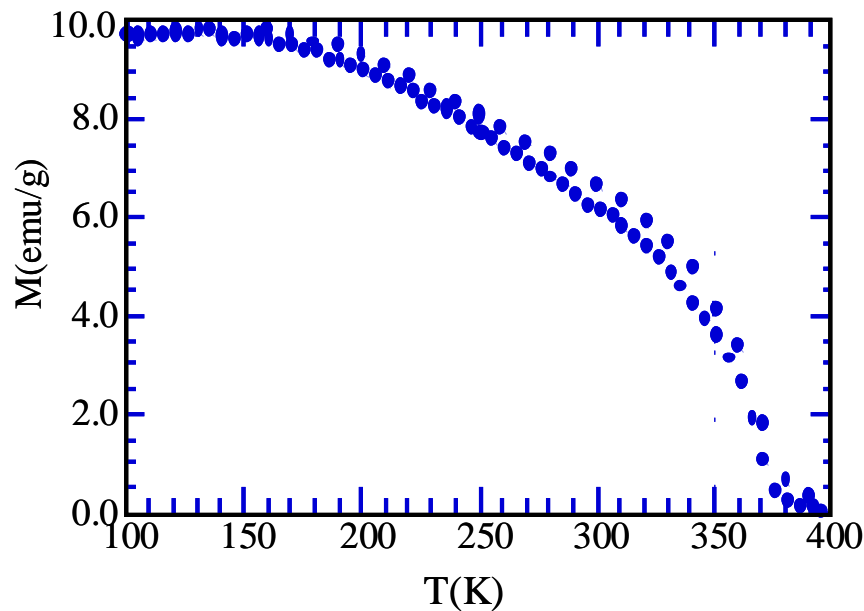
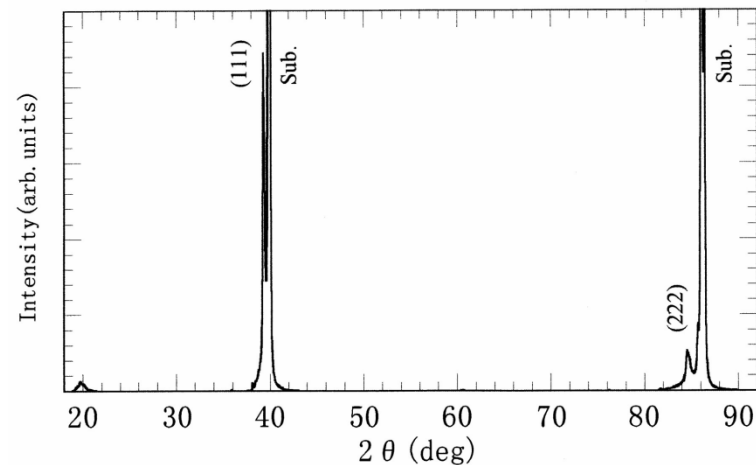
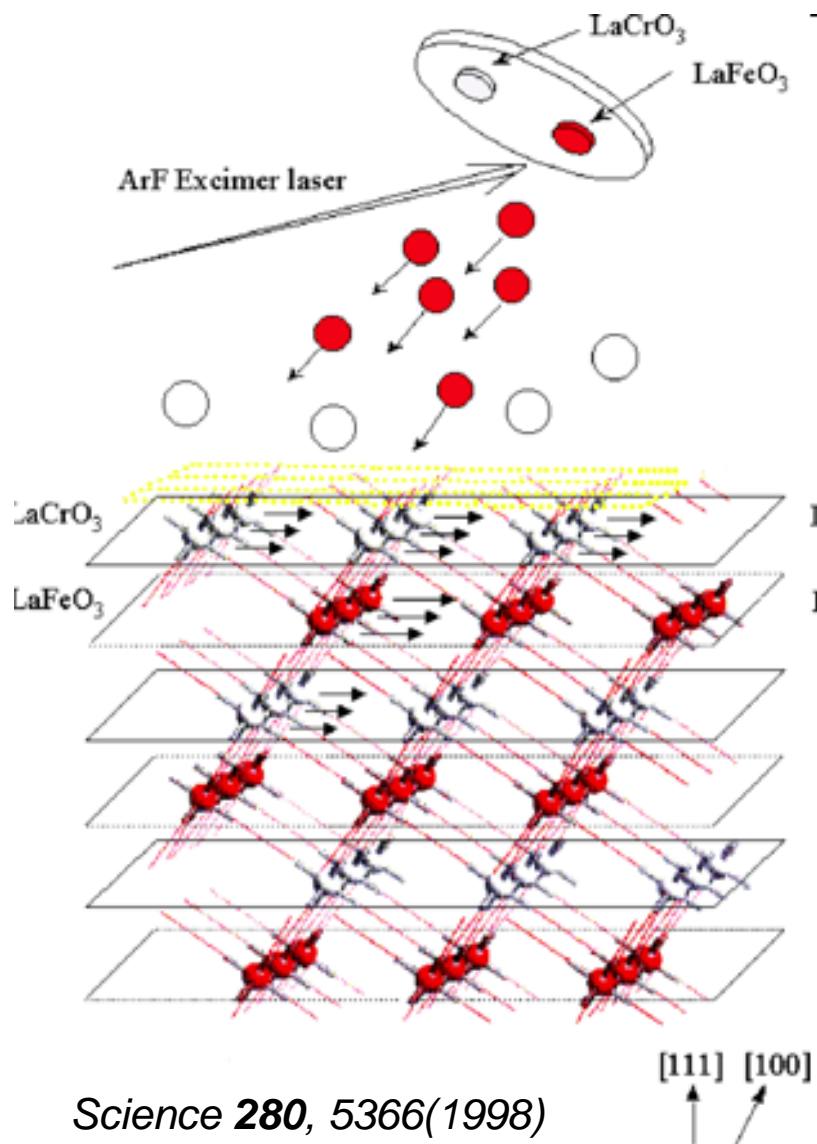
Na layer

Lattice-direction control superlattice



J. Appl. Phys. **89**, 2847(2001)

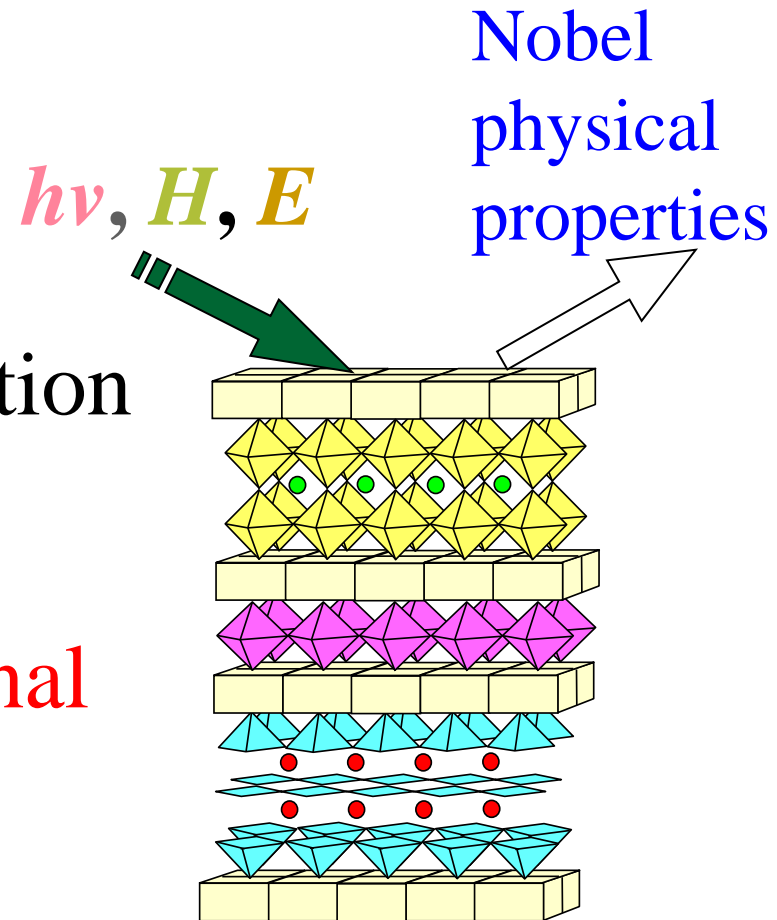
Lattice-direction control superlattice





Integration of different functional materials

- (1) Introduce strain effect
- (2) Introduce magnetic interaction between different layers
- (3) Integrate different functional materials

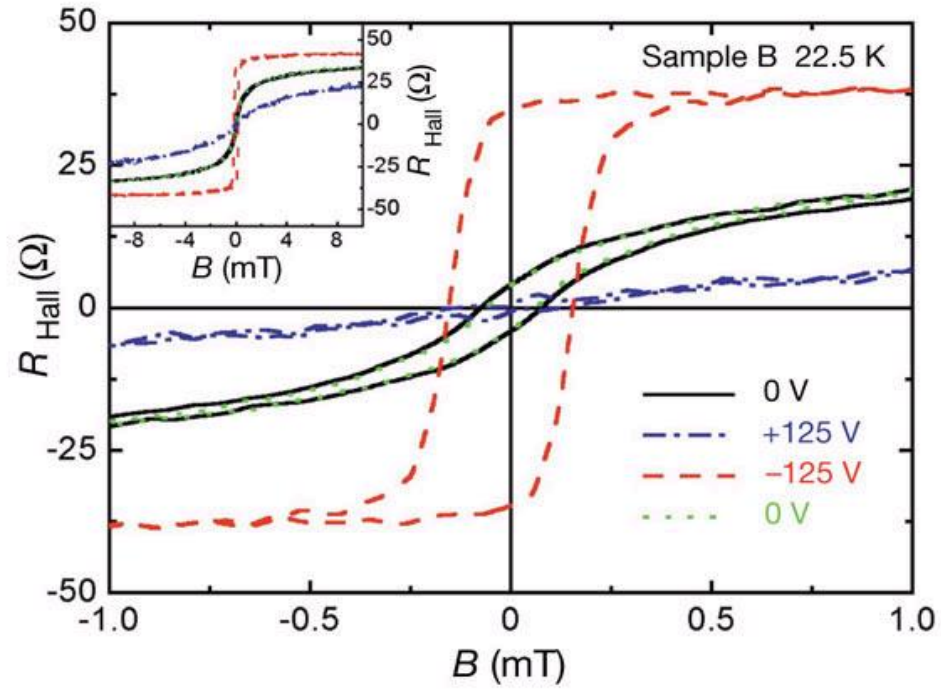
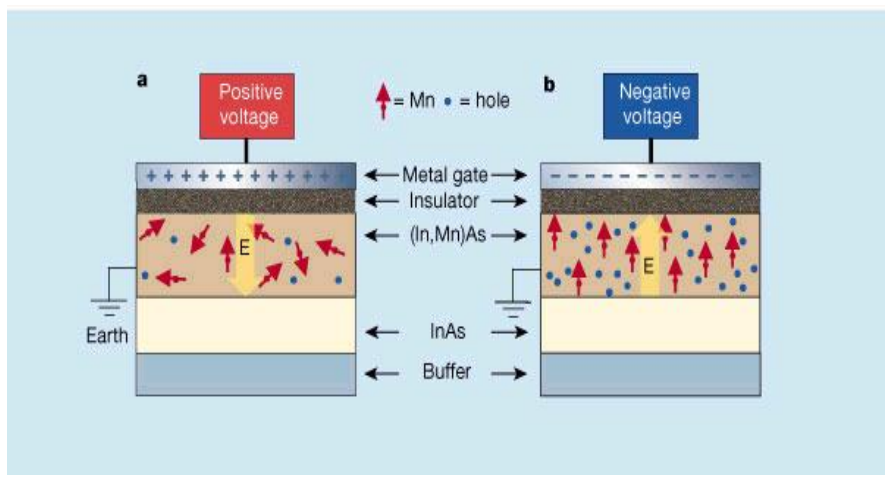




Ferromagnet/Ferroelectric material combination

Diluted magnetic semiconductor-- (In,Mn)As

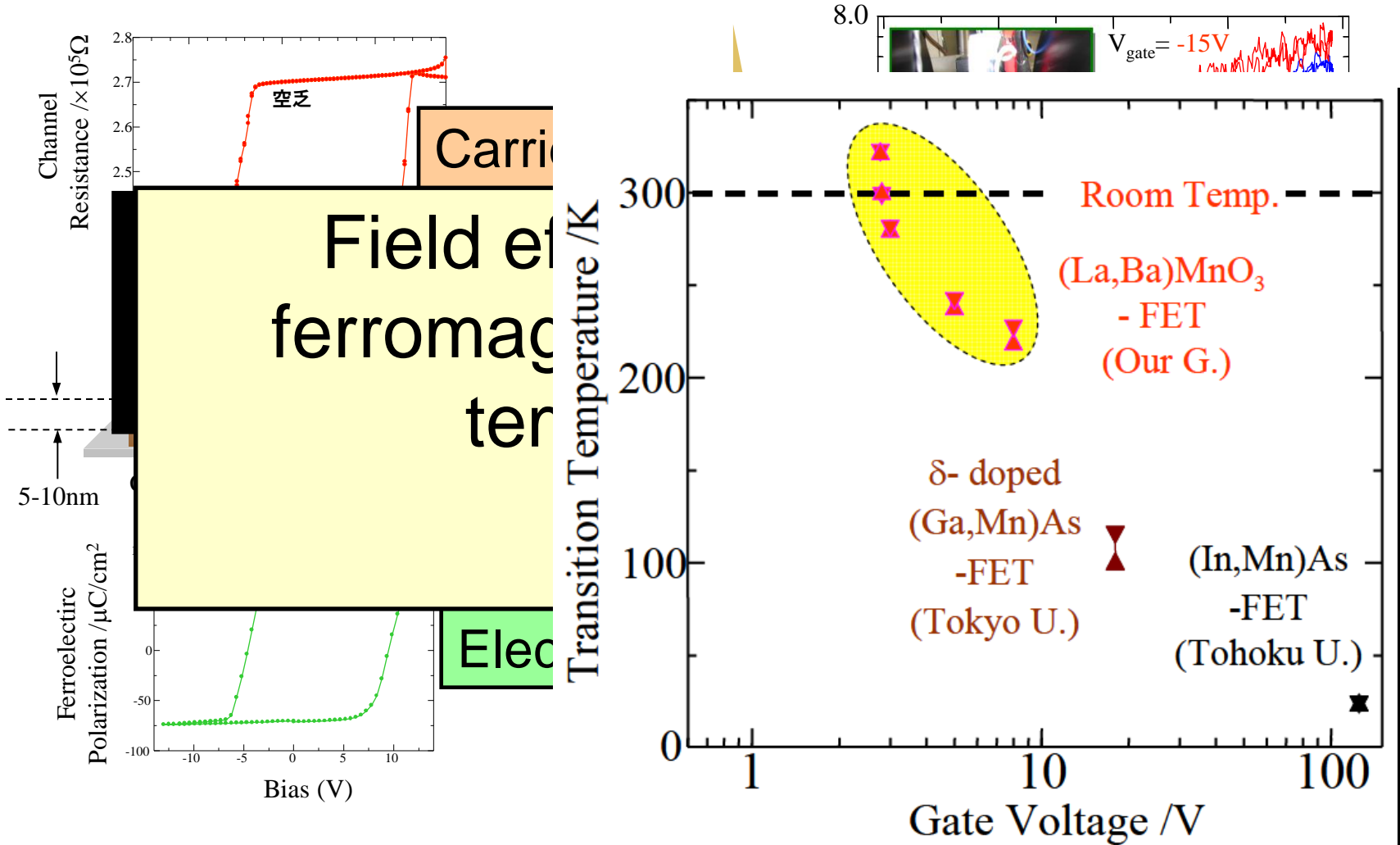
Field effect transistor



Nature **408**, 944(2000)



Ferromagnet/Ferroelectric material combination





Ferromagnet/Ferroelectric material combination

Conductive electron

$$H = -t_{\text{Mn-Mn}} \cos\left(\frac{\theta}{2}\right) - K_{\text{Hund}} \sigma \mathcal{S}_{\text{Mn}}$$

Localized spin

$$-J_{t2g} \sum_{LMnO} S_{\text{Mn}}^{t2g} S_{\text{Mn}}^{t2g}$$

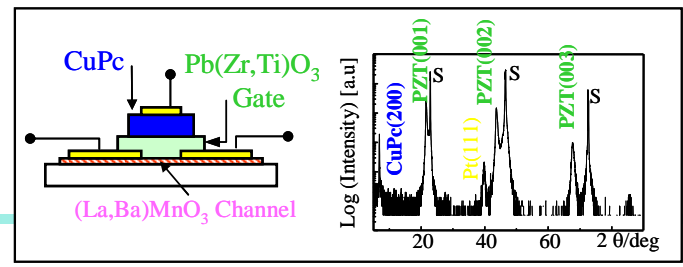
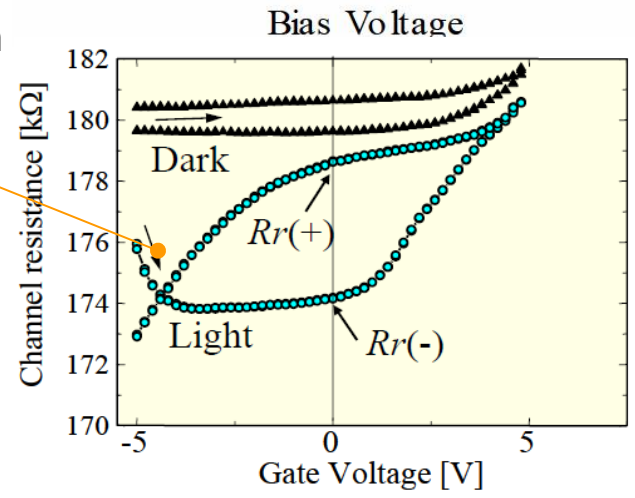
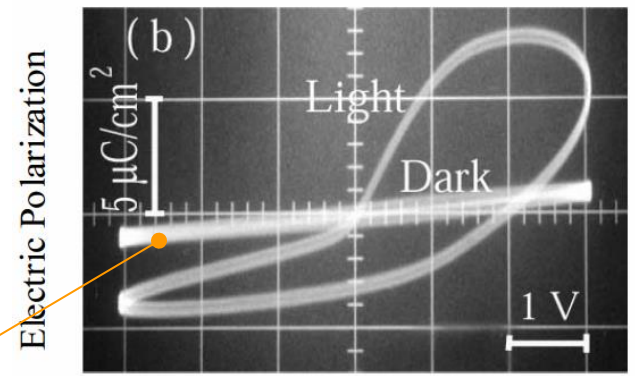
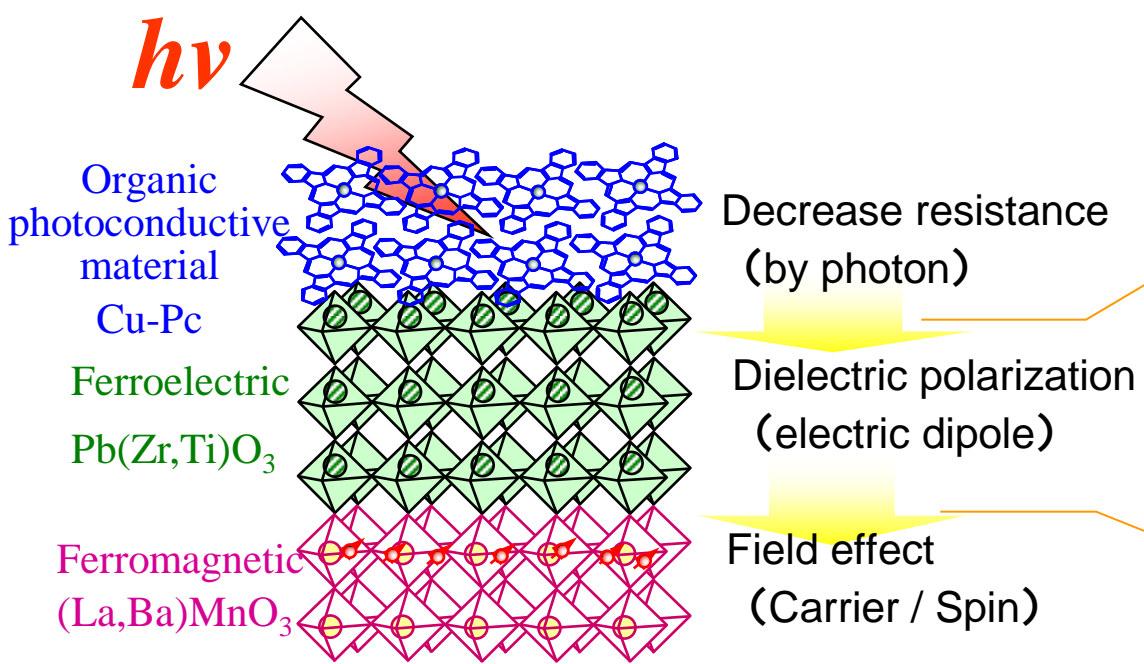
$$N \times$$

(The number of carriers)

Electric field

Photonic/Ferroelectric/magnetic material combination

Photon → Electric dipole → Carrier spin





Summary: Oxide spintronics

- (1) Introduce strain effect ----- Room temperature CMR
- (2) Introduce magnetic interaction --- Magnetic superlattice
between different layers Design of magnetic susceptibility
- (3) Integrate different functional ----- Ferromagnetism
materials + Ferroelectric