Computational Materials Design (CMD®) Workshop

Spintronic Design Course

Spintronic · Design · Magnetic control II

Materials Design based on band structures

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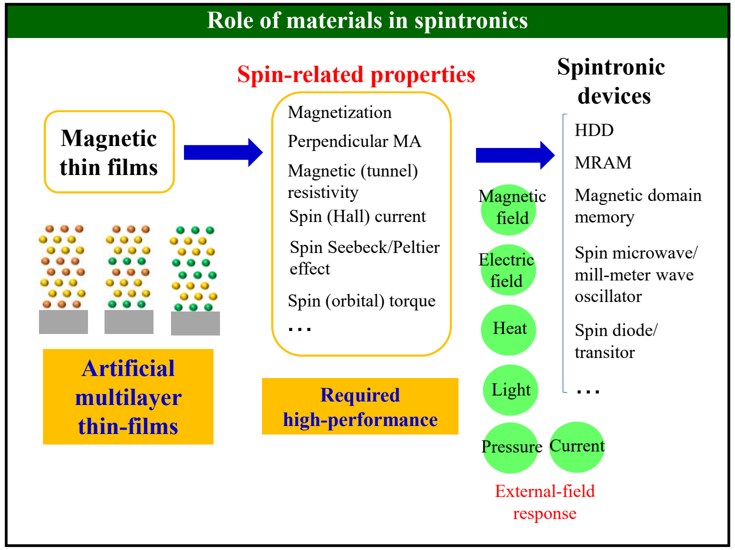
Mie University

Outline
- Introduction
- Electronic structures and magnetism in transition-metals
- Electronic structures and magnetism at surfaces/thin films
- Control of magnetism by tuning atomic-layer alignments
- Control of magnetism by external electric field
- Summary



Role of materials in spintronics

Magnetic thin films

Artificial multilayer thin-films

Spin-related properties
- Magnetization
- Perpendicular MA
- Magnetic (tunnel) resistivity
- Spin (Hall) current
- Spin Seebeck/Peltier effect
- Spin (orbital) torque
- …

Required high-performance

Magnetic field

Electric field

Heat

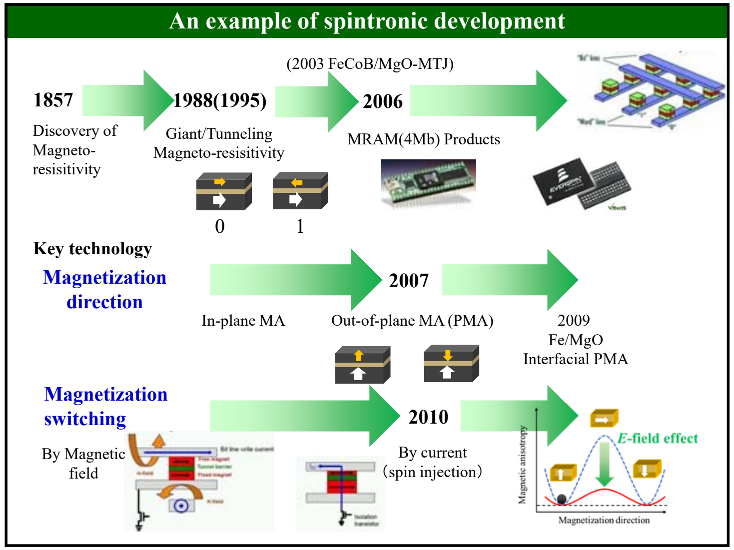
Light

Pressure

Current

External-field response

Spintronic devices
- HDD
- MRAM
- Magnetic domain memory
- Spin microwave/ mill-meter wave oscillator
- Spin diode/ transitor
- …



An example of spintronic development

1857 Discovery of Magneto-resisitivity

1988(1995) Giant/Tunneling Magneto-resisitivity

(2003 FeCoB/MgO-MTJ)

2006 MRAM(4Mb) Products

Key technology

Magnetization direction

In-plane MA → **2007** Out-of-plane MA (PMA) → 2009 Fe/MgO Interfacial PMA

Magnetization switching

By Magnetic field → **2010** By current （spin injection） → *E*-field effect

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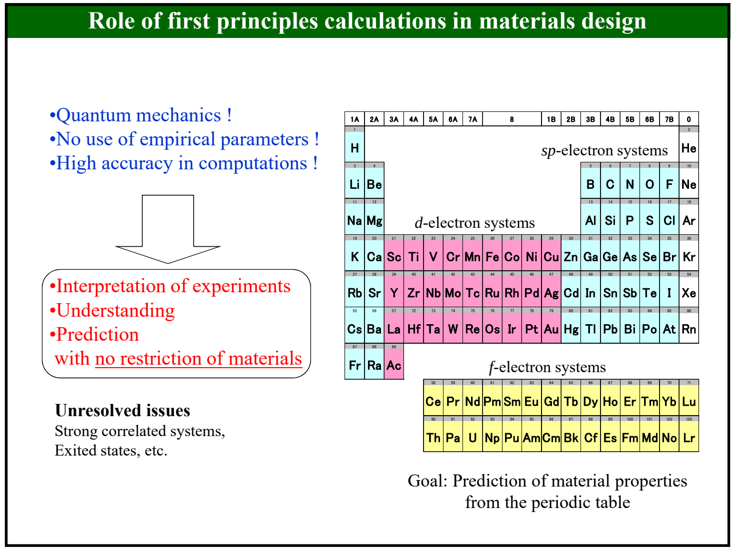

Role of first principles calculations in materials design

- •Quantum mechanics !
- •No use of empirical parameters !
- •High accuracy in computations !

- •Interpretation of experiments
- •Understanding
- •Prediction

with <u>no restriction of materials</u>

Unresolved issues
Strong correlated systems,
Exited states, etc.

sp-electron systems

d-electron systems

f-electron systems

1A	2A	3A	4A	5A	6A	7A	8			1B	2B	3B	4B	5B	6B	7B	0
1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac															
				58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
				90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Goal: Prediction of material properties from the periodic table

First principles calculations

①Kohn-Sham equation

exchange correlation potential

$$\boxed{\left[-\nabla^2+V_c(\mathbf{r})+V_{\text{eff}}(\mathbf{r})\right]\psi_i(\mathbf{r})=\varepsilon_i\psi_i(\mathbf{r})}$$

$$E_{\text{xc}}^{\text{LDA}}[n]\approx\int n(\mathbf{r})\varepsilon_{\text{ex}}^{\text{LDA}}(n(\mathbf{r}))$$

Coulomb potential **wave function (basis)**

②Total energy

$$E_{\text{total}}=\sum_{i=1,\varepsilon_i<E_F}^{N}\varepsilon_i$$

Kohn-Sham eigenvalues
(band structure, density of states)

$$-\frac{1}{2}\left[\int V_C(\mathbf{r})n(\mathbf{r})d\mathbf{r}+\sum_{\sigma}\int\left\{v_{\sigma}^{exc}(\mathbf{r})-\varepsilon_{\sigma}^{exc}(\mathbf{r})\right\}n_{\sigma}(\mathbf{r})d\mathbf{r}\right]-\frac{1}{2}\sum_{\mu}Z_{\mu}V_{C,\mu}(\mathbf{R}_{\mu})$$

double counting term

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Eigenvalues and eigenstates of electron orbitals in atoms

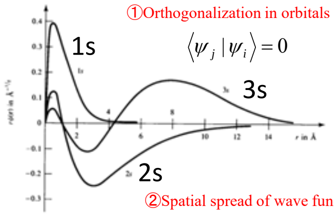
$$\boxed{\psi_{nlm}(\mathbf{r})\approx R_{nl}(r)Y_{lm}}$$

Li : $1s^2 2s$

Na : $1s^2 2s^2 2p^6 3s$

K : $1s^2 2s^2 2p^6 3s^2 3p^6 4s$

Atomic core

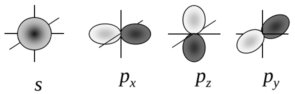


①Orthogonalization in orbitals

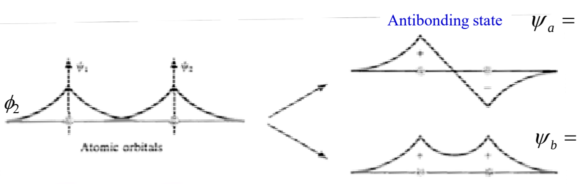
$$\langle\psi_j|\psi_i\rangle=0$$

②Spatial spread of wave function
Hybridization in crystals

FIGURE 1-2
The three s states of lowest energy for atomic hydrogen. The orbitals, multiplied by r, are plotted as a function of distance from the nucleus.

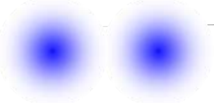


Hybridization : bonding and anti-bonding orbitals

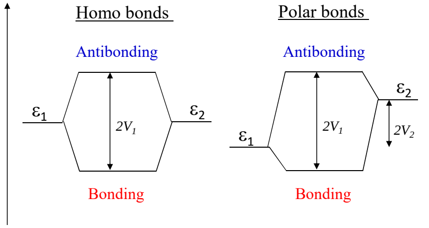


$$\psi_a=\frac{1}{\sqrt{2}}(\phi_1-\phi_2)$$

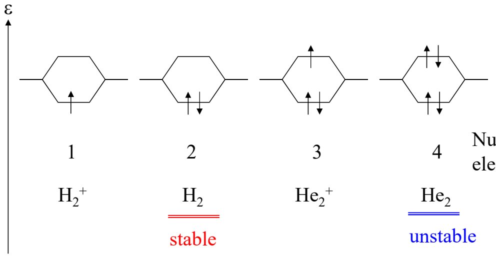
$$\psi_b=\frac{1}{\sqrt{2}}(\phi_1+\phi_2)$$



$$V_2=\langle\phi_2|V|\phi_1\rangle$$



Occupation of electrons



H_2^+ H_2 He_2^+ He_2

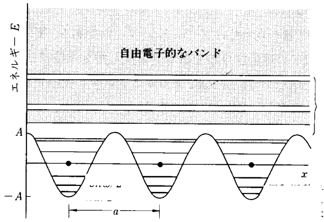
stable

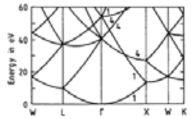
unstable

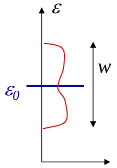
Electrons in crystal

Free-electron-like

$$\left(-\frac{\nabla^2}{2}+V_0\right)\psi=\varepsilon\psi \quad \varepsilon\propto\frac{k^2}{2}$$







Density of states, $D(\varepsilon)$

$$\left.\begin{aligned}&\left(-\frac{\nabla^2}{2}+V(\mathbf{r})\right)\psi_v=\varepsilon\psi_v\\&V(\mathbf{r}+\mathbf{R}_j)=V(\mathbf{r})\end{aligned}\right\}$$

Bloch function

$$\psi_{\mathbf{k}}(\mathbf{r})=e^{i\mathbf{k}\cdot\mathbf{r}}u_{\mathbf{k}}(\mathbf{r})$$

$$u_{\mathbf{k}}(\mathbf{r}+\mathbf{R}_j)=u_{\mathbf{k}}(\mathbf{r})$$

$$\langle\psi_v|\psi_c\rangle=0$$

Orthogonal

atomic-like

$$\left(-\frac{\nabla^2}{2}+V_{atom}(r)\right)\psi_c=\varepsilon\psi_c \quad \varepsilon=\varepsilon_{n\ell}$$

Cohesive energy and spin polarization in transition-metals

Non-spin Polarized

LDA results vs. experiments

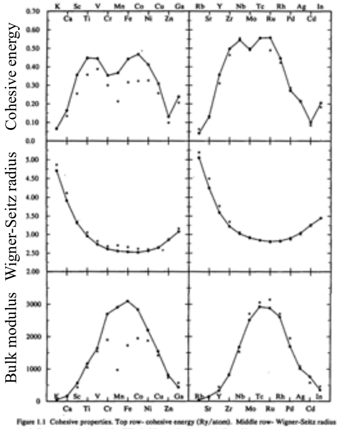


Figure 1.1 Cohesive properties. Top row- cohesive energy (Ry/atom). Middle row- Wigner-Seitz radius (a.u.). Bottom row- bulk modulus (Kbar). Measured values are indicated by crosses.

V. L. Moruzzi, J.F. Janak, A.R. Williams, Calculated electronic properties of metals (Pergamon Press, New York, 1978)

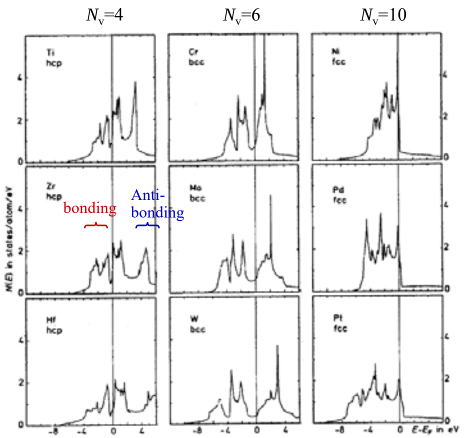
Magnetism

Question:
Why do ferromagnetism appear only in Fe, Co and Ni?

1A	2A	3A	4A	5A	6A	7A	8			1B	2B	3B	4B	5B	6B	7B	0
H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn

	Magnetic order	Transition Temperature(K)	Crystal structure	Number of valence
Fe	Ferromagnetic	1043	bcc	8
Co	Ferromagnetic	1388	hcp	9
Ni	Ferromagnetic	627	fcc	10

Band structures of transition-metals



J. Kübler, Theory of itinerant electron magnetism (Oxford University Press, Oxford, 2000)

Band structure

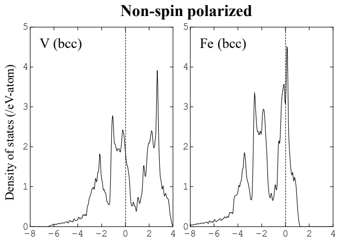
$D^{3d}(E_F)$
$> D^{4d}(E_F)$
$> D^{5d}(E_F)$

W^{3d}
$> W^{4d}$
$> W^{5d}$

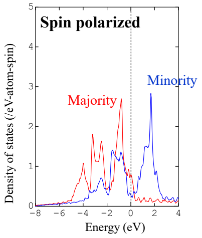
Fermi level

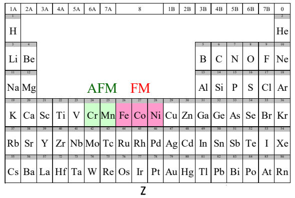
E_F^{Ti}
$< E_F^{Cr}$
$< E_F^{Ni}$

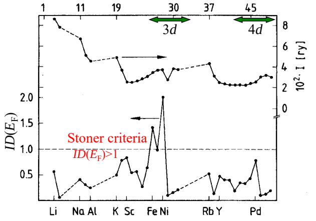
Magnetism in transition metals



LDA results







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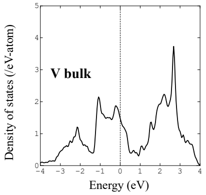
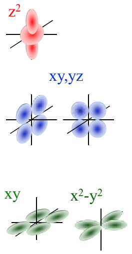
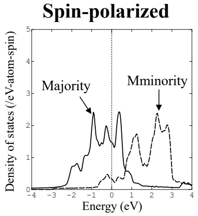
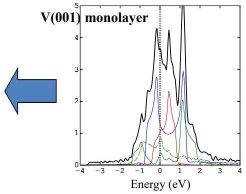
Band structures and spin polarization in transition metal monolayers

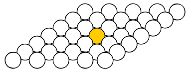
LDA results





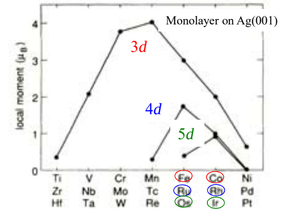


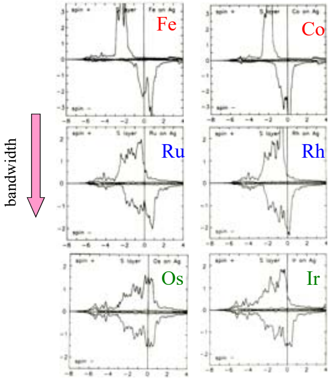




Ferromagnetism in transition metal monolayers

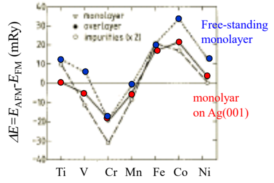
Magnetic moments





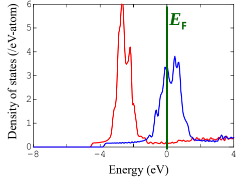
S. Blügel, Phys. Rev. Lett. 68, 851(1992)

Energy difference between FM and AFM

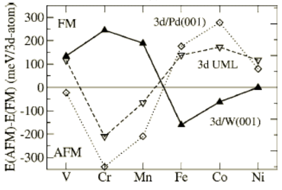


Effect of substrates to magnetism in transition metal monolayers

Fe(001) monolayer (*a*=2.87Å)



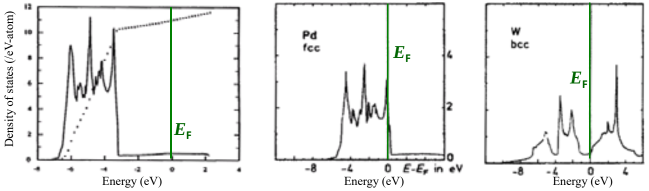
Total energy difference



P. Ferriani et.al., Phys. Rev. B 72, 024452 (2005)

Substrates

Ag (*a*=2.89Å) Pd (*a*=2.75Å) W (*a*=2.23Å)



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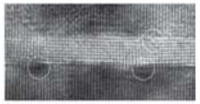
Magnetocrystalline anisotropy (MCA)

MTJ device



[1]

Ferromagnetic

Insulator

Ferromagnetic

✓Non-volatility
✓Large capacity
✓High-speed

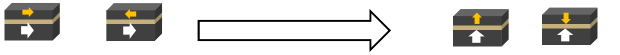
Many Applications
- MRAM
- Magnetic sensor

[1] S. Yuasa, *et al*., Nature Materials **3**, 868 (2004).

In-plane MCA

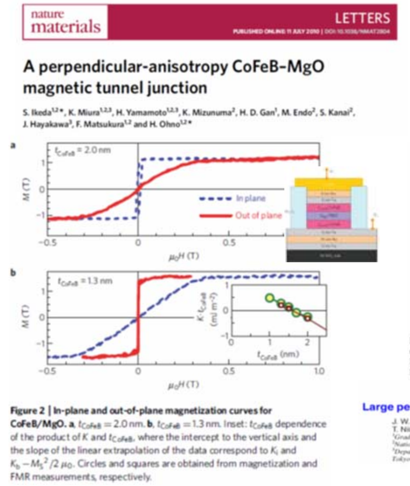
Large advance for applications

Out-of-plane MCA



We, here, design thin films with large MCA

Perpendicular MCA of Fe thin film on MgO(001): experiments



nature materials | LETTERS

PUBLISHED ONLINE 11 JULY 2010 | DOI: 10.1038/NMAT2804

A perpendicular-anisotropy CoFeB–MgO magnetic tunnel junction

S. Ikeda[1,2]*, K. Miura[1,2,3], H. Yamamoto[1,2,3], K. Mizunuma[2], H. D. Gan[1], M. Endo[2], S. Kanai[2], J. Hayakawa[3], F. Matsukura[1,2] and H. Ohno[1,2]*

Figure 2 | In-plane and out-of-plane magnetization curves for CoFeB/MgO. a, $t_{CoFeB} = 2.0$ nm. **b**, $t_{CoFeB} = 1.3$ nm. Inset: t_{CoFeB} dependence of the product of K and t_{CoFeB}, where the intercept to the vertical axis and the slope of the linear extrapolation of the data correspond to K_i and $K_b - M_S^2/2\mu_0$. Circles and squares are obtained from magnetization and FMR measurements, respectively.

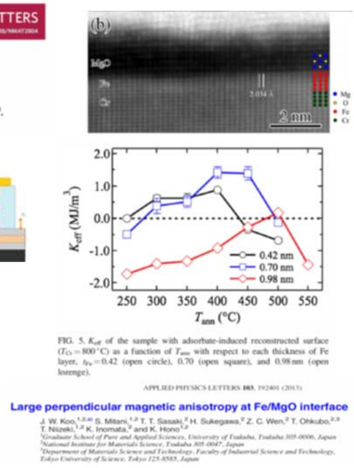


FIG. 5. K_{eff} of the sample with adsorbate-induced reconstructed surface (T_{Cr} = 800 °C) as a function of T_{ann} with respect to each thickness of Fe layer, t_{Fe} = 0.42 (open circle), 0.70 (open square), and 0.98 nm (open lozenge).

APPLIED PHYSICS LETTERS **103**, 192401 (2013)

Large perpendicular magnetic anisotropy at Fe/MgO interface

J. W. Koo,[1,2,a)] S. Mitani,[1,2] T. T. Sasaki,[2] H. Sukegawa,[2] Z. C. Wen,[2] T. Ohkubo,[2,3] T. Niizeki,[1,2] K. Inomata,[2] and K. Hono[1,2]

[1]Graduate School of Pure and Applied Sciences, University of Tsukuba, Tsukuba 305-0006, Japan
[2]National Institute for Materials Science, Tsukuba 305-0047, Japan
[3]Department of Materials Science and Technology, Faculty of Industrial Science and Technology, Tokyo University of Science, Tokyo 125-8585, Japan

First principles calculations of MCA energy

Spin-orbit coupling

$$H^{SOC} = \underline{\underline{\frac{1}{4c^2}\frac{1}{r}\frac{dV}{dr}}}\,\ell\cdot\boldsymbol{\sigma} = \xi(r)\begin{bmatrix}\ell_z & \ell_- \\ \ell_+ & -\ell_z\end{bmatrix}$$

Admixture of spin-up and down components

SOC strength, $\xi(r)$

~50 meV for 3d-metals

Magnetocrystalline anisotropy energy

$$E_{MCA} = E_{total}(\rightarrow) - E_{total}(\uparrow)$$

~0.1 meV/atom

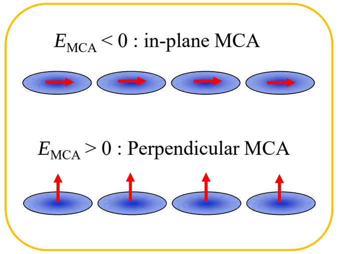
Force theorem

$$\approx \{E[\rho_0, \mathbf{m}_0(\rightarrow)] - E[\rho_0, \mathbf{m}_0(\uparrow)]\}$$

$$= \sum_{\mathbf{k}}\left[\sum_{i\in o'}\varepsilon_{\mathbf{k},i}(\rightarrow) - \sum_{i\in o''}\varepsilon_{\mathbf{k},i}(\uparrow)\right]$$

$E_{MCA} < 0$: in-plane MCA

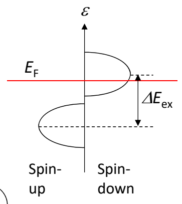
$E_{MCA} > 0$: Perpendicular MCA



Perturbation method of MCA energy

$$E_{MCA}(\sigma) = E^{SOC}(x) - E^{SOC}(z)$$

$$\approx \Delta E^{dd} + \Delta E^{ud}$$



$$\Delta E^{dd} = E^{dd}(x) - E^{dd}(z) = \xi^2 \sum_{o_-}\sum_{u_-} \frac{|\langle o_- | \mathbf{L}_z | u_- \rangle|^2 - |\langle o_- | \mathbf{L}_x | u_- \rangle|^2}{\varepsilon_{u_-} - \varepsilon_{o_+}}$$

$$\Delta E^{ud} = E^{ud}(x) - E^{ud}(z) = \frac{\xi^2}{\Delta E_{ex}} \sum_{o_-} \langle o_- | 3\mathbf{L}_z^2 - \mathbf{L}^2 | o_- \rangle$$

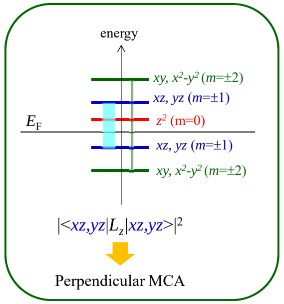
R. Wu, A.J. Freeman, J. Magn. Magn. Mater. 200, 498(1999)

Rule in origin of MCA in ΔE^{dd}

$$\Delta E^{dd} = \xi^2 \sum_{o_-}\sum_{u_-} \frac{|\langle o_- | \mathbf{L}_z | u_- \rangle|^2 - |\langle o_- | \mathbf{L}_x | u_- \rangle|^2}{\varepsilon_{u_-} - \varepsilon_{o_+}}$$

Positive E_{MCA}

$|\langle o|L_z|u\rangle|^2$

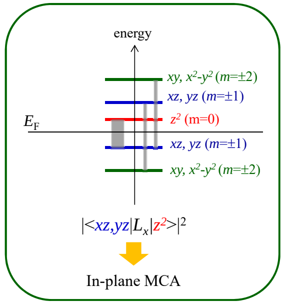


$|\langle xz,yz|L_z|xz,yz\rangle|^2$

Perpendicular MCA

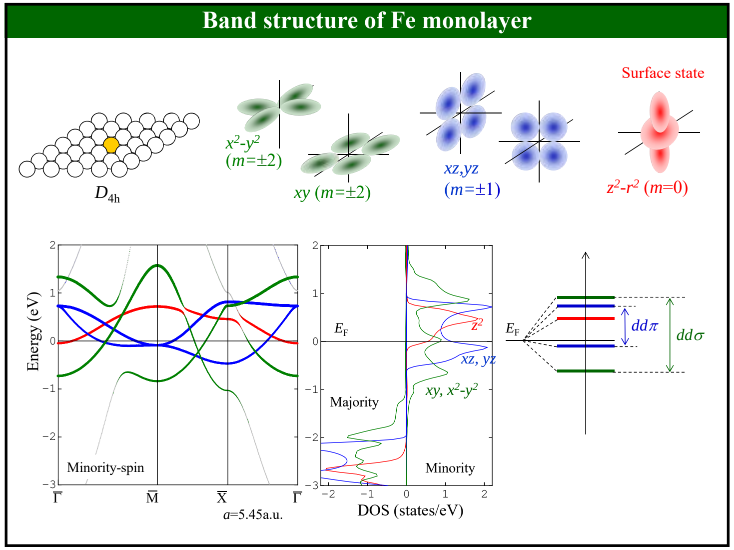
Negative E_{MCA}

$|\langle o|L_x|u\rangle|^2$

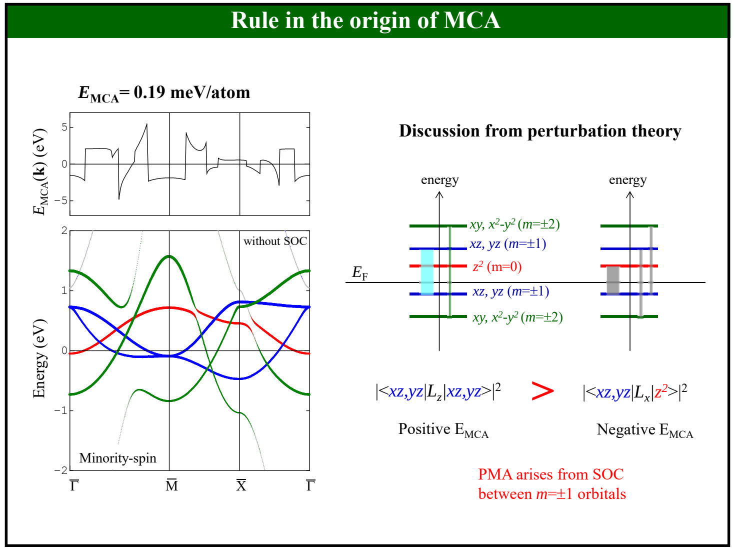


$|\langle xz,yz|L_x|z^2\rangle|^2$

In-plane MCA



Band structure of Fe monolayer



Rule in the origin of MCA

E_{MCA}= 0.19 meV/atom

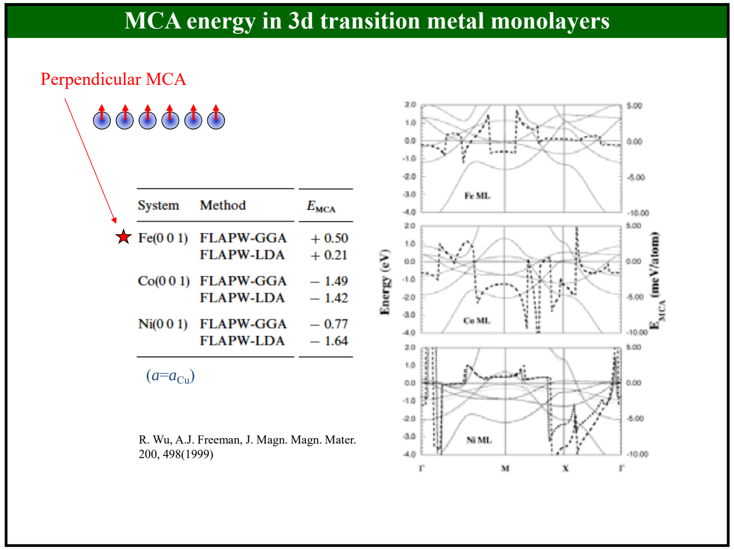
Discussion from perturbation theory

$|\langle xz,yz|L_z|xz,yz\rangle|^2$ > $|\langle xz,yz|L_x|z^2\rangle|^2$

Positive E_{MCA}

Negative E_{MCA}

PMA arises from SOC between m=±1 orbitals



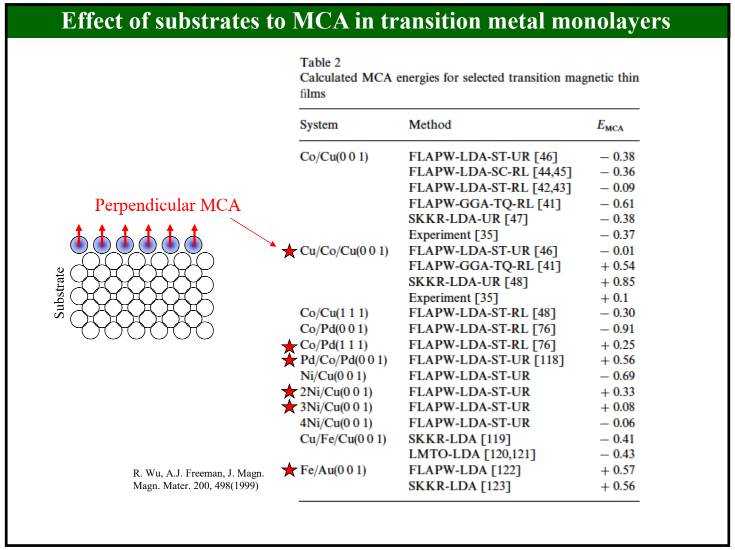
MCA energy in 3d transition metal monolayers

Perpendicular MCA

System	Method	E_{MCA}
★ Fe(0 0 1)	FLAPW-GGA	+ 0.50
	FLAPW-LDA	+ 0.21
Co(0 0 1)	FLAPW-GGA	– 1.49
	FLAPW-LDA	– 1.42
Ni(0 0 1)	FLAPW-GGA	– 0.77
	FLAPW-LDA	– 1.64

(a=a_{Cu})

R. Wu, A.J. Freeman, J. Magn. Magn. Mater. 200, 498(1999)



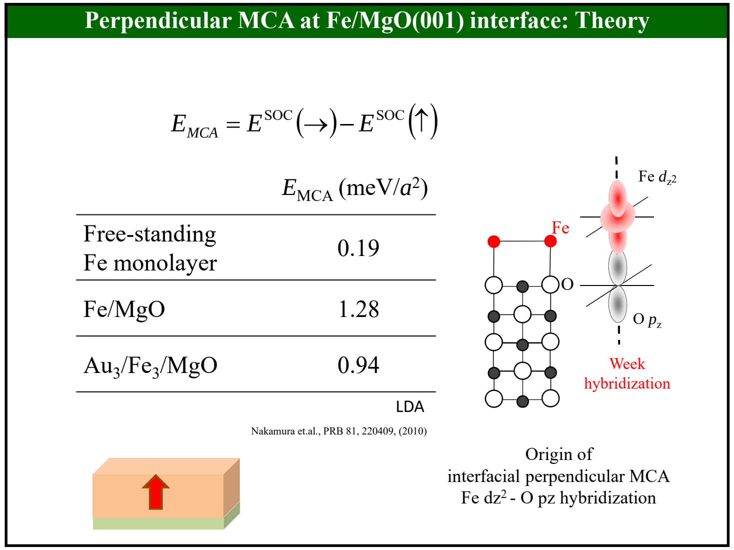
Effect of substrates to MCA in transition metal monolayers

Perpendicular MCA

Table 2
Calculated MCA energies for selected transition magnetic thin films

System	Method	E_{MCA}
Co/Cu(0 0 1)	FLAPW-LDA-ST-UR [46]	– 0.38
	FLAPW-LDA-SC-RL [44,45]	– 0.36
	FLAPW-LDA-ST-RL [42,43]	– 0.09
	FLAPW-GGA-TQ-RL [41]	– 0.61
	SKKR-LDA-UR [47]	– 0.38
	Experiment [35]	– 0.37
★ Cu/Co/Cu(0 0 1)	FLAPW-LDA-ST-UR [46]	– 0.01
	FLAPW-GGA-TQ-RL [41]	+ 0.54
	SKKR-LDA-UR [48]	+ 0.85
	Experiment [35]	+ 0.1
Co/Cu(1 1 1)	FLAPW-LDA-ST-RL [48]	– 0.30
Co/Pd(0 0 1)	FLAPW-LDA-ST-RL [76]	– 0.91
★ Co/Pd(1 1 1)	FLAPW-LDA-ST-RL [76]	+ 0.25
★ Pd/Co/Pd(0 0 1)	FLAPW-LDA-ST-UR [118]	+ 0.56
Ni/Cu(0 0 1)	FLAPW-LDA-ST-UR	– 0.69
★ 2Ni/Cu(0 0 1)	FLAPW-LDA-ST-UR	+ 0.33
★ 3Ni/Cu(0 0 1)	FLAPW-LDA-ST-UR	+ 0.08
4Ni/Cu(0 0 1)	FLAPW-LDA-ST-UR	– 0.06
Cu/Fe/Cu(0 0 1)	SKKR-LDA [119]	– 0.41
	LMTO-LDA [120,121]	– 0.43
★ Fe/Au(0 0 1)	FLAPW-LDA [122]	+ 0.57
	SKKR-LDA [123]	+ 0.56

R. Wu, A.J. Freeman, J. Magn. Magn. Mater. 200, 498(1999)



Perpendicular MCA at Fe/MgO(001) interface: Theory

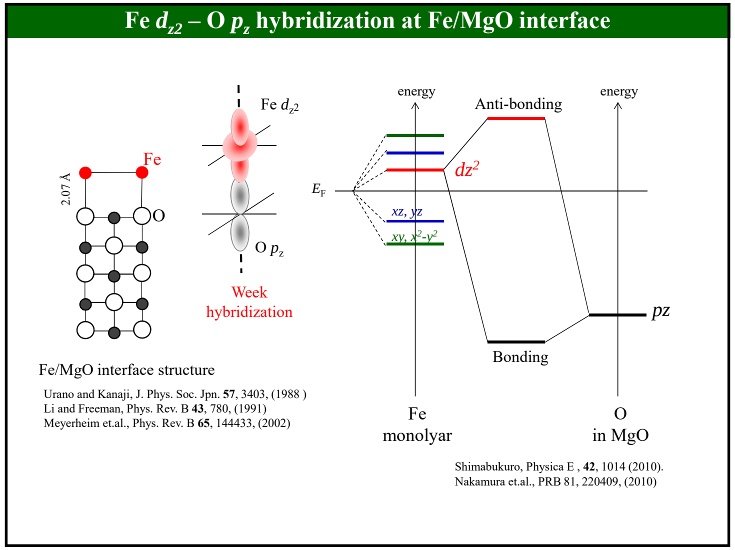
$$E_{MCA} = E^{\mathrm{SOC}}(\rightarrow) - E^{\mathrm{SOC}}(\uparrow)$$

	E_{MCA} (meV/a^2)
Free-standing Fe monolayer	0.19
Fe/MgO	1.28
$Au_3/Fe_3/MgO$	0.94

LDA

Nakamura et.al., PRB 81, 220409, (2010)

Origin of
interfacial perpendicular MCA
Fe dz^2 - O pz hybridization



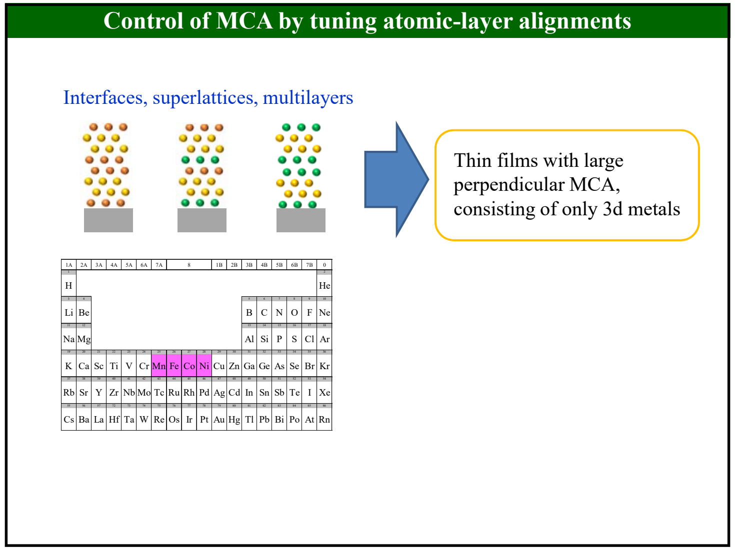
Fe d_{z2} – O p_z hybridization at Fe/MgO interface

Fe/MgO interface structure

Urano and Kanaji, J. Phys. Soc. Jpn. **57**, 3403, (1988)
Li and Freeman, Phys. Rev. B **43**, 780, (1991)
Meyerheim et.al., Phys. Rev. B **65**, 144433, (2002)

Shimabukuro, Physica E , **42**, 1014 (2010).
Nakamura et.al., PRB 81, 220409, (2010)

- Introduction
- Electronic structures and magnetism in transition-metals
- Electronic structures and magnetism at surfaces/thin films
- Control of magnetism by tuning atomic-layer alignments
- Control of magnetism by external electric field
- Summary



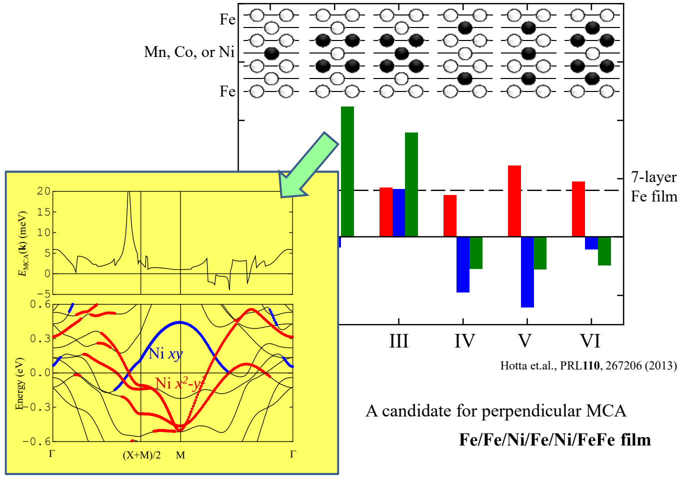
Control of MCA by tuning atomic-layer alignments

Interfaces, superlattices, multilayers

Thin films with large perpendicular MCA, consisting of only 3d metals

1A	2A	3A	4A	5A	6A	7A	8			1B	2B	3B	4B	5B	6B	7B	0
1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn

MCA of 3d transition metal thin films with seven-atomic-layer



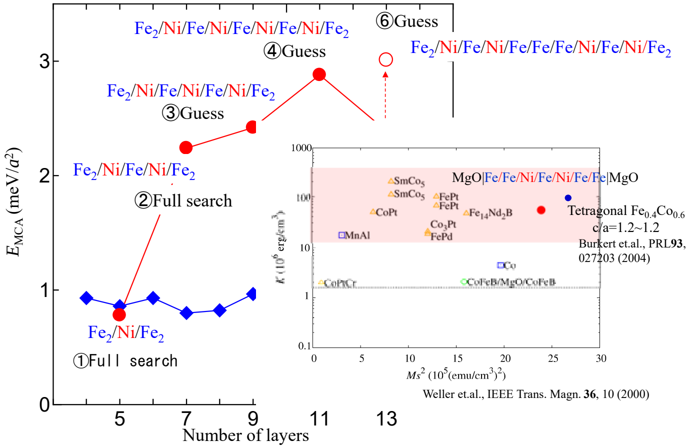
Hotta et.al., PRL**110**, 267206 (2013)

A candidate for perpendicular MCA

Fe/Fe/Ni/Fe/Ni/FeFe film

Search for *3d* thin films with giant perpendicular MCA

Upper limit for perpendicular MCA in 3*d* thin films



Burkert et.al., PRL**93**, 027203 (2004)

Weller et.al., IEEE Trans. Magn. **36**, 10 (2000)

- ➢ Introduction
- ➢ Electronic structures and magnetism in transition-metals
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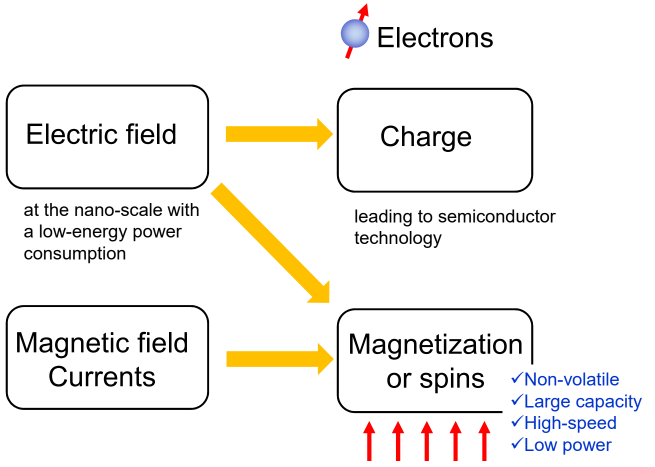
- ➢ Control of magnetism by tuning atomic-layer alignments
- ➢ Control of magnetism by external electric field
- ➢ Summary

E-field-control of magnetism



Electrons

Electric field

Charge

at the nano-scale with a low-energy power consumption

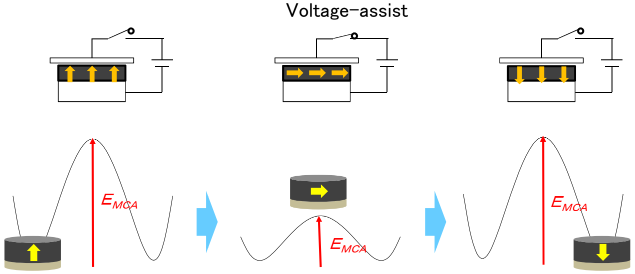
leading to semiconductor technology

Magnetic field
Currents

Magnetization
or spins

✓Non-volatile
✓Large capacity
✓High-speed
✓Low power

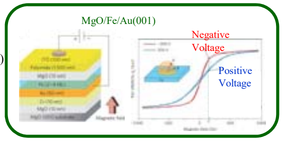
An example:
Voltage-assist magnetization switching



Control of magnetism of metal thin films by electric field

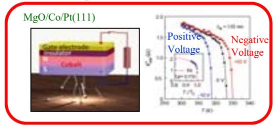
- Magnetocrystalline anisotropy (MCA)
  Weisheit et.al., Science 315, 349 (2007)
  Maruyama et.al., Nature Nanotech. 4, 349 (2009)
  Duan et.al., PRL**101**, 137201 (2008)
  Nakamura et.al., PRL**102**, 187201 (2009); PRB **80**, 172402 (2009)
  Tsujikawa et.al., PRL**102**, (2009)
  ….
- Curie temperature (T_C)
  Chiba et.al., Nat. Mater. 10, 853-856 (2011)
  Oba et.al., PRL**114**, 107202 (2015)
- Dzyaloshinskii-Moriya interaction (DMI)
  Nawaoka et.al., Appl. Phys. Express 8, 063004(2015)
  Nakamura et.al., (2015)
- Magnetic moments
  Obinata et.al., Sci. Rep. 5, 14303 (2015)
- Magneto-optical conductivity
  Hibino et.al., (2015)
  Nakamura et.al., J. Korean Phys. Soc. **63**, 612 (2013)
- Magnetic dumping
  Okada et.al., Appl. Phys. Lett. 105, 052415 (2014)
- Magnetic phase-transition (bcc Fe vs fcc Fe)
  Gerhard et.al., Nat. Nanotech., **5**, 792 (2010)
- etc.

Magnetocrystalline anisotropy



Maruyama et.al., Nature Nanotech. 4, 349 (2009)

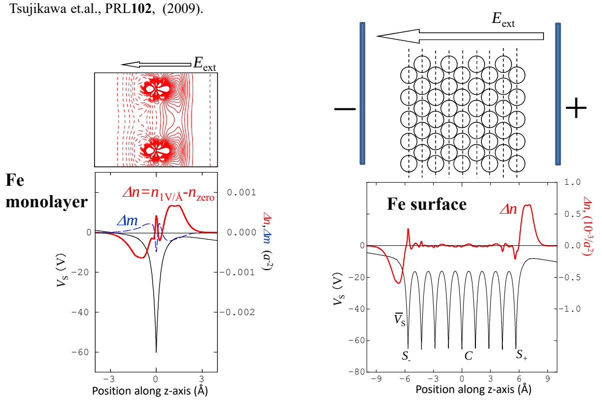
Curie temperatures



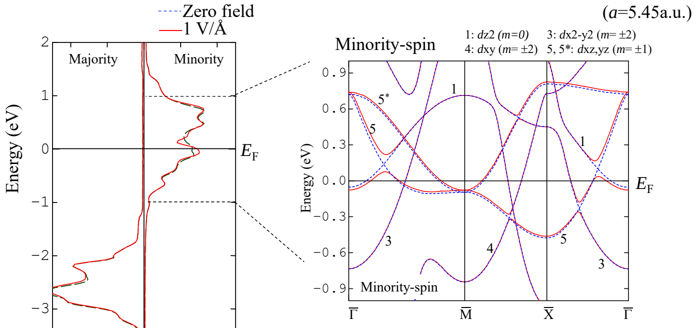
Chiba et.al., Nat. Mater. 10, 853-856 (2011)

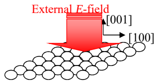
Electric-field-induced charges at surfaces

- ***Redistribution in charge/spin densities at surfaces/interfaces by E-field*.**
  Duan et.al., PRL**101**, 137201 (2008),
  Nakamura et.al., PRL**102**, 187201 (2009); PRB **80**, 172402 (2009),
  Tsujikawa et.al., PRL**102**, (2009).



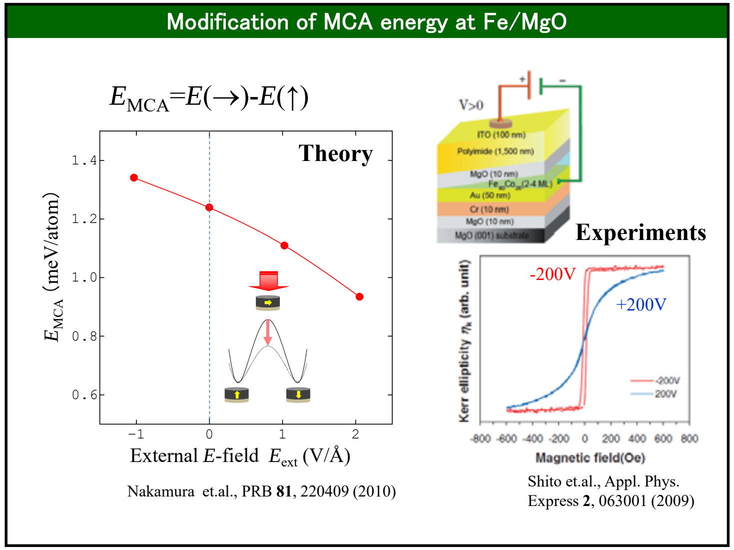
Modification of band structure of Fe monolayer by electric field





Change in band structure around Fermi level

Change of MCA energy

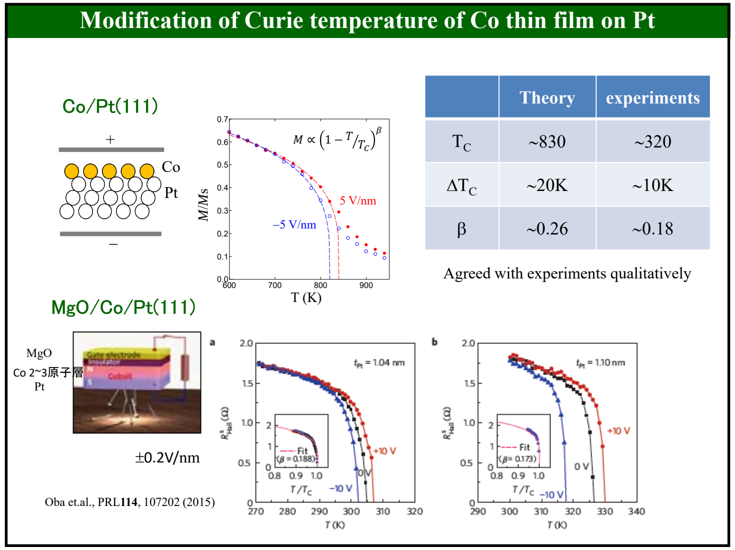


Modification of MCA energy at Fe/MgO

E_{MCA}=E(→)-E(↑)

Nakamura et.al., PRB **81**, 220409 (2010)

Shito et.al., Appl. Phys. Express **2**, 063001 (2009)



Modification of Curie temperature of Co thin film on Pt

Co/Pt(111)

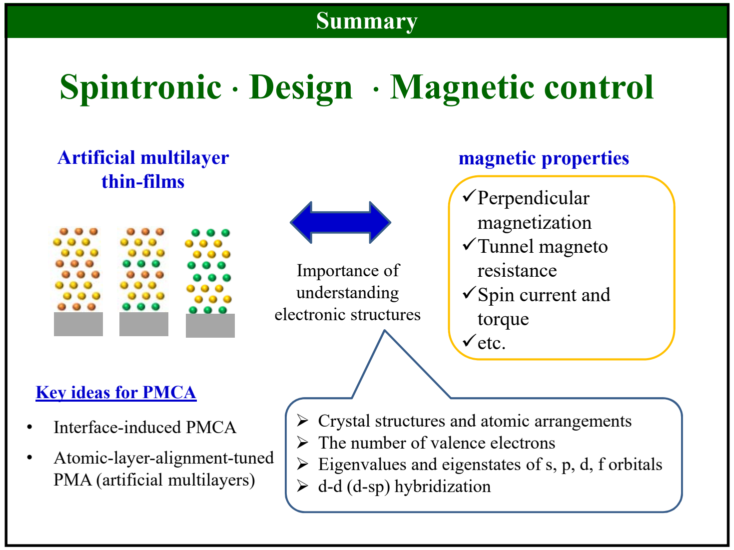
	Theory	experiments
T_C	~830	~320
ΔT_C	~20K	~10K
β	~0.26	~0.18

Agreed with experiments qualitatively

MgO/Co/Pt(111)

±0.2V/nm

Oba et.al., PRL**114**, 107202 (2015)



Summary

Spintronic · Design · Magnetic control

Artificial multilayer thin-films

Importance of understanding electronic structures

magnetic properties

✓Perpendicular magnetization
✓Tunnel magneto resistance
✓Spin current and torque
✓etc.

Key ideas for PMCA

- Interface-induced PMCA
- Atomic-layer-alignment-tuned PMA (artificial multilayers)

- Crystal structures and atomic arrangements
- The number of valence electrons
- Eigenvalues and eigenstates of s, p, d, f orbitals
- d-d (d-sp) hybridization