Computational Materials Design (CMD®) Workshop

Spintronic Design Course

Spintronic · Design · Magnetic control II

Materials Design based on band structures

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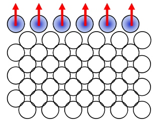
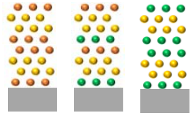
Outline
- Introduction
- Calculation method
- Electronic structures and magnetism in bulk and at surfaces/thin films
- Control of magnetism by atomic-layer alignments and external electric field



Role of materials in spintronics

Magnetic thin films → **Spin-related properties** → **Spintronic devices**



Artificial multilayer thin-films

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

External-field response: Magnetic field, Electric field, Heat, Light, Pressure, Current

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

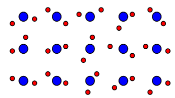
- Introduction
- Calculation method
- Electronic structures and magnetism

  in bulk and at surfaces/thin films
- Control of magnetism

  by tuning atomic-layer alignments and by external electric field

Basic: Density functional theory and Kohn-Sham equation

Many-body problem for electrons



$$\hat{\mathcal{H}}_e \Psi(\boldsymbol{R}_1,\boldsymbol{R}_2,\cdots;\boldsymbol{r}_1,\boldsymbol{r}_2,\cdots) = E\,\Psi(\boldsymbol{R}_1,\boldsymbol{R}_2,\cdots;\boldsymbol{r}_1,\boldsymbol{r}_2,\cdots)$$

① Adiabatic (Born-Oppenheimer) approximation

②Non-interacting one particle approximation

Kohn-Sham equation (one-electron equation)

$$\left[-\frac{\nabla^2}{2}+v_{\mathrm{H}}(n(\mathbf{r}))+v_{\mathrm{XC}}(n(\mathbf{r}))\right]\phi_b(\mathbf{r})=\varepsilon_b\,\phi_b(\mathbf{r})$$

Basic: Case of non spin-polarized systems

Kohn-Sham equation in one-electron approximation

$$\left[-\frac{\nabla^2}{2} + v_{\mathrm{H}}(n(\mathbf{r})) + v_{\mathrm{XC}}(n(\mathbf{r}))\right]\phi_b(\mathbf{r}) = \varepsilon_b\,\phi_b(\mathbf{r})$$

↑ Local Density Approximation (LDA)

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

$$E_{\mathrm{xc}}^{\mathrm{GGA}}[n] \approx \int n(\mathbf{r})\varepsilon_{\mathrm{xc}}^{\mathrm{GGA}}(n(\mathbf{r}),\nabla n(\mathbf{r}))$$

Electron density

$$n(\boldsymbol{r}) = \langle\psi(\boldsymbol{r})|\hat{n}|\psi(\boldsymbol{r})\rangle$$

$$\sim |\phi_1(r)|^2 + |\phi_2(r)|^2 + \cdots = \sum_{b=1}^{N}|\phi_b(r)|^2$$

Basic: Case of spin-polarized systems

Kohn-Sham equation in one-electron approximation

$$\left[-\frac{\nabla^2}{2} + v_{\mathrm{H}}(n(\mathbf{r})) + v_{\mathrm{XC}}(n(\mathbf{r}), m(\boldsymbol{r}))\right]\phi_{b,\sigma}(\mathbf{r}) = \varepsilon_{b,\sigma}\phi_{b,\sigma}(\mathbf{r})$$

↑ Local Spin Density Approximation (LSDA)

Electron density

$$n(\boldsymbol{r}) \sim \sum_{b=1}^{N_\uparrow}|\phi_{b,\uparrow}(\boldsymbol{r})|^2 + \sum_{b=1}^{N_\downarrow}|\phi_{b,\downarrow}(\boldsymbol{r})|^2$$

$$= n_\uparrow(\boldsymbol{r}) + n_\downarrow(\boldsymbol{r})$$

$$m(\boldsymbol{r}) = n_\uparrow(\boldsymbol{r}) - n_\downarrow(\boldsymbol{r})$$

Basic: Variational principle method

Cut-off of basis

$$\psi_{\boldsymbol{k},\sigma}(\boldsymbol{r}) = \sum_{\boldsymbol{G}}^{<K_{\max}} C_{\boldsymbol{k+G},\sigma}|\phi_{\boldsymbol{k+G},\sigma}\rangle$$

Basis

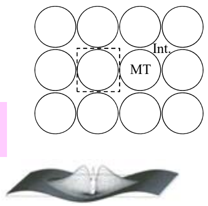
⇨

Eigenvalue problem

$$\hat{H}_{\mathrm{KS}}|\psi_{\boldsymbol{k},\sigma}\rangle = \varepsilon_b|\psi_{\boldsymbol{k},\sigma}\rangle$$

Example: Linearized Augmented Plane Wave basis

$$\phi_{\boldsymbol{k+G},\sigma}(\boldsymbol{r}) = \begin{cases} \text{Interstitial} \\ e^{i(\boldsymbol{k+G})\cdot\vec{r}} \\ \text{MT sphere} \\ \sum_{l=0}^{l_{max}}\left[A_{l,\sigma}(\boldsymbol{k}+\boldsymbol{G})u_{l,\sigma}(r) + B_{l,\sigma}(\boldsymbol{k}+\boldsymbol{G})\dot{u}_{l,\sigma}(r)\right]iY_l(\hat{\boldsymbol{r}}) \\ \left[-\frac{\partial}{\partial r^2} + \frac{l(l+1)}{r^2} + v_{l=0,\sigma}(r) - E_{l,\sigma}\right]ru_{l,\sigma}(r) = 0 \end{cases}$$



E. Wimmer *et.al.*, PRB 24, 864, (1981); PRB 26, 4571 (1982)

Basic: SOC and Second variational method

Spin-orbit coupling

$$\hat{H}_{SOC} = \frac{1}{4c^2}\frac{1}{r}\frac{dV_{l=0}^{\sigma}}{dr}\hat{l}\cdot\hat{\sigma} = \xi(r)\begin{pmatrix}\hat{l}_z & \hat{l}_- \\ \hat{l}_+ & -\hat{l}\end{pmatrix}$$

$\hat{l}$: Angular momentum operator

$\hat{\sigma}$: Dirac operator

① Redefine basis by the KS eigenfunctions

$$|\psi_b\rangle = C_{b,\uparrow}|\psi_{b,\uparrow}\rangle + C_{b,\downarrow}|\psi_{b,\downarrow}\rangle$$

② Generate SOC matrix

$$\hat{H} = \hat{H}_{\mathrm{KS}} + \hat{H}_{\mathrm{SOC}}$$

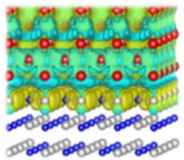
$$= \begin{pmatrix}\hat{H}_{KS}^{\uparrow} & 0 \\ 0 & \hat{H}_{KS}^{\downarrow}\end{pmatrix} + \xi(r)\begin{pmatrix}\hat{l}_z & \hat{l}_- \\ \hat{l}_+ & -\hat{l}\end{pmatrix}$$

③Eigenvalue problem

$$(\hat{H}_{\mathrm{KS}} + \hat{H}_{\mathrm{SOC}})|\psi_b\rangle = \varepsilon_b|\psi_b\rangle$$

Li et.al., PRB **42**, 5433 (1990).

Basic: Self-consistent field (SCF)



Input electron density

$n_{\mathrm{in}}(\mathbf{r})$

Kohn-Sham equation

$$\left[-\frac{\nabla^2}{2} + v_{\mathrm{H}}(n_{\mathrm{in}}(\mathbf{r})) + v_{\mathrm{XC}}(n_{\mathrm{in}}(\mathbf{r}))\right]\phi_{b,\boldsymbol{k}}(\mathbf{r}) = \varepsilon_b\, \phi_{b,\boldsymbol{k}}(\mathbf{r})$$

$$\sum_{\boldsymbol{k}}^{BZ} \sum_{b=1}^{N(\le E_F)} \left|\phi_{b,\boldsymbol{k}}\right|^2 \rightarrow n_{\mathrm{out}}(\boldsymbol{r})$$

Output electron density

SCF: Input and output electron densities should be identical.

Basic: Total energy

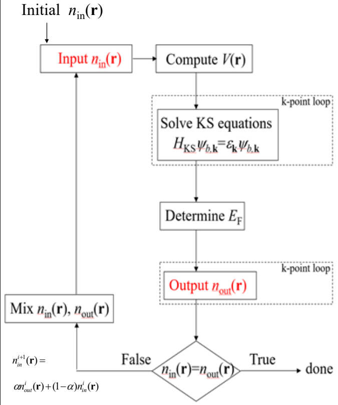
$$E_{\mathrm{Total}} = \sum_{i=1}^{N(\le E_F)} \varepsilon_b$$ Kohn-Sham eigenvalues

$$-\frac{1}{2}\left[\int v_H(\mathbf{r}) n(\mathbf{r})\, d\mathbf{r} + \sum_{\sigma}\int\{v_{XC,\sigma}(\mathbf{r}) - \varepsilon_{XC,\sigma}(\mathbf{r})\} n_\sigma(\mathbf{r}) d\mathbf{r}\right]$$

$$-\frac{1}{2}\sum_{\mu} Z_\mu V_{C,\mu}(\mathbf{R}_\mu)$$ Double counting term

Coding: Program

Flowchart



kohji@red27:~/CLASS/SCF

```
      subroutine sub_flapw

      write(ofh,'(/,1x,a)') 'Self-consistent field iteration ...'

      self_loop: do it=1,itmax
        write(ofh,'(/,1x,a,i5)') 'iteration=',it

!       load charge density
        call wrtdop('load')

!       check neutrity and generate potential
        call fix_charge
        call gen_potential

!       generate H and S matrixes and eigen-problem
        k_loop: do k=1,nkpt
          call gen_hsmatrix
          call get_eigen
        end do k_loop

!       get fermi energy
        call get_fermi

!       generate charge density
        k_loop: do k=1,nkpt
          call gen_charge
        end do k_loop

!       get charge distance and check
        call get_distance(distance)
        if(distance.lt.converged) exit slf_loop

!       mixing charge density and save
        call mix_charge(distance)
        call wrtdop('save')

      end do self_loop

!     calculation of totale energy
      call get_tote

!     calculation of band structure and dos
      call get_band
      call get_dos

      write(ofh,'(/,1x,a)') '... completed'

      return
      end
```

Coding: Execution

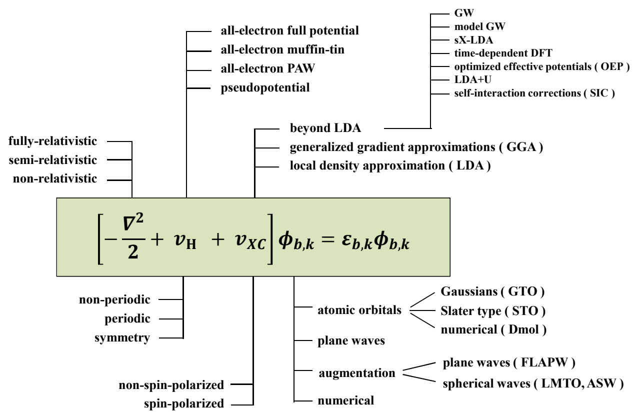
Charge distance :

$$\Delta = \frac{1}{\Omega}\int_{\mathrm{cell}} \sqrt{\left(n_{\mathrm{out}}(\boldsymbol{r}) - n_{\mathrm{in}}(\boldsymbol{r})\right)^2}\, d\boldsymbol{r}$$

kohji@red27:~/FLAPW/current/work

```
[kohji@red27 work]$ FLchk
** Total energy
   total energy for it=    9:              -75.9859905662 htr
*** Charge distance
 distance of charge densities for it=    1:      15.418023 me/bohr**3
 distance of charge densities for it=    2:      12.714097 me/bohr**3
 distance of charge densities for it=    3:      10.269848 me/bohr**3
 distance of charge densities for it=    4:       2.465512 me/bohr**3
 distance of charge densities for it=    5:       1.862776 me/bohr**3
 distance of charge densities for it=    6:       0.363891 me/bohr**3
 distance of charge densities for it=    7:       0.086428 me/bohr**3
 distance of charge densities for it=    8:       0.079364 me/bohr**3
 distance of charge densities for it=    9:       0.025358 me/bohr**3
***
 FLAPW calculations were done
```

Coding: Implementation

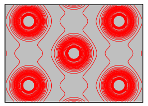


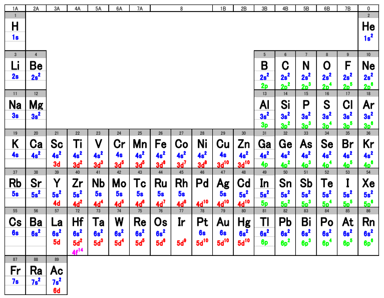
- ➢ Introduction
- ➢ Calculation method
- ➢ Electronic structures and magnetism

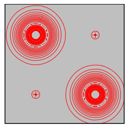
  in bulk and at surfaces/thin films
- ➢ Control of magnetism

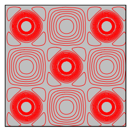
  by tuning atomic-layer alignments and by external electric field

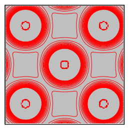
Demo: Electron density

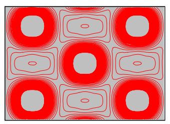

bcc Na: (110)

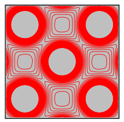


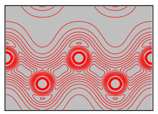

NaCl: (100)


fcc Al: (100)


fcc Ar: (100)


bcc V: (110)


fcc Cu: (100)


Diamond C: (110)

Demo: Band structure of non-magnetic system

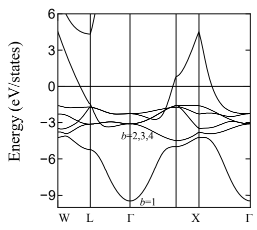
fcc Cu (non spin-polarized system)

Kohn-Sham equation

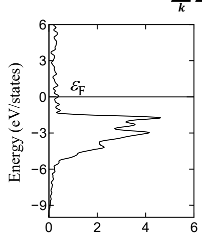
$$-\frac{\nabla^2}{2} + v_{\mathrm{H}} + v_{\mathrm{xc}}\,|\phi_{b,\boldsymbol{k}}\rangle = \varepsilon_{b,\boldsymbol{k}}|\phi_{b,\boldsymbol{k}}\rangle$$

Wave function of system

$$|\psi\rangle = \sum_{\boldsymbol{k}}\sum_{b} C_{b,\boldsymbol{k}}|\phi_{b,\boldsymbol{k}}\rangle$$



k in Bloch function



Density of states, $D(\varepsilon)$

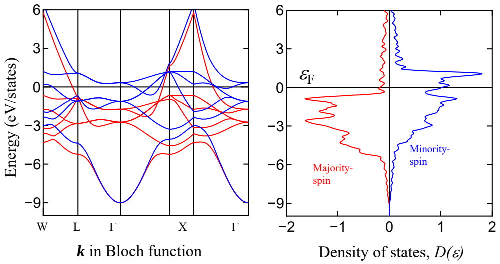
Demo: Band structure of ferromagnetic system

Kohn-Sham equation

fcc Co (spin-polarized system)

$$-\frac{\nabla^2}{2}+v_{\mathrm{H}}+v_{\mathrm{xc},\uparrow}|\phi_{b,\boldsymbol{k},\uparrow}\rangle=\varepsilon_{b,\boldsymbol{k},\uparrow}|\phi_{b,\boldsymbol{k},\uparrow}\rangle$$ spin-up state

$$-\frac{\nabla^2}{2}+v_{\mathrm{H}}+v_{\mathrm{xc},\downarrow}|\phi_{b,\boldsymbol{k},\uparrow}\rangle=\varepsilon_{b,\boldsymbol{k},\downarrow}|\phi_{b,\boldsymbol{k},\uparrow}\rangle$$ spin-down state



Magnetic moment

$$m=\int_{-\infty}^{\varepsilon_F}\boldsymbol{D}_{\uparrow}(\boldsymbol{\varepsilon})d\varepsilon-\int_{-\infty}^{\varepsilon_F}\boldsymbol{D}_{\downarrow}(\boldsymbol{\varepsilon})d\varepsilon$$

Demo: Band structure of antiferromagnetic system

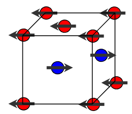
fcc Mn (spin-polarized system)

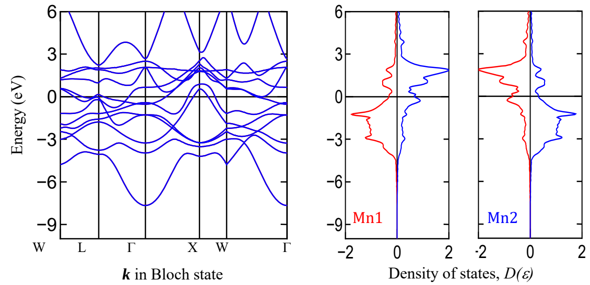
Kohn-Sham equation

$$-\frac{\nabla^2}{2}+v_{\mathrm{H}}+v_{\mathrm{xc},\uparrow}|\phi_{b,\boldsymbol{k},\uparrow}\rangle=\varepsilon_{b,\boldsymbol{k},\uparrow}|\phi_{b,\boldsymbol{k},\uparrow}\rangle$$

$$-\frac{\nabla^2}{2}+v_{\mathrm{H}}+v_{\mathrm{xc},\downarrow}|\phi_{b,\boldsymbol{k},\uparrow}\rangle=\varepsilon_{b,\boldsymbol{k},\downarrow}|\phi_{b,\boldsymbol{k},\uparrow}\rangle$$

AFM



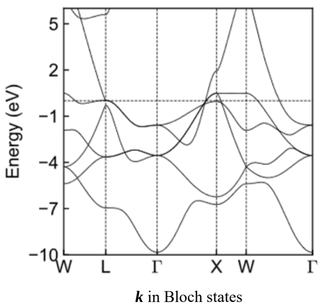


Demo: Band structure of Pt with SOC

Pt (non spin-polarized system)

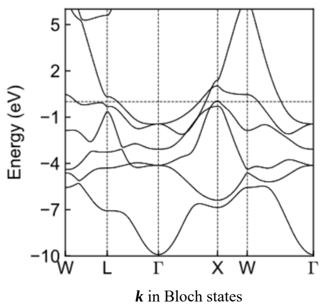
Without SOC

$$\hat{H}_{\mathrm{KS}}|\phi_{b,\boldsymbol{k}}\rangle=\varepsilon_{b,\boldsymbol{k}}|\phi_{b,\boldsymbol{k}}\rangle$$



With SOC

$$(\hat{H}_{\mathrm{KS}}+\hat{H}_{\mathrm{SOC}})|\psi_{b,\boldsymbol{k}}\rangle=\varepsilon_{b,\boldsymbol{k}}|\psi_{b,\boldsymbol{k}}\rangle$$



Spin-orbit coupling-induced properties

Fundamental properties
- ☐ Magnetic spin/orbital and dipole moments
- ☐ Exchange interaction
- ☐ Magnetocrystalline anisotropy (MCA)
- ☐ Dzyaloshinskii-Moriya interaction (DMI)

Conductivity
- ☐ Anomalous hall conductivity
- ☐ Spin/orbital Hall conductivity
- ☐ Magneto-optical conductivity

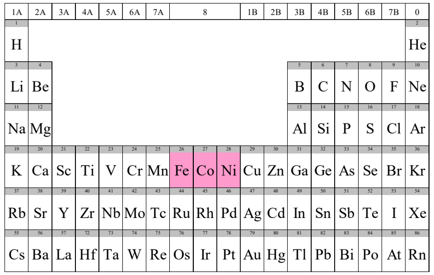
External field
- ☐ Magnetic field
- ☐ Electric field

Dynamics
- ☐ Magnetic damping constant
- ☐ Spin-orbit torque

Spin textures
- ☐ Non-collinear magnetic structures

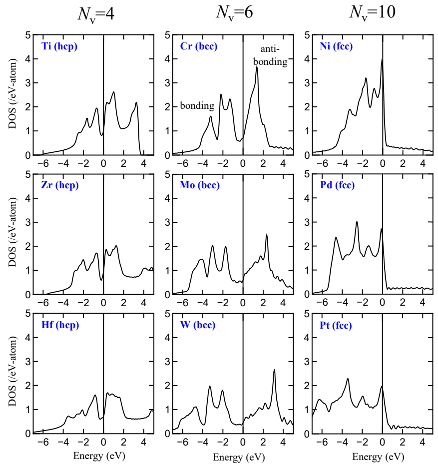
Magnetism

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



	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



Trends in band structures in transition metals

1) Bandwidth

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

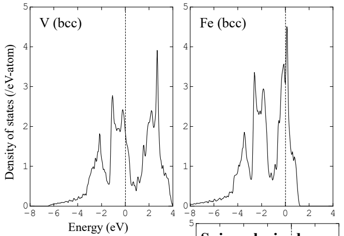
2) Density of states at E_F

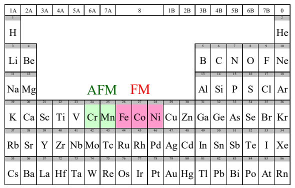
$D^{3d}(E_F) > D^{4d}(E_F) > D^{5d}(E_F)$

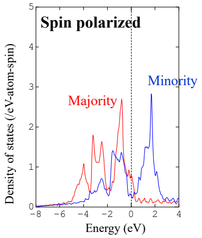
J. Kübler, Theory of itinerant electron magnetism (Oxford University Press, Oxford, 2000)

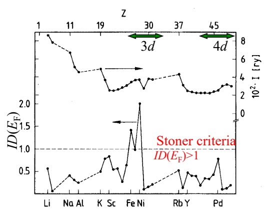
Magnetism in transition metals

Non-spin polarized







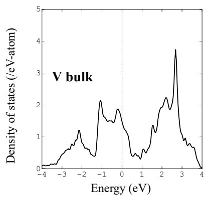


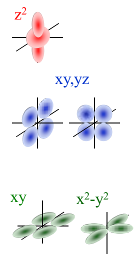
LDA results

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

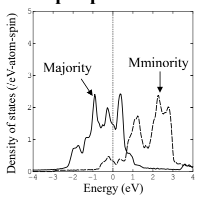
Band structures and spin polarization in transition-metal layers

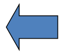
LDA results

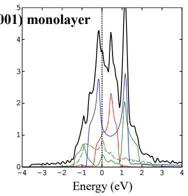


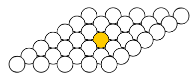


Spin-polarized



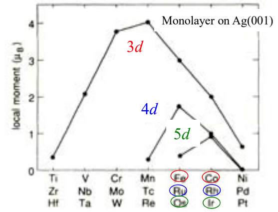




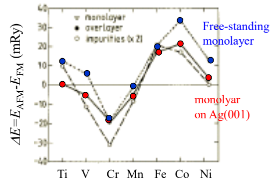


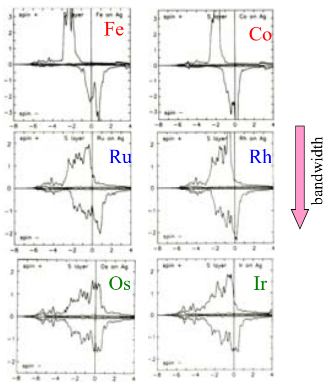
Ferromagnetism in transition-metal layers

Magnetic moment (assumed FM)



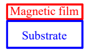
Energy difference between FM and AFM



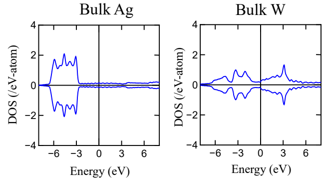


S. Blügel, Phys. Rev. Lett. 68, 851(1992)

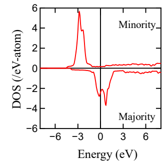
Effect of substrates to magnetism



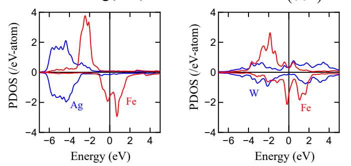
Substrate



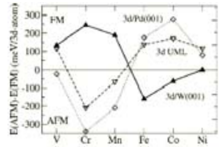
Fe(001) monolayer



Fe/Substrate



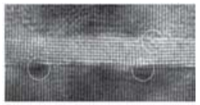
Stability of magnetic structures



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

Magnetocrystalline anisotropy (MCA)

MTJ device



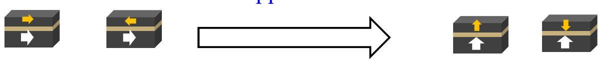
[1]
Ferromagnetic
Insulator
Ferromagnetic

✓Non-volatility
✓Large capacity
✓High-speed

Many Applications
- MRAM
- Magnetic sensor

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

In-plane MCA → Advanced applications → Out-of-plane MCA



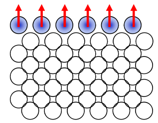
How to design thin films with large PMCA

Magnetocrystalline anisotropy

Spin-orbit coupling

$$H_{SOC} = \xi(r)\, l \cdot \sigma$$

SOC strength, ζ~50 meV for 3d-metals



Magnetocrystalline anisotropy energy

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

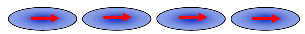
~0.1 meV/atom

Force theorem

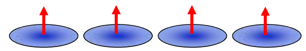
$$\approx \{E[\rho_0, \mathbf{m}_0(\rightarrow)] - E[\rho_0, \mathbf{m}_0(\uparrow)]\}$$

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

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

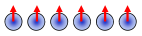


$E_{MCA} > 0$: Perpendicular MCA



MCA energy in 3d transition metal monolayers

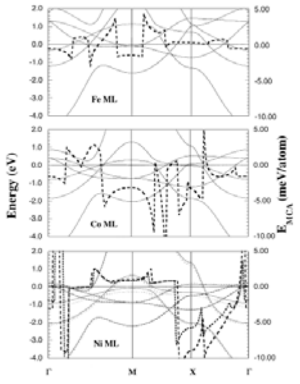
Perpendicular MCA



	System	Method	E_{MCA} (meV)
★	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

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

Perpendicular MCA

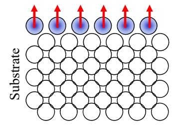


Table 2
Calculated MCA energies for selected transition magnetic thin films

	System	Method	E_{MCA} (meV)
	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)

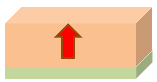
Perpendicular MCA at Fe/MgO(001) interface: Theory

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

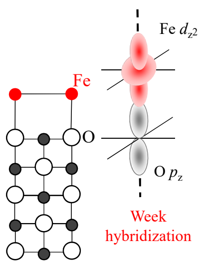
	E_{MCA} (meV/a^2)
Free-standing Fe monolayer	0.19
Fe/MgO	1.28
$Au_3/Fe_3/MgO$	0.94

LDA

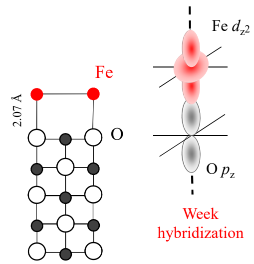
Nakamura et.al., PRB 81, 220409, (2010)



Origin of interfacial PMA

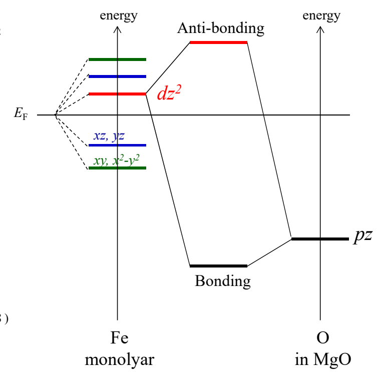


Fe d_{z2} – O p_z hybridization at Fe/MgO interface



Fe/MgO interface

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)

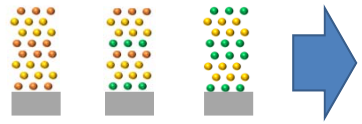


Shimabukuro, Physica E , **42**, 1014 (2010).
Nakamura et.al., PRB 81, 220409, (2010)

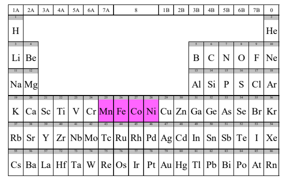
- Introduction
- Calculation method
- Electronic structures and magnetism
  in bulk and at surfaces/thin films
- Control of magnetism
  by tuning atomic-layer alignments and by external electric field

Control of MCA by tuning atomic-layer alignments

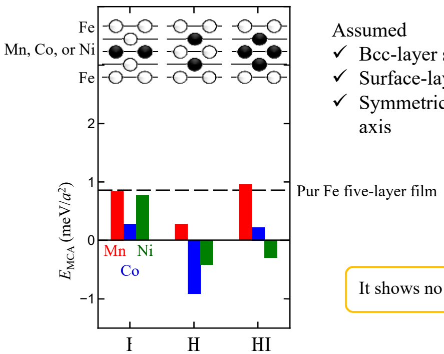
Interfaces, superlattices, multilayers



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



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

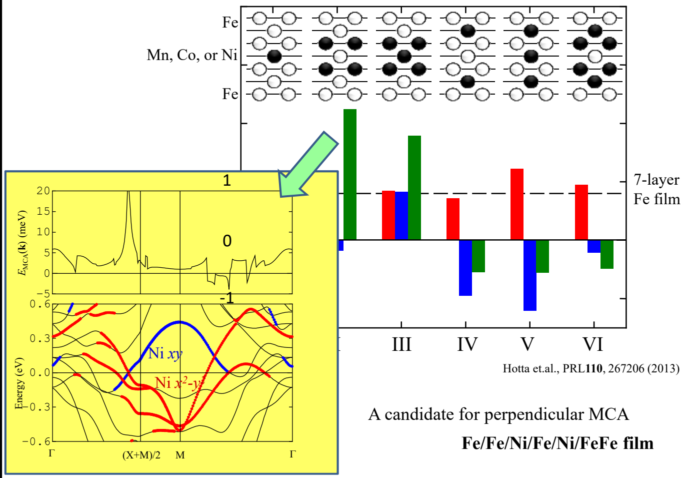


Hotta et.al., PRL **110**, 267206 (2013)

Assumed
- ✓ Bcc-layer stacking
- ✓ Surface-layer to be Fe
- ✓ Symmetric atomic alignment along z-axis

It shows no perpendicular MCA

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



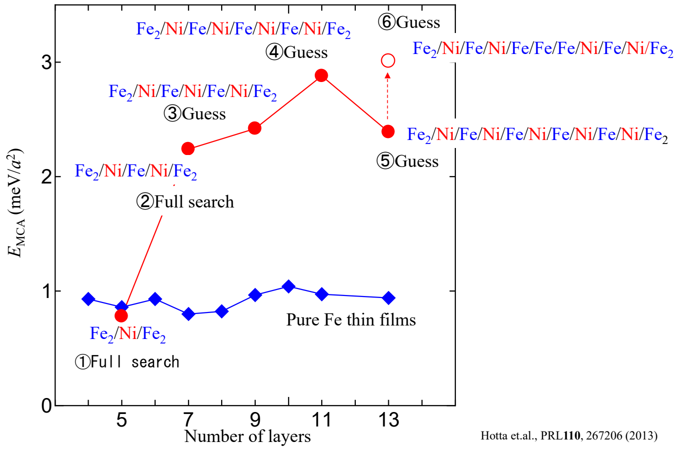
Hotta et.al., PRL **110**, 267206 (2013)

A candidate for perpendicular MCA

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

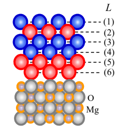
Search for 3*d* thin films with giant perpendicular MCA

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

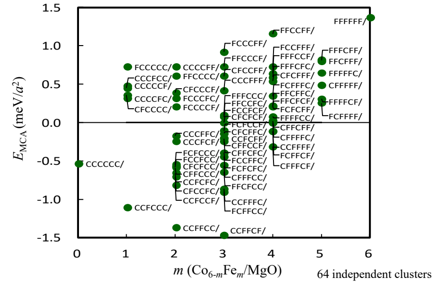


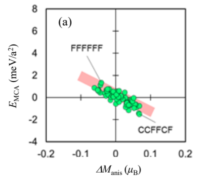
Hotta et.al., PRL**110**, 267206 (2013)

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

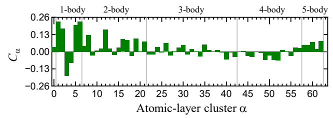


PMCA is enhanced Fe double-layer stacking





$$E_{MCA}(\vec{\sigma}_n) = \sum_{\alpha=0}^{2^N-1} C_\alpha \xi_\alpha(\vec{\sigma}_n)$$

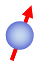


64 independent clusters

α		α		α		α	
0		16	(34)	32	(234)	48	(1345)
1	(1)	17	(35)	33	(235)	49	(1346)
2	(2)	18	(36)	34	(236)	50	(1356)
3	(3)	19	(45)	35	(245)	51	(1456)
4	(4)	20	(46)	36	(246)	52	(2345)
5	(5)	21	(56)	37	(256)	53	(2346)
6	(6)	22	(123)	38	(345)	54	(2356)
7	(12)	23	(124)	39	(346)	55	(2456)
8	(13)	24	(125)	40	(356)	56	(3456)
9	(14)	25	(126)	41	(456)	57	(12345)
10	(15)	26	(134)	42	(1234)	58	(12346)
11	(16)	27	(135)	43	(1235)	59	(12356)
12	(23)	28	(136)	44	(1236)	60	(12456)
13	(24)	29	(145)	45	(1245)	61	(13456)
14	(25)	30	(146)	46	(1246)	62	(23456)
15	(26)	31	(156)	47	(1256)	63	(123456)

Nakamura, et.al., J.Magn. Magn. Mater. 537, 168175 (2021)
Nawa, et.al., Comput. Mater. Sci. 219, 112032 (2023)

E-field (Voltage)-control of magnetism



Electrons

Electric field → Charge

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

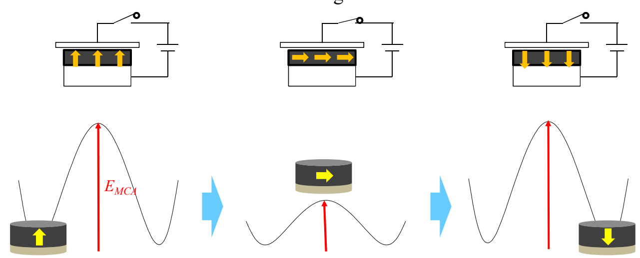
leading to semiconductor technology

Magnetic field /Currents → Magnetization or spins

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

Example: voltage-assist magnetization switching

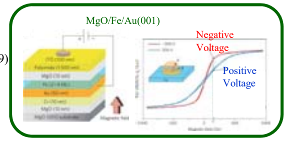
Voltage-assist



Control of magnetism of metal thin films by electric field

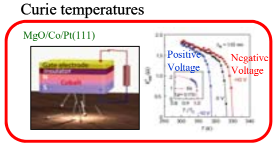
- Magnetocrystalline anisotropy (MCA)
  Weisheit et.al., Science 315, 349 (2007)
  Maruyama et.al., Nature Nanotech. 4, 349 (2009)
  Duan et.al., PRL **101**, 137201 (2008)
  Nakamura et.al., PRL **102**, 187201 (2009); PRB **80**, 172402 (2009)
  Tsujikawa et.al., PRL **102**, (2009)
  ….
- Curie temperature (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)

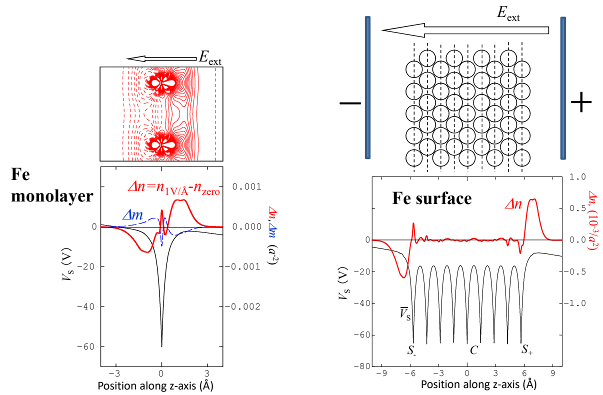
Curie temperatures



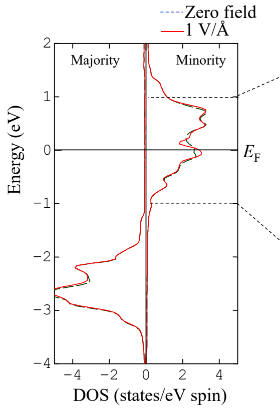
Chiba et.al., Nat. Mater. 10, 853-856 (2011)

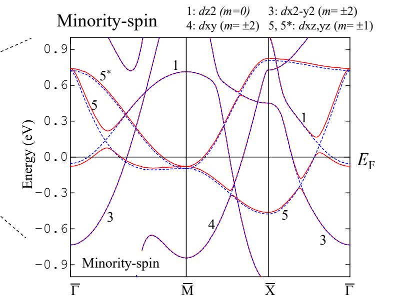
Electric-field-induced charges at surfaces/interfaces

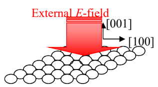
- ***Redistribution in charge/spin densities at surfaces/interfaces by E-field.***
  Duan et.al., PRL **101**, 137201 (2008),
  Nakamura et.al., PRL **102**, 187201 (2009); PRB **80**, 172402 (2009),
  Tsujikawa et.al., PRL **102**, (2009).



Modification of band structure of Fe monolayer by electric field





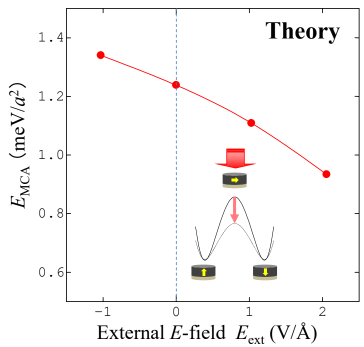


Change in band structure around Fermi level

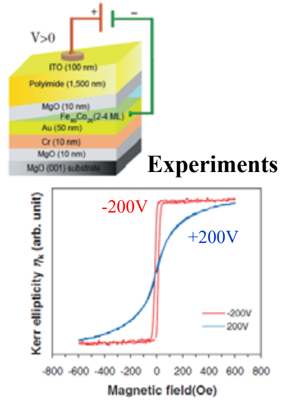
MCA energy modification

Modification of MCA energy at Fe/MgO(001)

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



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

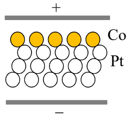


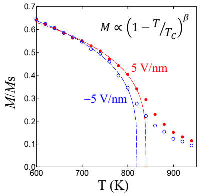
Shito et.al., Appl. Phys. Express **2**, 063001 (2009)

Modification of Curie temperature of Co/Pt(111)

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

Co/Pt(111)





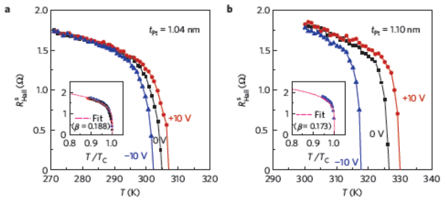
	Theory	Experiments
T_C	~830	~320
ΔT_C	~20K	~10K
β	~0.26	~0.18

Agreed with experiments qualitatively

MgO/Co/Pt(111)

±0.2V/nm

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



Summary

Spintronic · Design · Magnetic control

Outline

- Introduction
- Calculation method
- Electronic structures and magnetism
  in bulk and at surfaces/thin films
- Control of magnetism
  by atomic-layer alignments and external electric field