2011/10/14-15, PF研究会
「磁性薄膜を究める：キャラクタリゼーションから新奇材料の創製へ」

表面修飾によるFe_3O_4最表面ハーフメタル性回復現象

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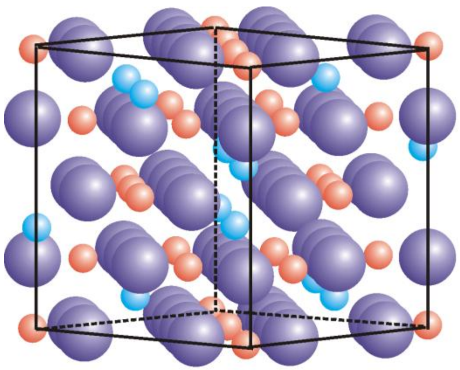
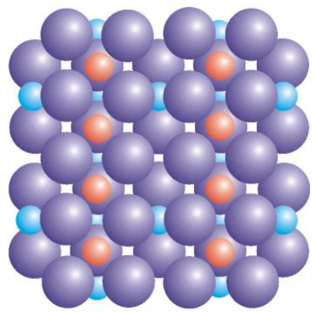
Bulk Fe_3O_4

1. 物性、結晶構造

- Tc=858 K、逆スピネル構造



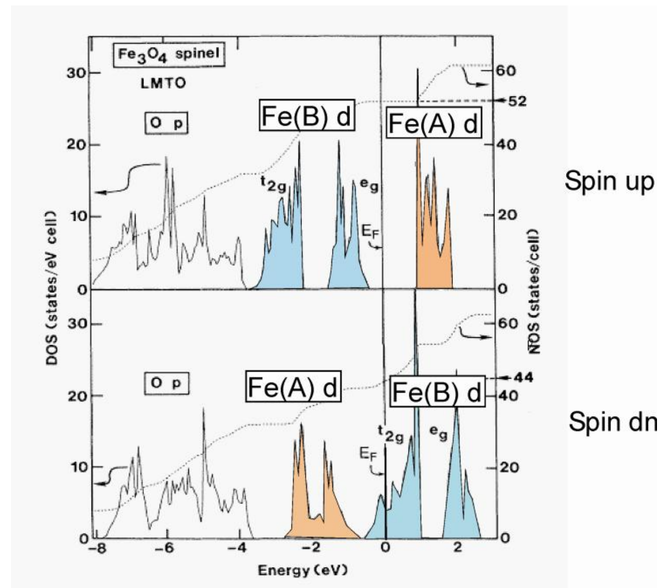
Bulk



Ideal (100) surface

O　　Fe-A site (Fe^{3+})　　Fe-B site (Fe^{2+}, Fe^{3+})

2.　電子状態計算



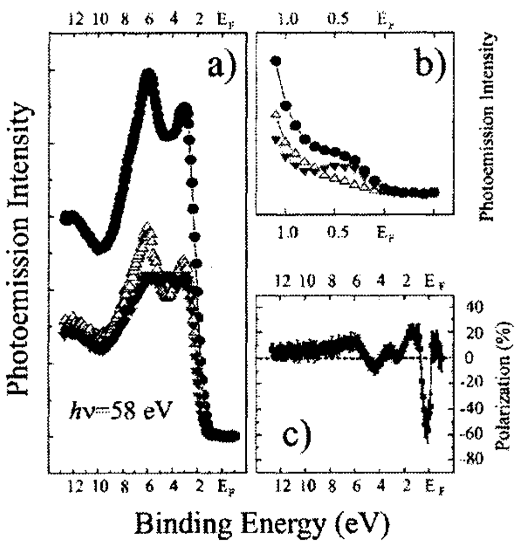
Z. Zhang and S. Satpathy, PRB 44, 13319 (1991)

Spin up -- band gap
Spin down --- metallic
→ $P(E_F)$= -100%

Fe_3O_4表面,界面スピン偏極

1. SPPES

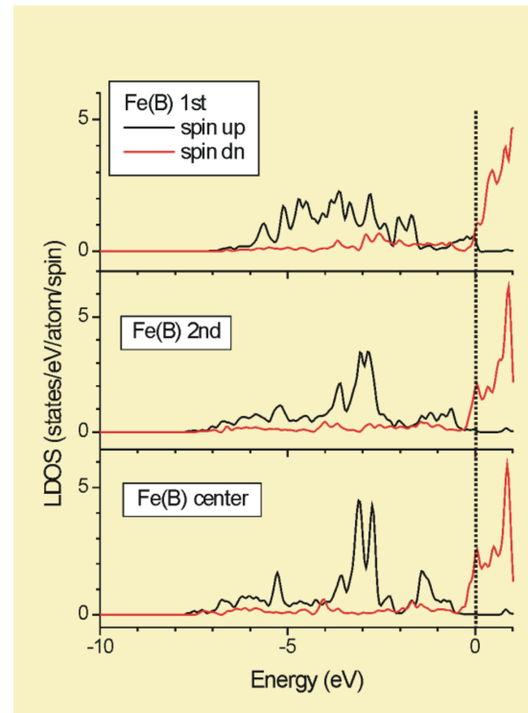
・(100) : $P(E_F)$= -40～-60%
・(111) : ～ -80 %



SPPES
--- probing depth
→ $P(E_F)$ at topmost surface?

[M. Fonin et al.,
Phys. Rev. B 72, 104436(2005)]

表面電子状態計算
(Fe_3O_4(100)理想表面)



low
～-80%
-100%

2. 伝導測定

・TMR --- -26 % (RT)

[T. Kado, APL, 92, 092502 (2008)]

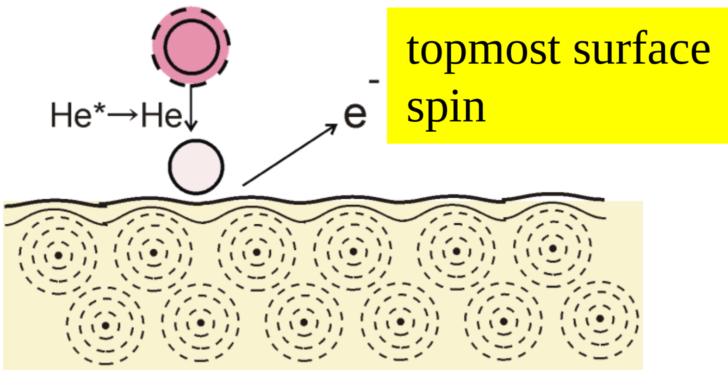
本研究の内容

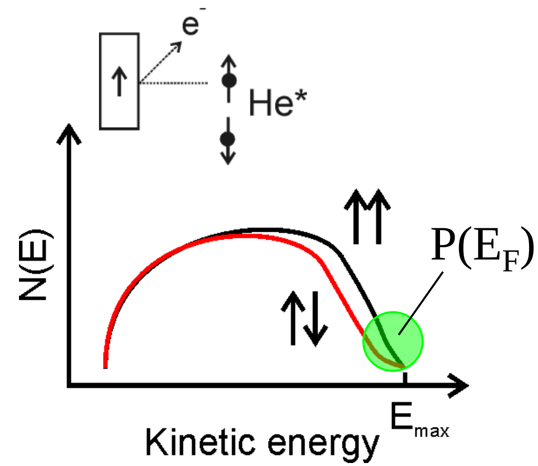
1. スピン偏極Heビーム法
   → Fe_3O_4(100)最表面E_Fスピン偏極
   (5%以下)

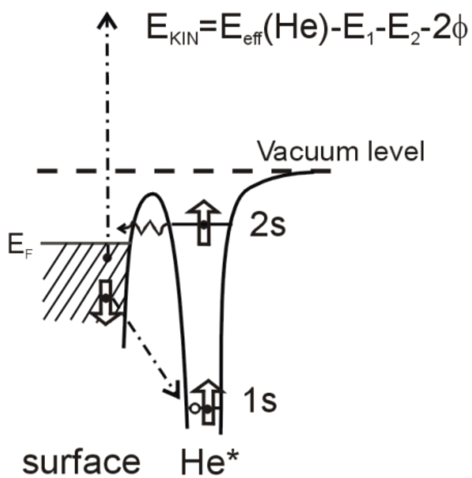
2. 表面の水素終端
   → $P(E_F)$が著しく増大　（室温で-50%以上）
   ハーフメタル性回復　(計算)

スピン偏極He*ビームによる表面計測

He* (1s)↑(2s)↑ (M_S=+1)







$$N_{\uparrow}(E_{\max}-E)=\int_0^E D_{\downarrow}(E')D_{tot}(E-E')dE'$$

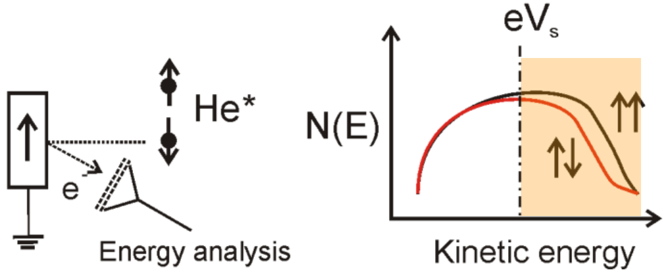
$$N_{\uparrow}(E_{\max})\propto D_{\downarrow}(E_F)$$

$$A=\frac{N_{\uparrow}-N_{\downarrow}}{N_{\uparrow}+N_{\downarrow}}$$

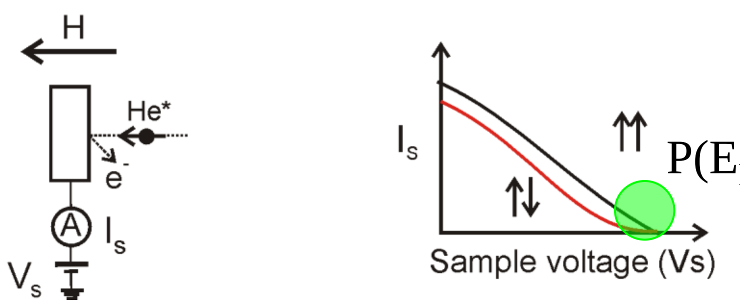
$$\rightarrow A(E_{\max})\cong -P(E_F)$$

強磁場下表面スピン偏極計測

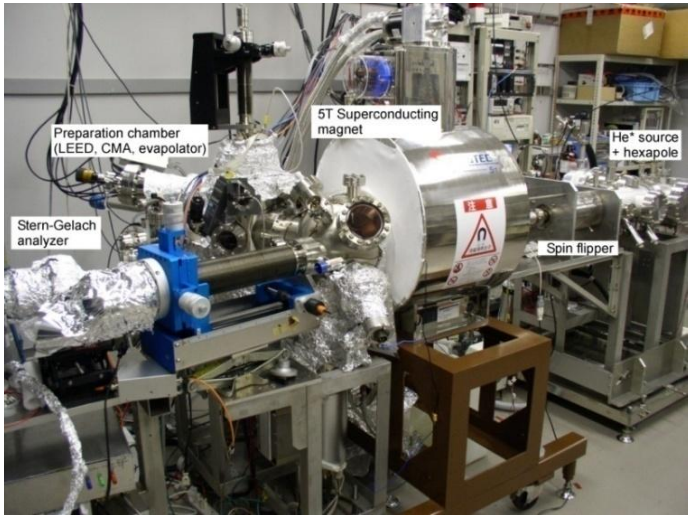
1, SPMDS

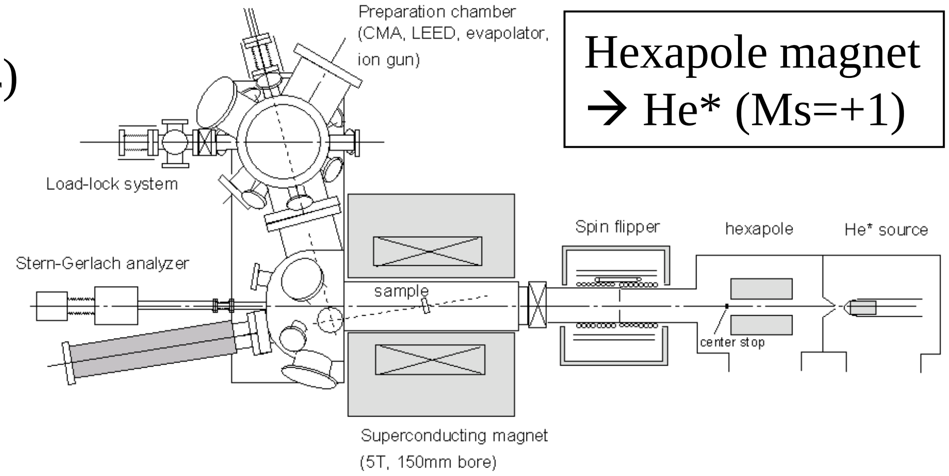


2, sample current (H—allowed)



$$I(V_S) = \int_{eV_s}^{\infty} N(E)dE$$





Hexapole magnet
→ He* (Ms=+1)

M. Kurahashi et al. RSI 79, 073902(2008), APL93 (2008) 132505.

Sample

・Fe_3O_4(100) surface

1, **epitaxial film** (20 nm)

・Fe deposition (0.1nm/min) at $P(O_2)=3x10^{-6}$ Torr

・Ts=250-300℃

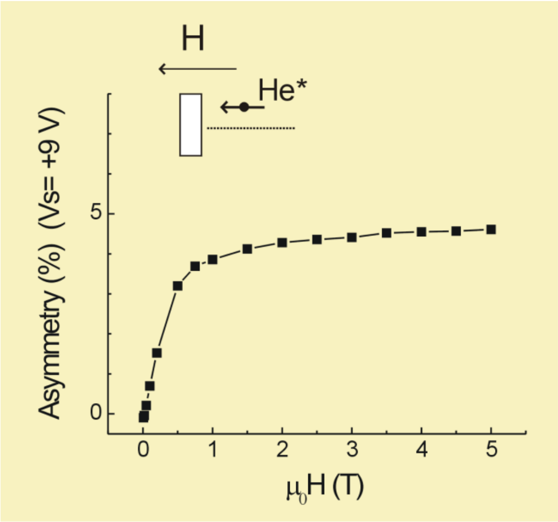
2, **natural single crystal**

・sputter+annealing (500℃)

・300℃ annealing at $P(O_2)$～10^{-6} Torr

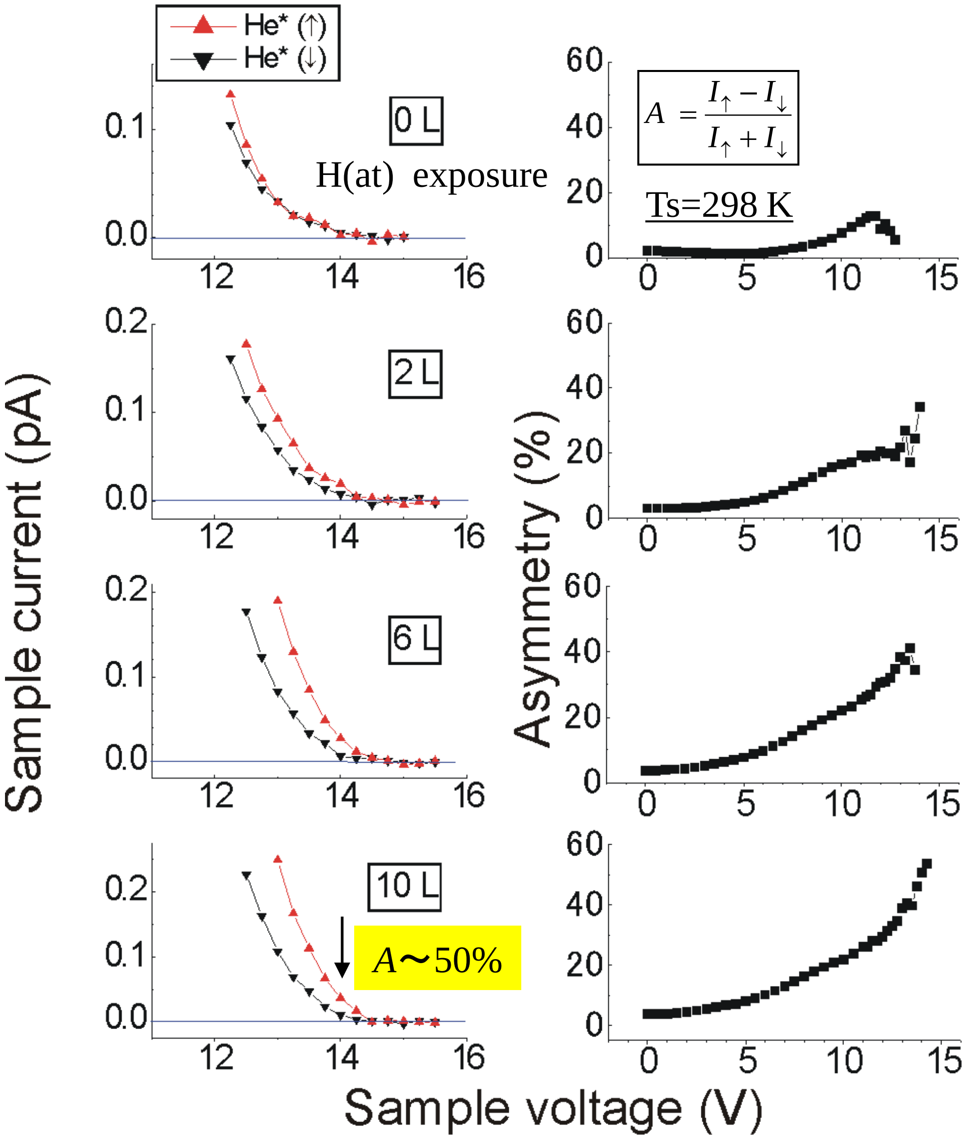
・Atomic H

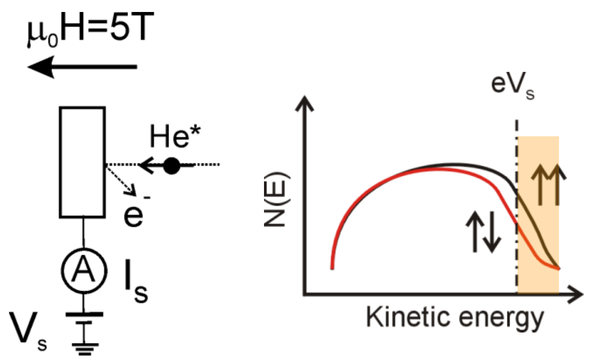
-- thermal dissociation of H_2



Fe_3O_4(100)薄膜の最表面磁化曲線 (磁場は面垂直方向)

$Fe_3O_4(100)/MgO(100)$+atomic H



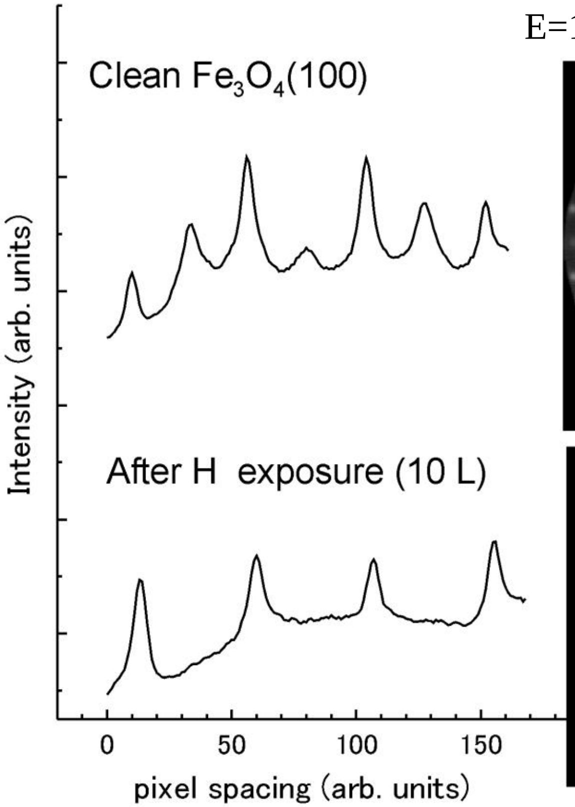


*Fe_3O_4(100) clean surface
--low P(E_F)

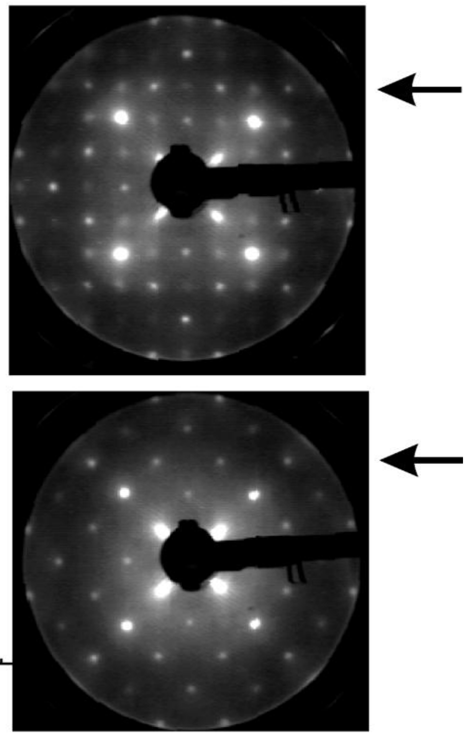
･H termination
→ strong increase in P(E_F)

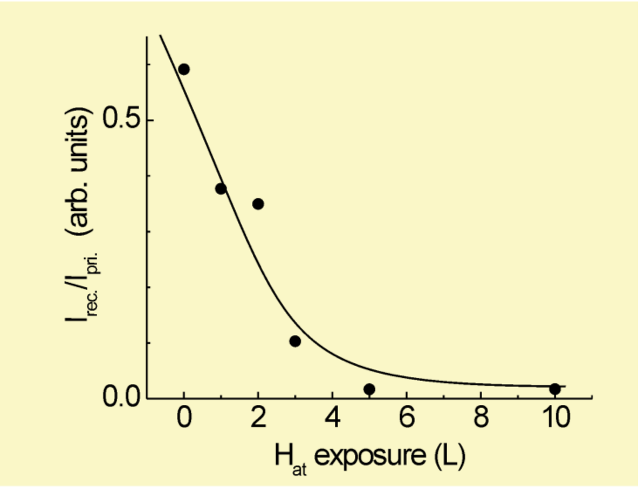
M. Kurahashi et al., Phys. Rev. B, **81**, 193402 (2010).

$Fe_3O_4(100)$ /MgO(100): LEED

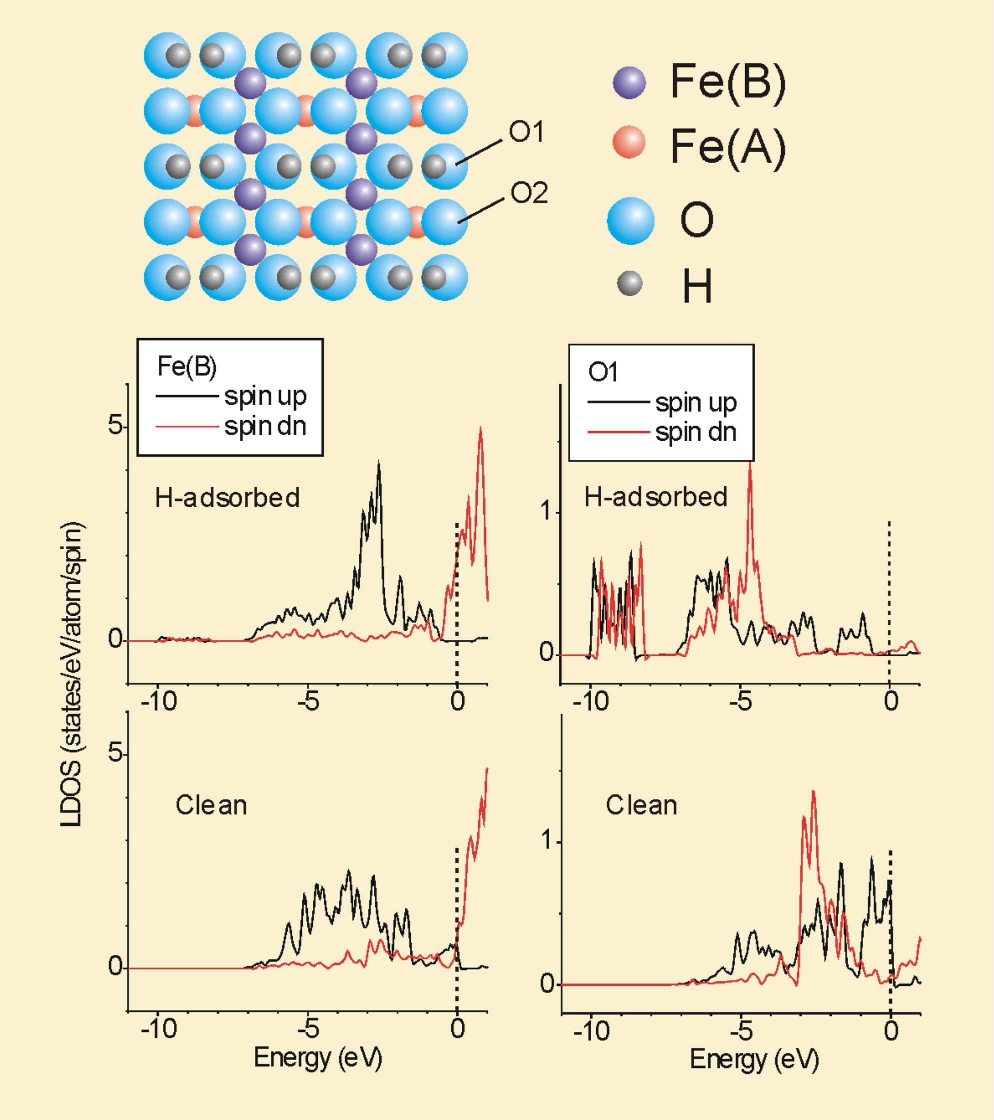


E=107eV





$Fe_3O_4(100)$ /H: DFT calculation



- ideal B-terminated $Fe_3O_4(100)$ surface + H (O1 site)
  (*only H position was optimized.)
- O2 site– unfavorable (ΔE_{ad}∼0.6 eV)

- H termination
  → half-metallic at surface Fe(B)
- OH bonding
  electron donation to $Fe_{\downarrow}$ band

まとめ、今後の課題

Fe_3O_4(100)最表面フェルミ面スピン偏極

- 清浄面----低。非対称率は5%以下。
- 表面の水素終端→ 最表面$P(E_F)$が著しく増大
  （298Kで-50%以上、 計算ではhalf-metallic。)
- 表面酸素結合状態の変化、水素からの電子供与
  → $P(E_F)$増大の要因

今後の課題

- 分子への高スピン偏極誘起
- 温度依存性、面方位依存性