# Enhanced Spin Hall Effect by Resonant Skew Scattering in the Orbital-Dependent Kondo Effect

Yosinori Senshu

7/22

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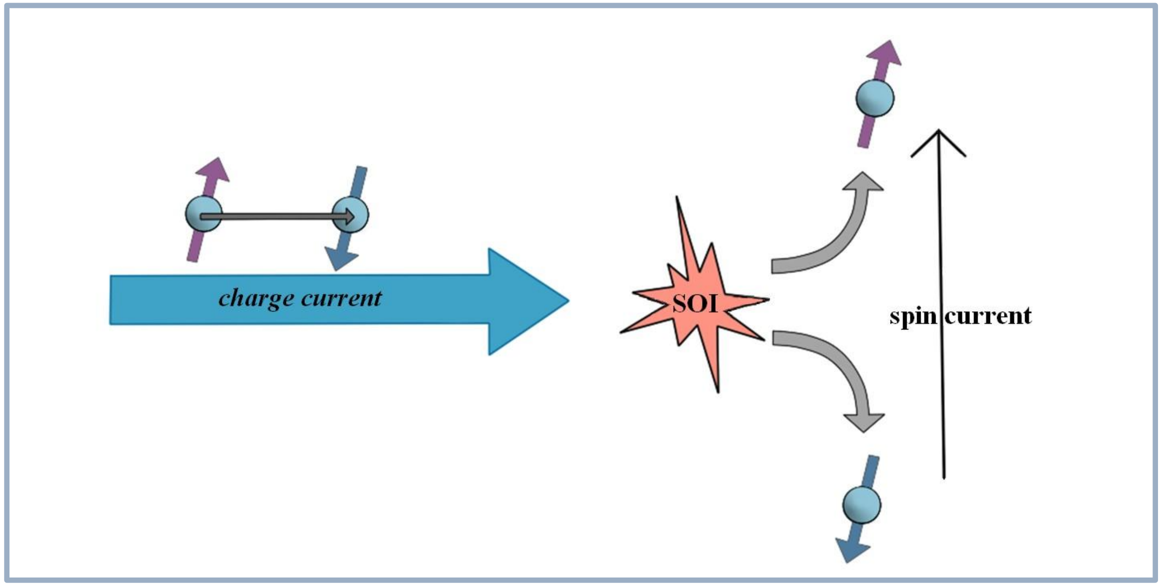
an effect where
the transverse spin current is
prodused by
the electric field or electric current

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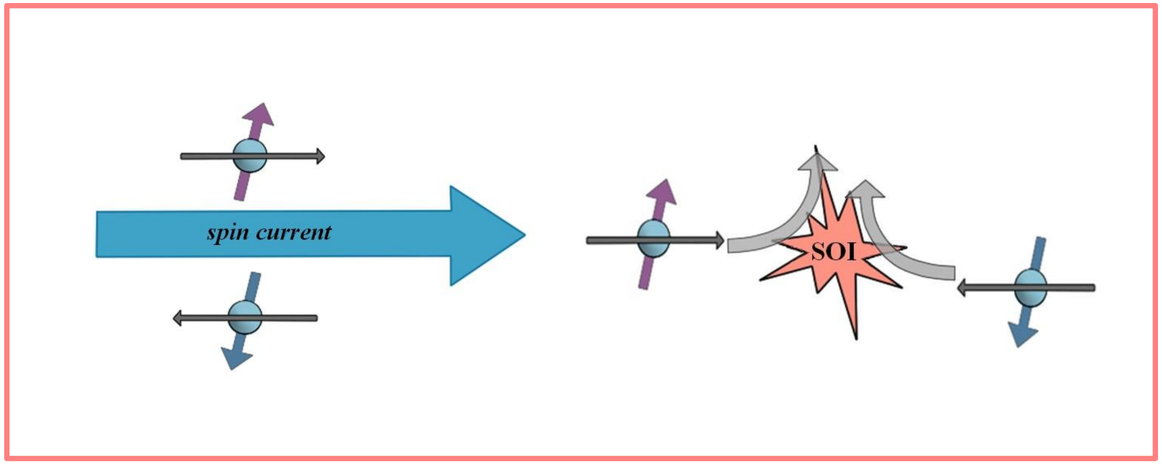

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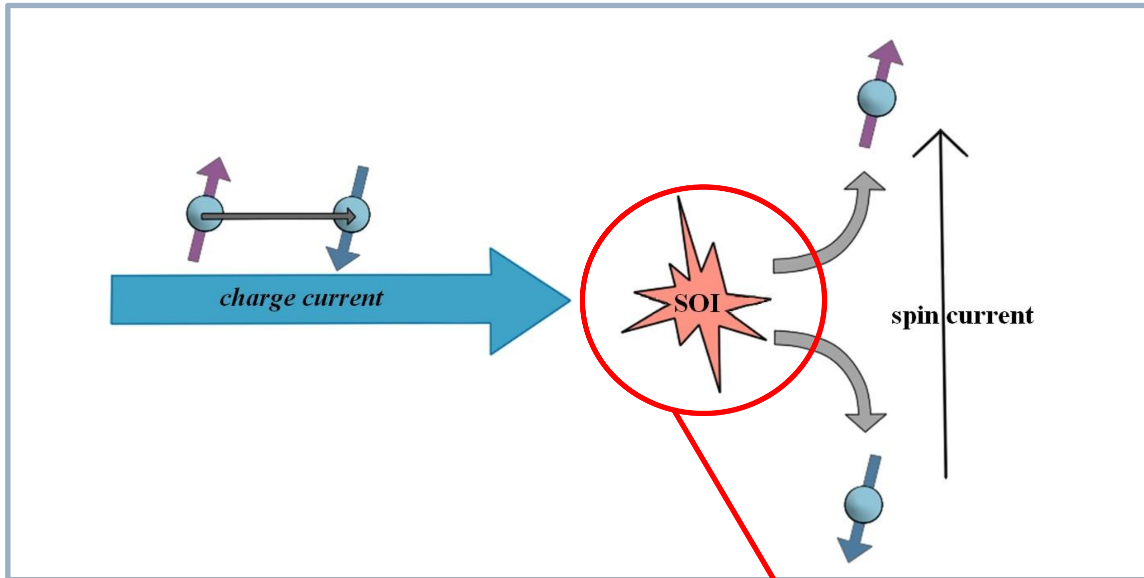


SOI plays an essential role

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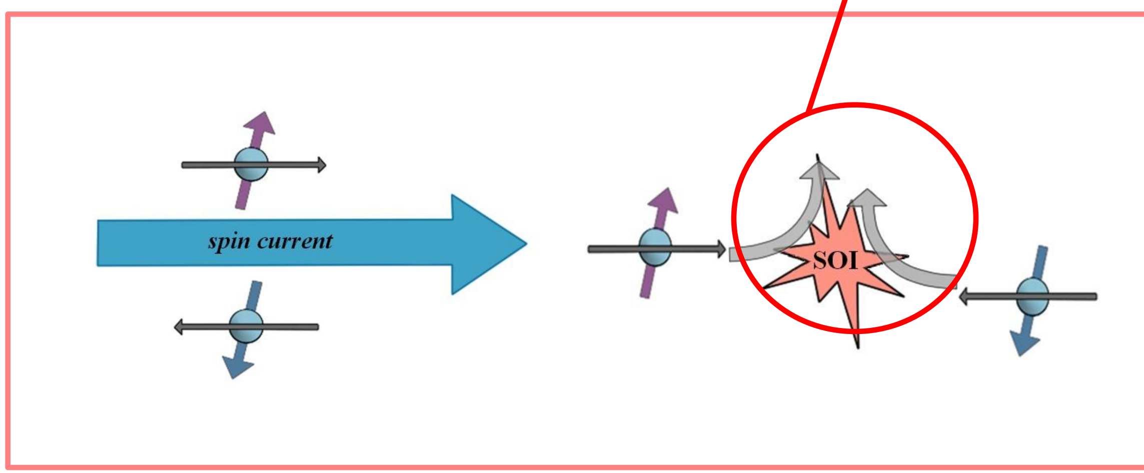
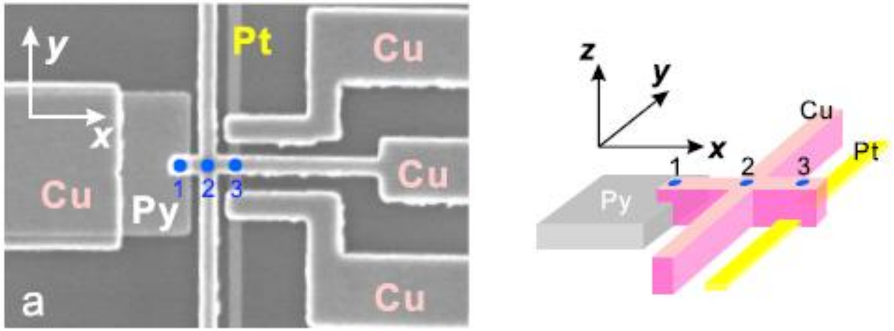


past experiment

Pt
observing large SHE due to the large SOI of Pt
($\gamma_S$ = 0.37)




(T. Kimura et al. PRL 98, 156610 (2007))

Au/FePt system
large SHE has been obserbed
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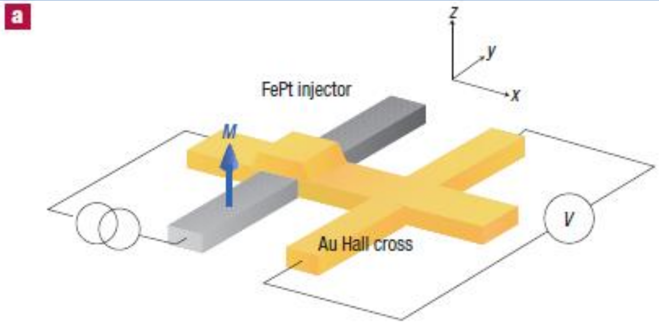


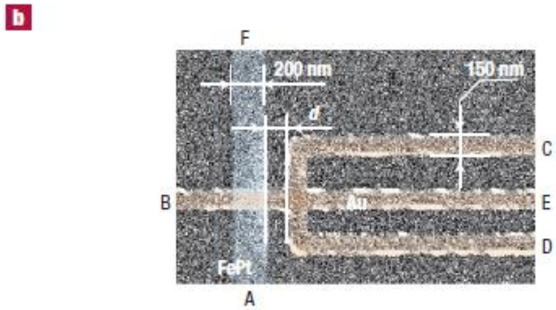


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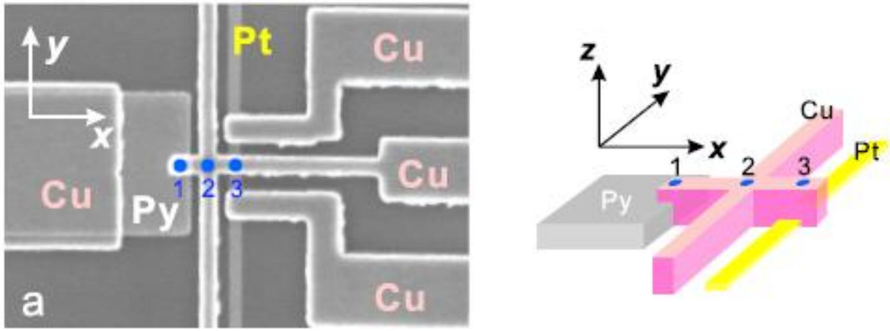


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Au/FePt system
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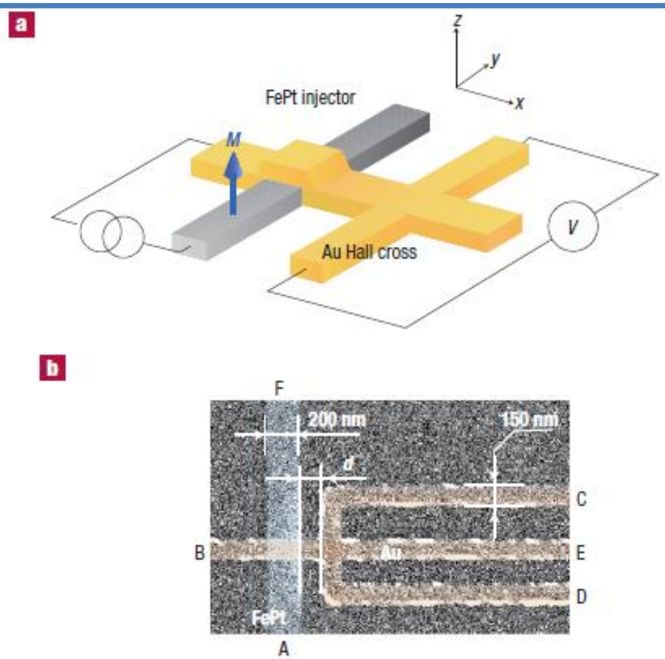
Actually
this value is surprisingly large value
with reratively small SOI of Au




(T. Seki et al. nature materials VOL7 FEBURARY 2008) expression of anomalous Hall angle due to skew scattering

$$\gamma \sim (\lambda/\Delta)\sin\delta_1$$

$\lambda$ : spin orbit interaction
$\Delta$ : hybridization energy
$\delta_1$ : phase shift of scattering

**(Guang-Yu Guo. et al. PRL 102, 036401 (2009))**

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experimental data or calcurated value

**(A. Fert, et al. PRL 28, 303 (1972))**

$$\gamma = 0.01 \sim 0.001$$

$\gamma_S \fallingdotseq 0.1$ is surplisingly large value expression of anomalous Hall angle due to skew scattering

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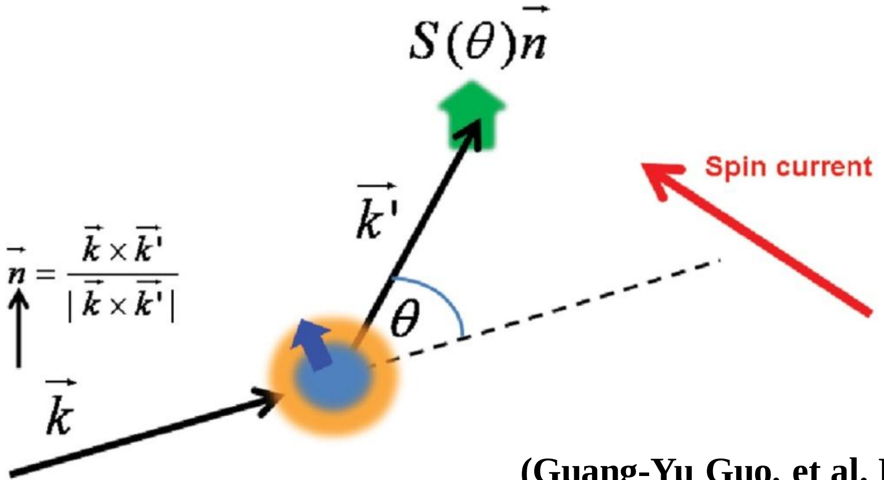
what is origin

## scattering

scattering by s = 1/2 particle due to SOI

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## scattering amplitude

$$f_{\uparrow}(\theta) = f_1(\theta)|\uparrow\rangle + ie^{i\varphi} f_2(\theta)|\downarrow\rangle,$$

$$f_{\downarrow}(\theta) = f_1(\theta)|\downarrow\rangle - ie^{-i\varphi} f_2(\theta)|\uparrow\rangle$$

$f_1$ : soin nonflip scattering amplitude

$f_2$ : soin flip scattering amplitude

$\theta$ : angle between incident and scattered waves scattering

scattering by s = 1/2 particle due to SOI

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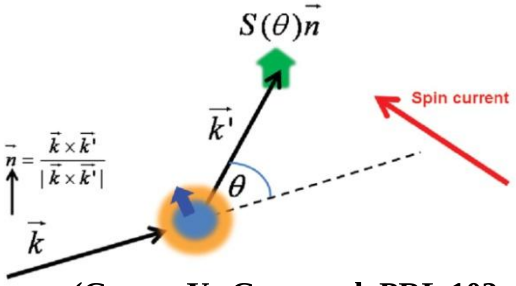


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$$S(\theta) = \frac{2\mathrm{Im}[f_1^*(\theta) f_2(\theta)]}{|f_1(\theta)|^2 + |f_2(\theta)|^2}$$ skewness

$$I(\theta) = |f_1(\theta)|^2 + f_2(\theta)|^2$$ scattering intensity

$$\gamma_S = \frac{\int d\Omega I(\theta) S(\theta) \sin\theta}{\int d\Omega I(\theta)(1-\cos\theta)}$$

← transverse spin current produced by scattering

← usual transport scattering rate

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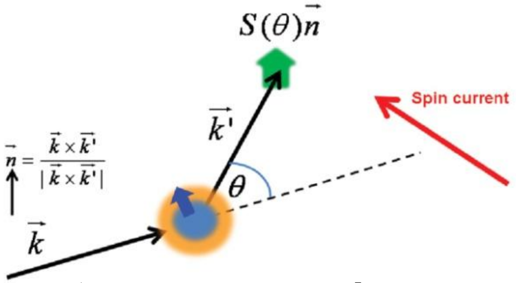


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← transverse spin current produced by scattering

← usual transport scattering rate

Hall angle is roughly estimated as $\gamma_S \fallingdotseq 0.001$ without resonant scattering

## 部分波展開

$$f_1(\theta) = \sum_l \frac{P_l(\cos\theta)}{2ik}[(l+1)(e^{2i\delta_l^+} - 1) + l(e^{2i\delta_l^-} - 1)]$$

$$f_2(\theta) = \sum_l \frac{\sin\theta}{2ik}(e^{2i\delta_l^+} - e^{2i\delta_l^-})\frac{d}{d\cos\theta}P_l(\cos\theta)$$

assuming resonant channel is the ***d*** wave (***l*** = 2) which is subject to SOI

$$\gamma_S = \frac{3\mathrm{Im}[(e^{-2i\delta_1} - 1)(e^{2i\delta_2^+} - e^{2i\delta_2^-})]}{9\sin^2\delta_2^+ + 4\sin^2\delta_2^- + 3[2 - \cos 2\delta_2^+ - \cos 2\delta_2^-]}$$

**(Guang-Yu Guo. et al. PRL 102, 036401 (2009))**

the p wave scattering is assmumed to
be spin independent and phase shift is small

$$\gamma_S = \frac{-6\delta_1(\cos 2\delta_2^+ - \cos 2\delta_2^-)}{9\sin^2\delta_2^+ + 4\sin^2\delta_2^- + 3[2 - \cos 2\delta_2^+ - \cos 2\delta_2^-]}$$

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most important factor

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difference in the phase shift of the $J = 2 \pm ½$ impurity state

this is related to that of occupation mumber

calcurate the local density of states for the d electrons several requirements to obtain the gigantic SHE

1, the resonance at Fermi energy due to Kondo peak or mixed valence

2, the orbiatl angular momentum should not be quenched

3, the peak must be split due to SOI by the energy
comparable or lager than the width of perk

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method

LDA : local density approximation

LDA + U (coulomb interaction)

# 計算対象

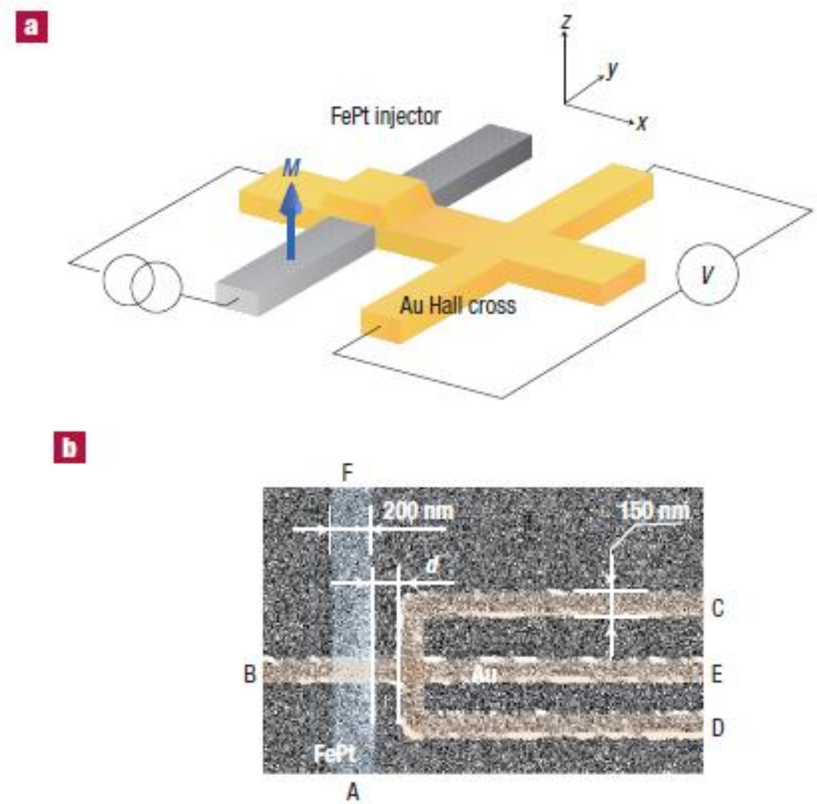
Au

relatively small SOI
difficult to explain the giant SHE

1, Au vacansies

2, Pt impurity

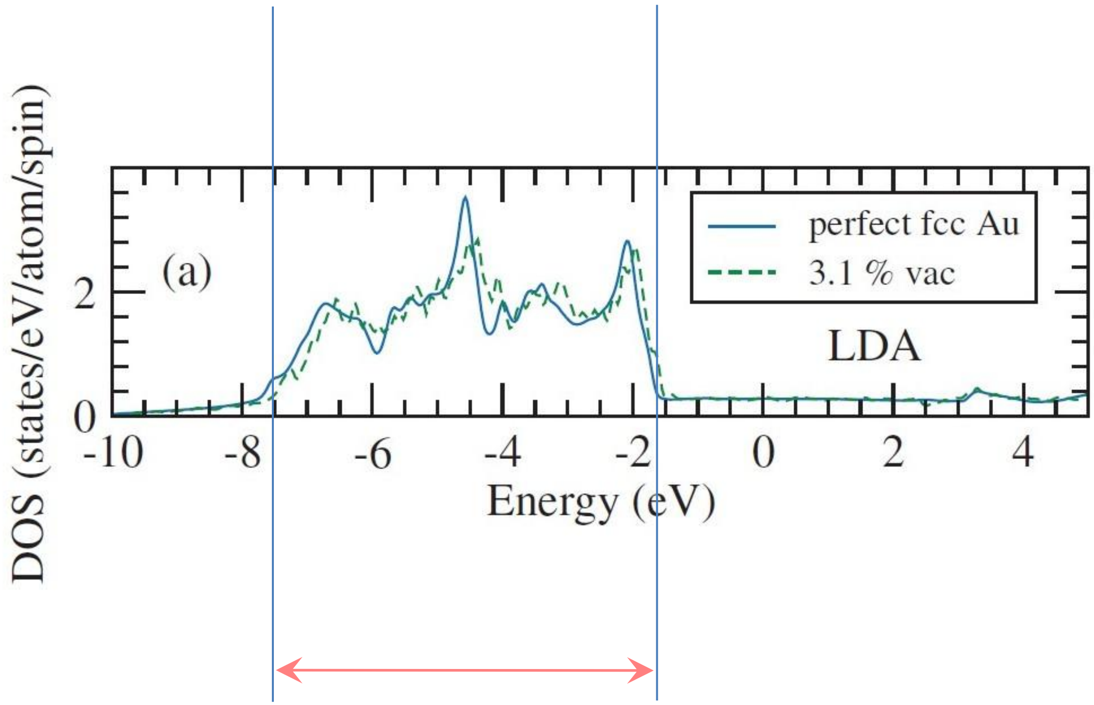
3, Fe impurity




**(T. Seki et al. nature materials VOL7 FEBURARY 2008)**

# 1, Au vacancies

The change of DOS is almost confined in the range of the 5*d* **b**and (-8 to -2 eV)

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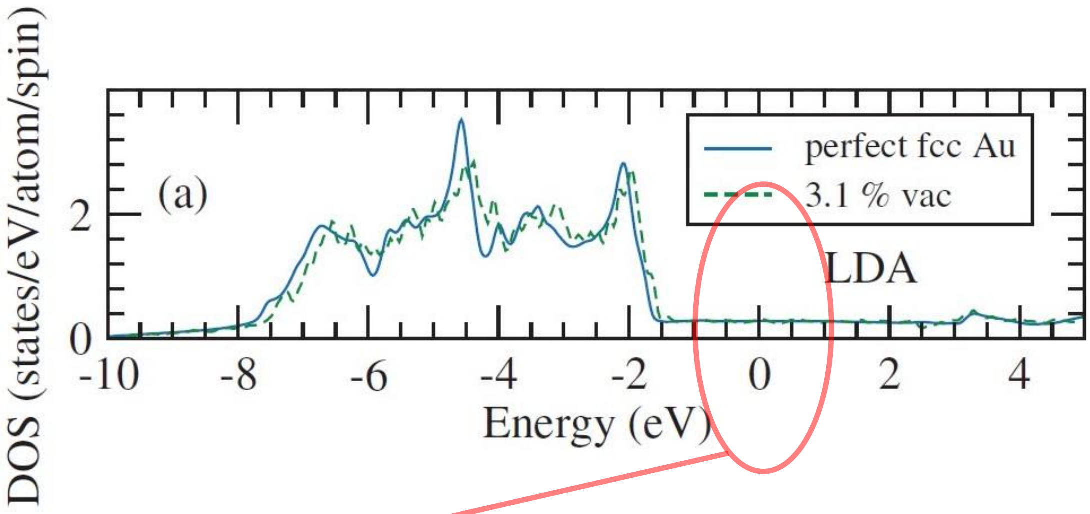


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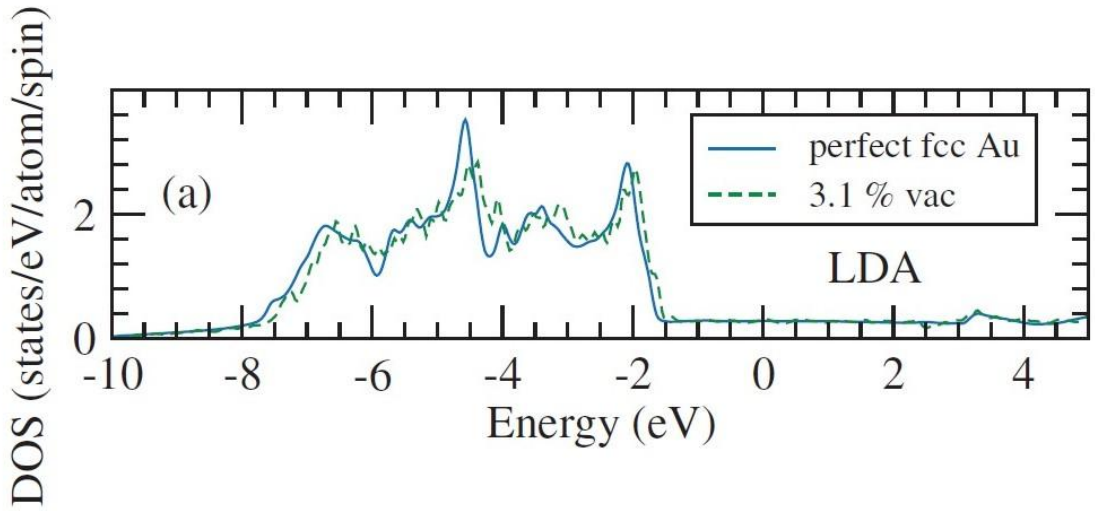


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This senario is difficult to explane large SHE

## 2, Pr impurities

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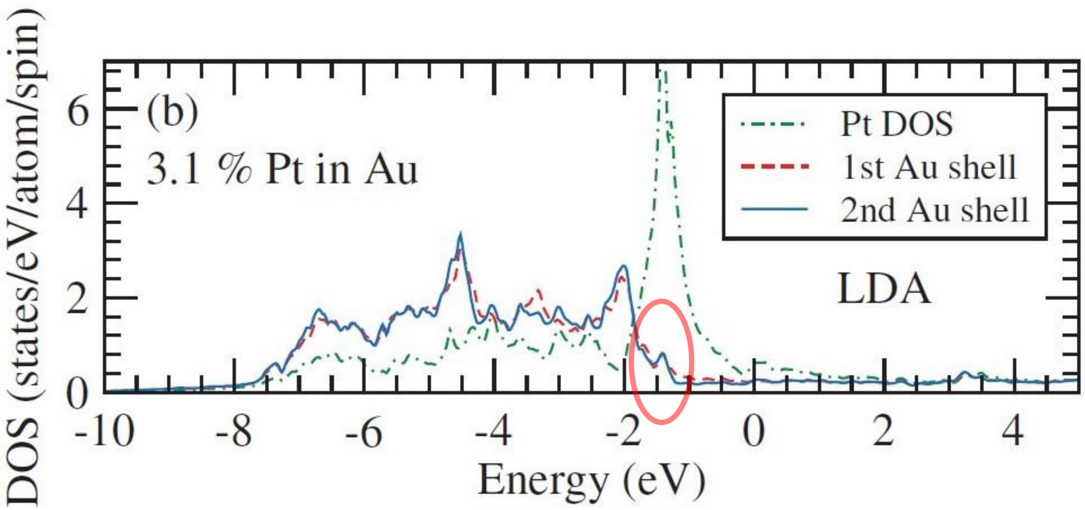


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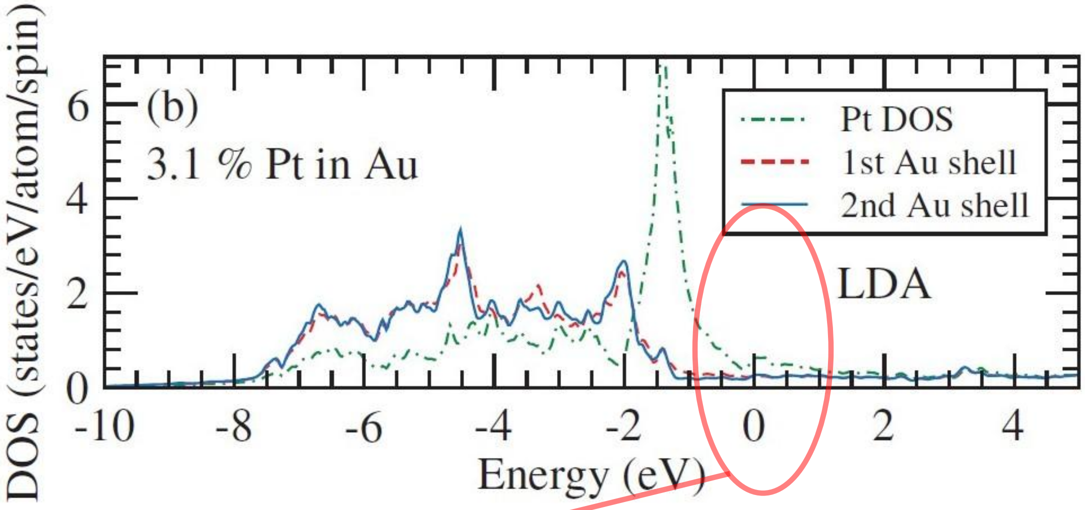


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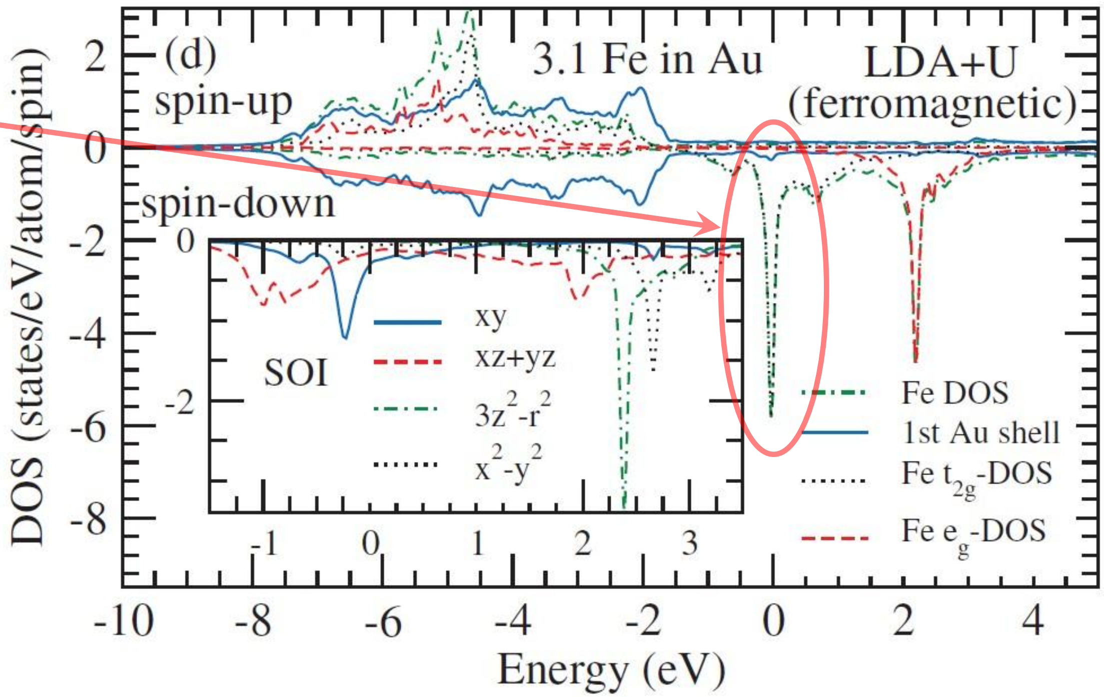
3, Fe impurities

Fe shows the spin splitting, and the down-spin DOS has sharp peak close to Fermi energy

valence fluctuation of Fe between $d^6$ and $d^7$

This is reasonable since the Fe in Au is known as a Kondo impurity

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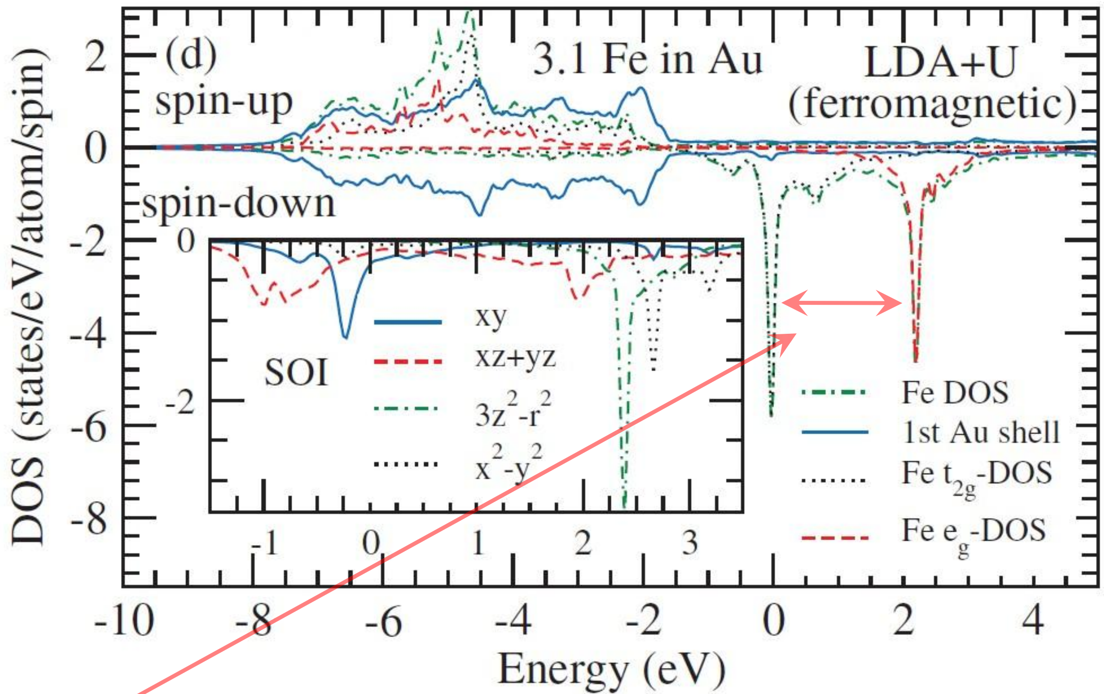


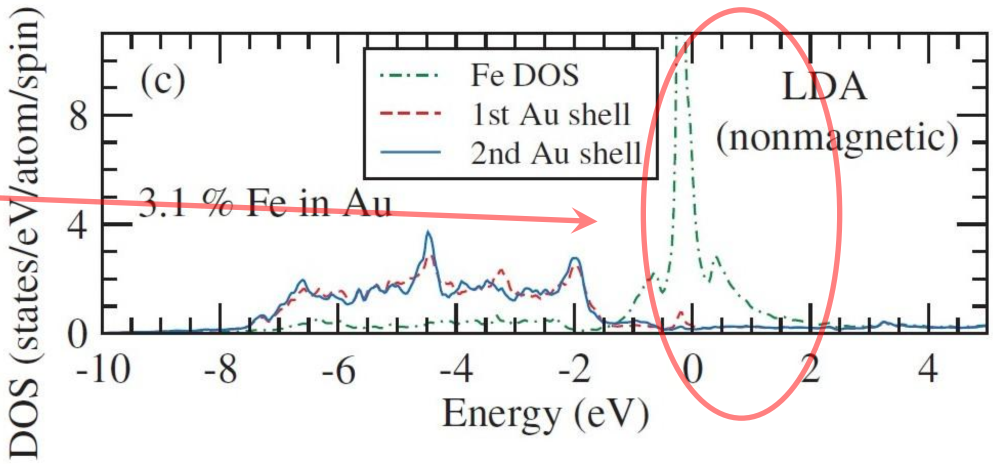

(Guang-Yu Guo. et al. PRL 102, 036401 (2009))

peak is split

## 3, Fe impurities

This is the result of LDA calculation (without Coulomb potential).

This has no magnetic state and no DOS splitting.




**(Guang-Yu Guo. et al. PRL 102, 036401 (2009))**

the orbital polarization due to the electron correlation (not by the crystal field)

orbital-dependent Kondo effect orrurs for Fe in Au

Fe impurities could be the origin of large SHE

## Fe orbital

$e_g$ : in the Kondo limit (around 2eV)

---

$t_{2g}$ : in the mixed valence region (at Fermi energy)
orbital angular momentum is not quenched

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→ play the major role in the transport properties

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orbital polarization

large orbital magnetic moment ($m_o = 1.5\mu_b$) is obtained

Table.1

| (a) | $xy$ | $xz$ | $yz$ | $3z^2 - r^2$ | $x^2 - y^2$ |
|---|---|---|---|---|---|
| No SOI | 0.459 | 0.459 | 0.459 | 0.053 | 0.053 |
| SOI | 0.559 | 0.453 | 0.453 | 0.050 | 0.128 |
| (b) | $m = -2$ | $m = -1$ | $m = 0$ | $m = 1$ | $m = 2$ |
| No SOI | 0.256 | 0.459 | 0.053 | 0.459 | 0.256 |
| SOI | 0.138 | 0.087 | 0.050 | 0.819 | 0.549 |

**down spin occupation numbers of 3*d* orbitals of the Fe impurity in Au**
**(Guang-Yu Guo. et al. PRL 102, 036401 (2009))**

## orbital polarization

$t_{2g}$ : effective orbital angular momentum $l_{eff} = 1$

| | |
|---|---|
| $zx + iyz$ | (m = 1) |
| $xy$ | (m = 0) |
| $zx - iyz$ | (m = -1) |

SOI is effective within the $t_{g2}$ states leading to the energy splitting between the $J_{eff}$ = 2/3 and $J_{eff}$ = 1/2 states

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Orbital ordering is determined by the competition between the hybridization energy **Δ** and the SOI splitting

## many body state

energy separation is typically the order of SOI (~ 0.01 eV)

→ much smaller than **Δ** (~ 1 eV)

Δ >> SOI

orbital  polarization should not occer due to the hybridization

↓

different contribution of Coulomb energy between ***xy*** and ***xz, yz*** orbitals

↓

energy splitting of ***xy*** and ***xz, yz*** orbitals is enhanced by Coulomb energy

↓

***U*** plays an essential role in orbital polarization

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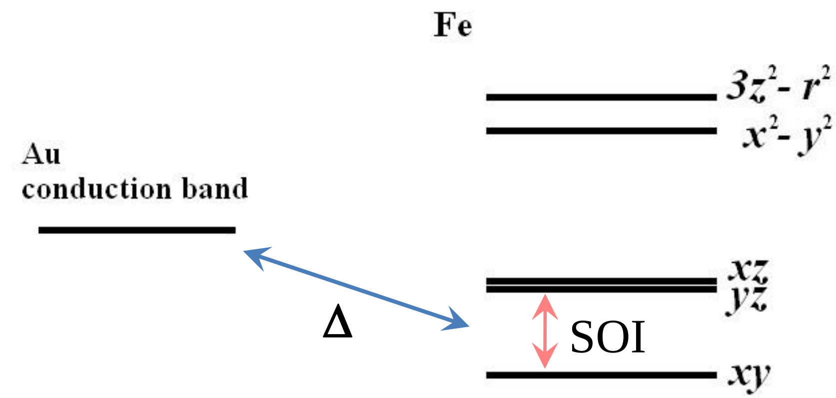

phase shift of $\boldsymbol{m}$ = 1 state is almost $\boldsymbol{\pi}$
and phase shift of $\boldsymbol{m}$ = -1 atate is almost 0

(***Friedel*** Sum Rule)

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AHE

$$\gamma \sim \sin\delta_1 \sin(2\delta_2^+ - \delta_1)$$

→ little contribution

**(A. Fert, et al. PRL 28, 303 (1972))**

SHE

$$\gamma_S = \frac{-6\delta_1(\cos 2\delta_2^+ - \cos 2\delta_2^-)}{9\sin^2\delta_2^+ + 4\sin^2\delta_2^- + 3[2-\cos 2\delta_2^+ - \cos 2\delta_2^-]}$$

→ large value

## Summary

large SHE in Au

Fe impurity in Au (Kondo impurity)

↓

DOS splitting due to the SOI

↓

energy splitting is enhanced by the Coulomb energy

↓

large SHE

**orbital dependent Kondo Effect enhance the Spin Hall Effect**

# Appendix

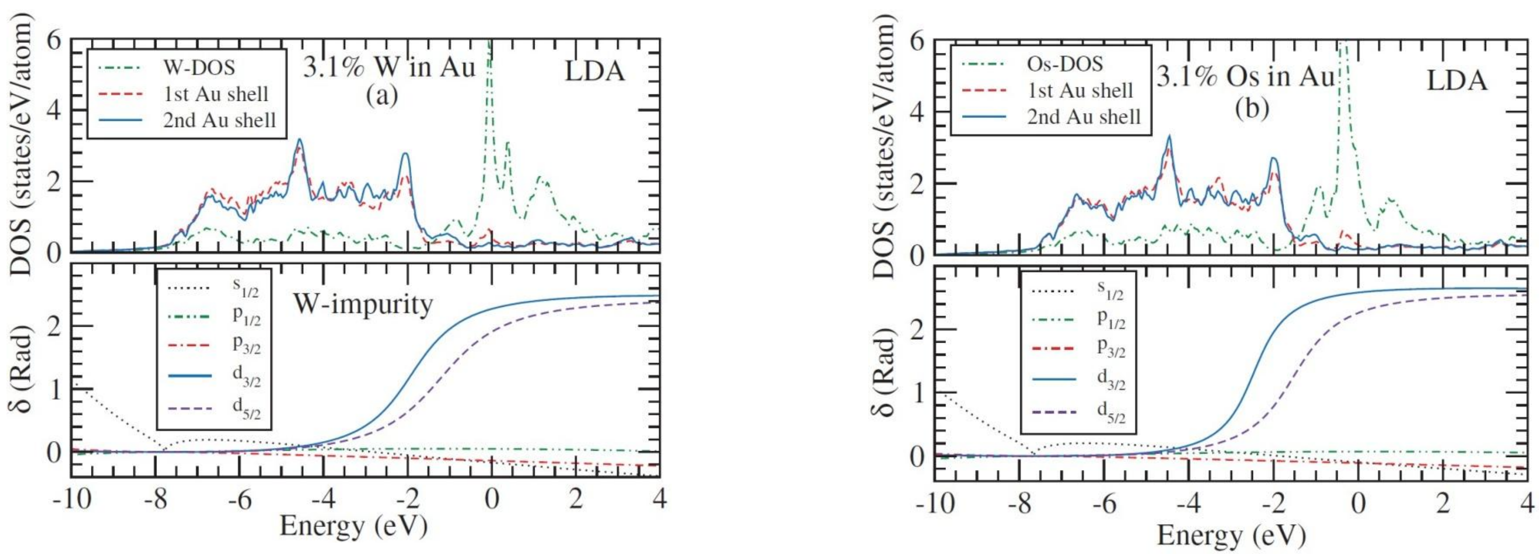
## W or Os impurities

there is no magnetic state

large SOI

resonanse peak at Fermi energy

large spin hall angle

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