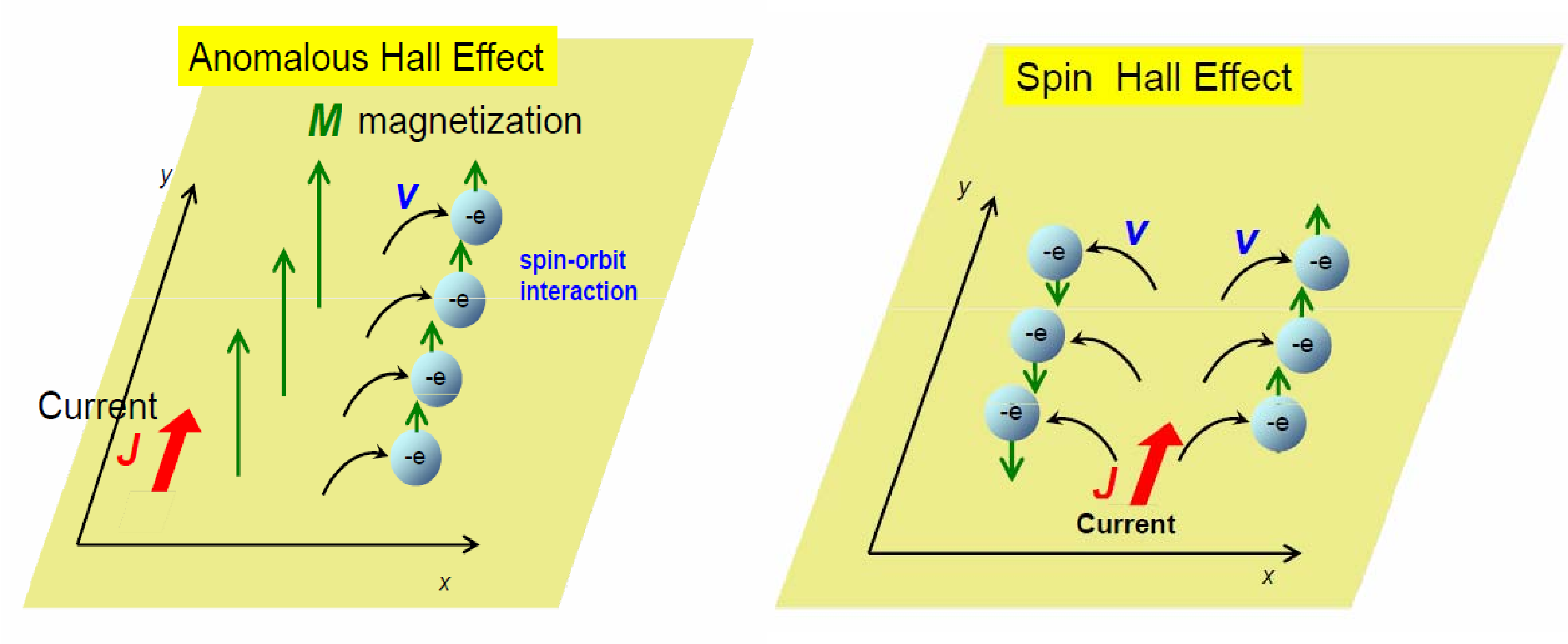
Kondo effect and Spin Hall Effect in Au metal

Jan 29 KITP

Naoto Nagaosa
Department of Applied Physics
The University of Tokyo

Collaborators:
G.Y. Guo , S. Maekawa,



Massage:

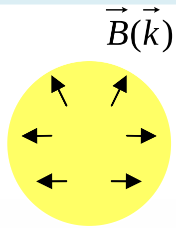
SHE is not the simple two copies of AHE for up and down spins.

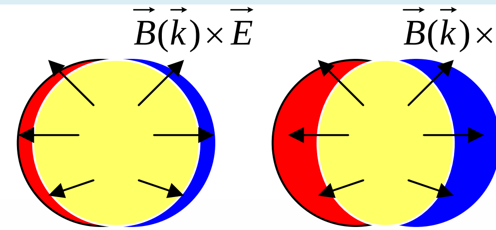
The spin fluctuation and electron correlation play crucial roles in SHE.

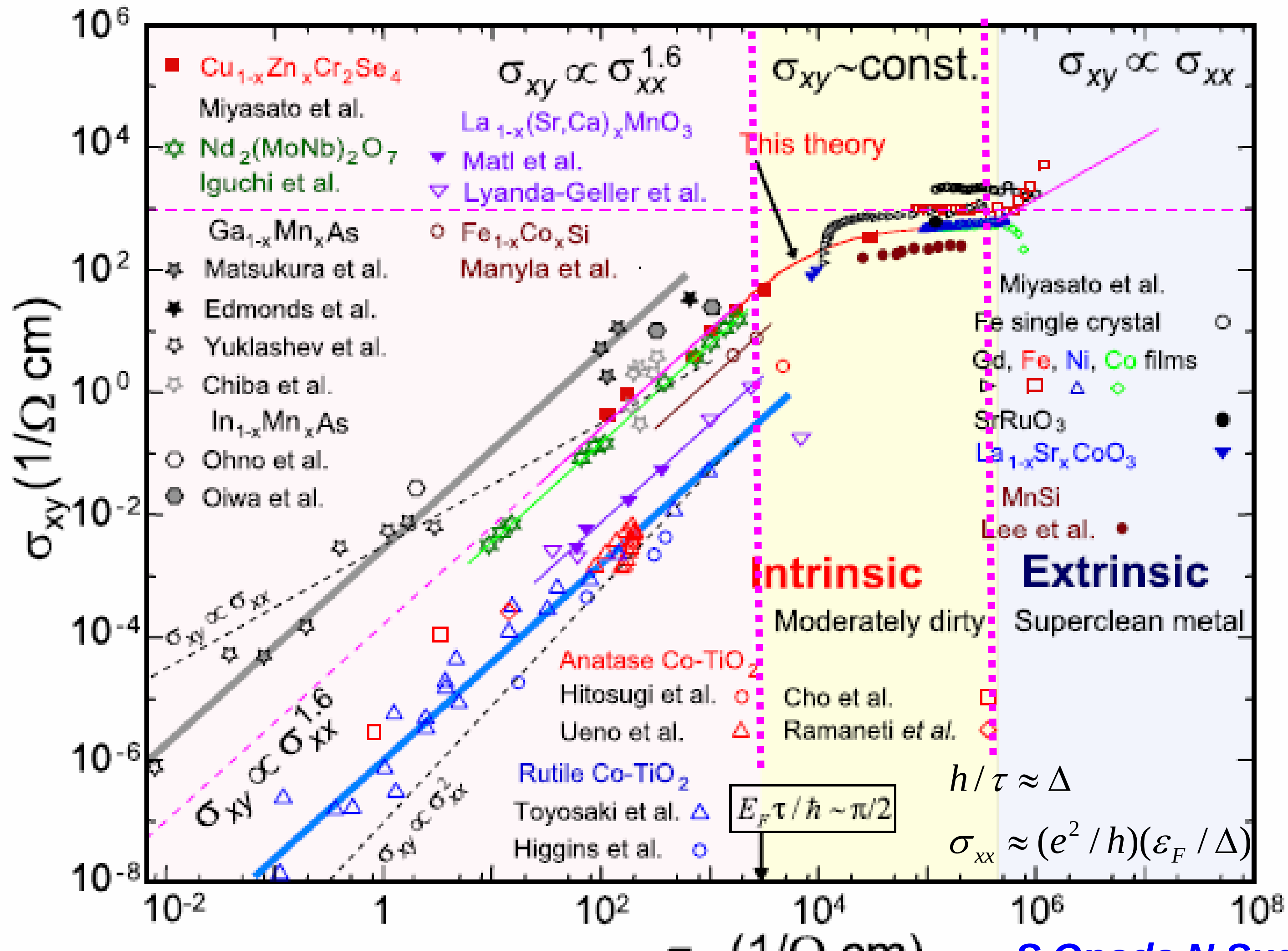
Intrinsic AHE is the quantum Hall effect hidden by metallicity

$$e^2/ha \approx 10^3 \Omega^{-1}\mathrm{cm}^{-1}$$

$$\sigma_{xx} \approx 10^3(\varepsilon_F \tau)\Omega^{-1}\mathrm{cm}^{-1}$$



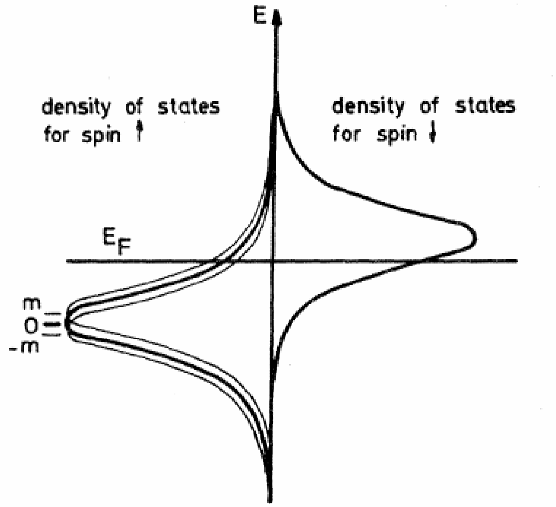




S.Onoda, N.Sugimoto, NN

Left-Right Asymmetry in the Scattering of Electrons by Magnetic Impurities, and a Hall Effect

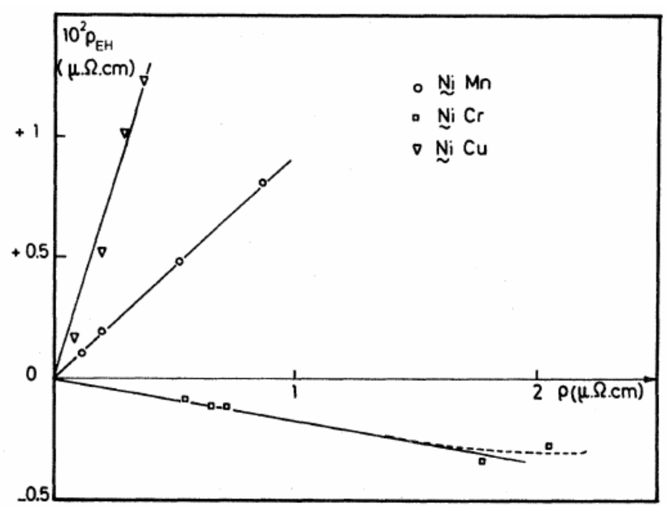
A. Fert and O. Jaoul
Laboratoire de Physique des Solides, Université de Paris-Sud, Orsay, France*
(Received 25 October 1971)

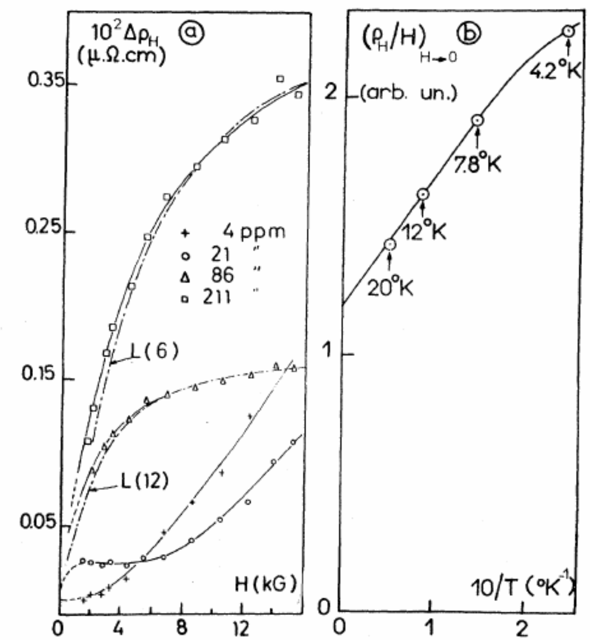


$$\varphi_\sigma = \pm(3\lambda_\sigma/5\Delta)\sin\eta_1 \sin(2\eta_{2\sigma}^{\,0} - \eta_1).$$

Anomalous Hall angle

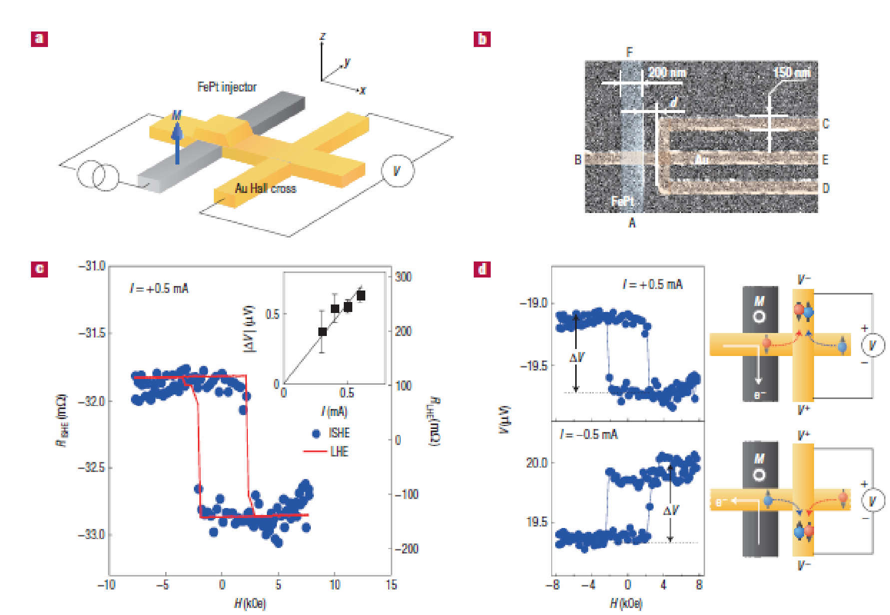
$$\approx 0.001 - 0.01$$

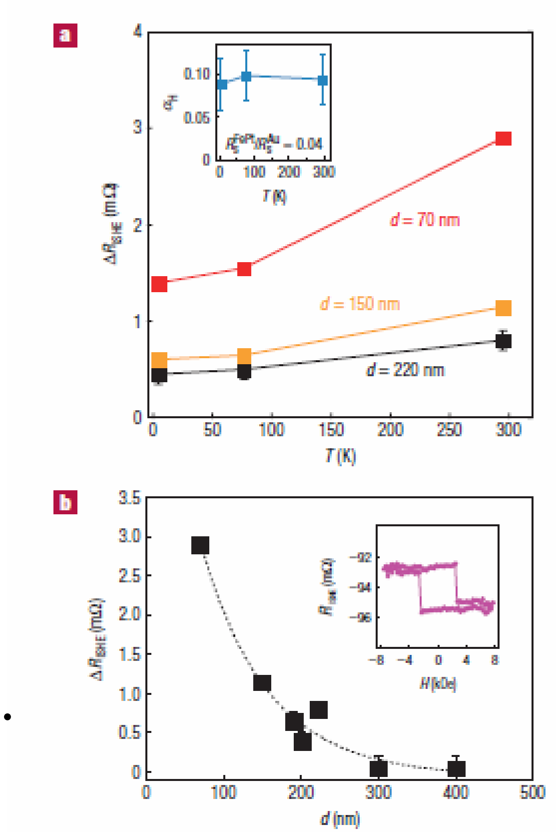




Giant spin Hall effect in perpendicularly spin-polarized FePt/Au devices

TAKESHI SEKI[1]*, YU HASEGAWA[1], SEIJI MITANI[1], SABURO TAKAHASHI[1,2], HIROSHI IMAMURA[2,3], SADAMICHI MAEKAWA[1,2], JUNSAKU NITTA[4] AND KOKI TAKANASHI[1]





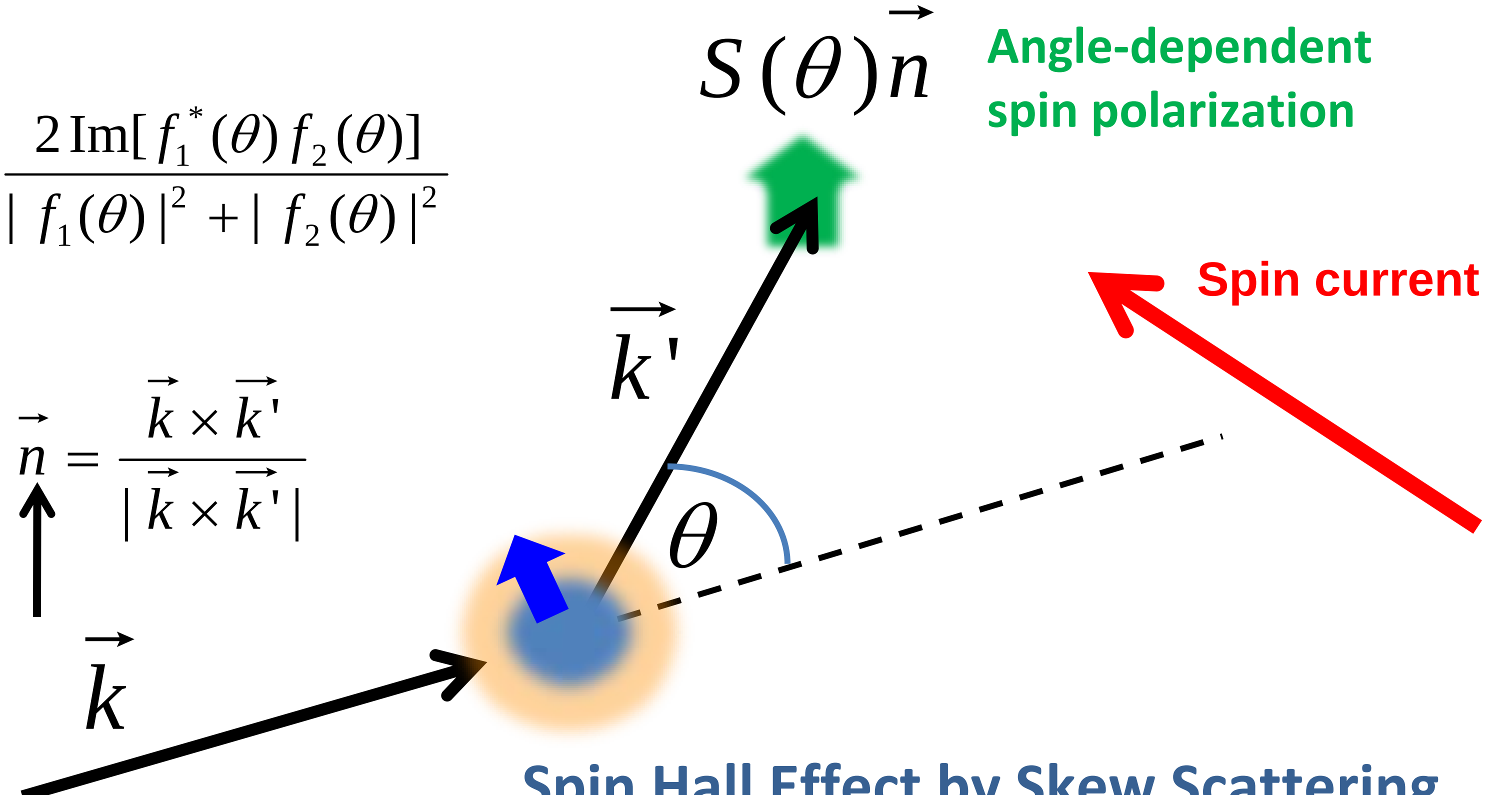
spin Hall angle $\alpha_H \approx 0.1$ at room temp.

$$\sigma_H^s \approx 10^5 \Omega^{-1} cm^{-1}$$

$\rho \approx 1\mu\Omega\text{cm} \rightarrow$ skew scattering

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

$$\vec{n} = \frac{\vec{k} \times \vec{k}'}{|\vec{k} \times \vec{k}'|}$$



Spin Hall Effect by Skew Scattering

$$\hat{f}(\vec{k}) = f_0(\vec{k})\hat{1} + \vec{k} \cdot \left[\vec{E} + \frac{\gamma}{2}(\vec{\sigma} \times \vec{E}) \right]$$

$$\sigma_H^s / \sigma_{xx} = \gamma = \frac{\int d\Omega I(\theta) S(\theta) \sin\theta}{\int d\Omega I(\theta)(1-\cos\theta)}$$

Spin Hall angle

S-matrix

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

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

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

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

$$\delta_l^{\pm} = \delta_{J=l\pm 1/2}$$

Friedel sum-rule

$$\pi Z = \sum_J (2J+1)\delta_J$$

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

$$\gamma = \frac{6\,\mathrm{Im}[(e^{-2i\delta_2} - 1)(e^{2i\delta_3^+} - e^{2i\delta_3^-})]}{|4(e^{2i\delta_3^+} - 1) + 3(e^{2i\delta_3^-} - 1)|^2 / 2 + |e^{2i\delta_3^+} - e^{2i\delta_3^-}|^2} \qquad \ell = 3$$

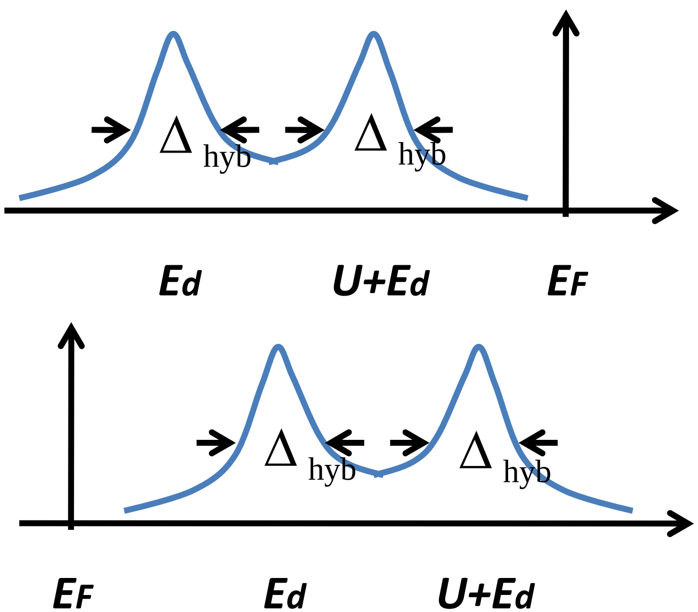
Anderson Hamiltonian as a generic model for impurity

$$H = \sum_{k,l,m,\sigma} \varepsilon_{k,l,m} c^{+}_{k,l,m,\sigma} c^{+}_{k,l,m,\sigma} + \sum_{k,l,m,\sigma} (V_{k,l,m} c^{+}_{k,l,m,\sigma} d_{l,m,\sigma} + h.c.) + H_d + H_U$$

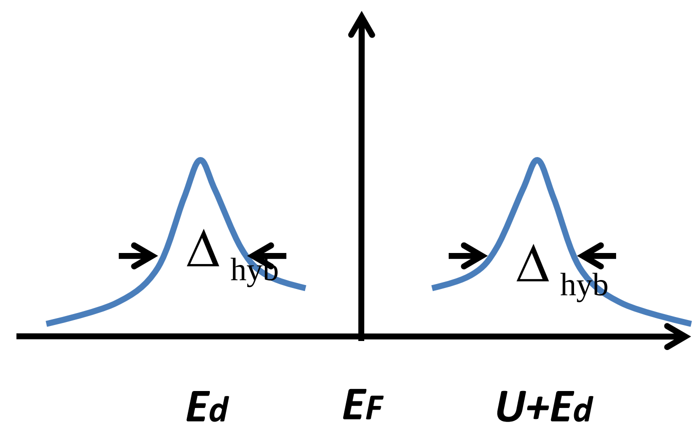
$$H_d = \sum_{l,m,\sigma} E_l d^{+}_{l,m} d_{l,m} + (\lambda/2) \sum_{l,m,m',\sigma,\sigma'} d^{+}_{l,m,\sigma} (\vec{l})_{mm'} \cdot (\vec{\sigma})_{\sigma\sigma'} d_{l,m',\sigma'} + D \sum_{l,m,\sigma} m^2 d^{+}_{l,m,\sigma} d_{l,m,\sigma}$$

$$H_U = U (\sum_{l,m,\sigma} d^{+}_{l,m,\sigma} d_{l,m,\sigma} - 1)^2$$

nonmagnetic



magnetic



mixed valence or Kondo

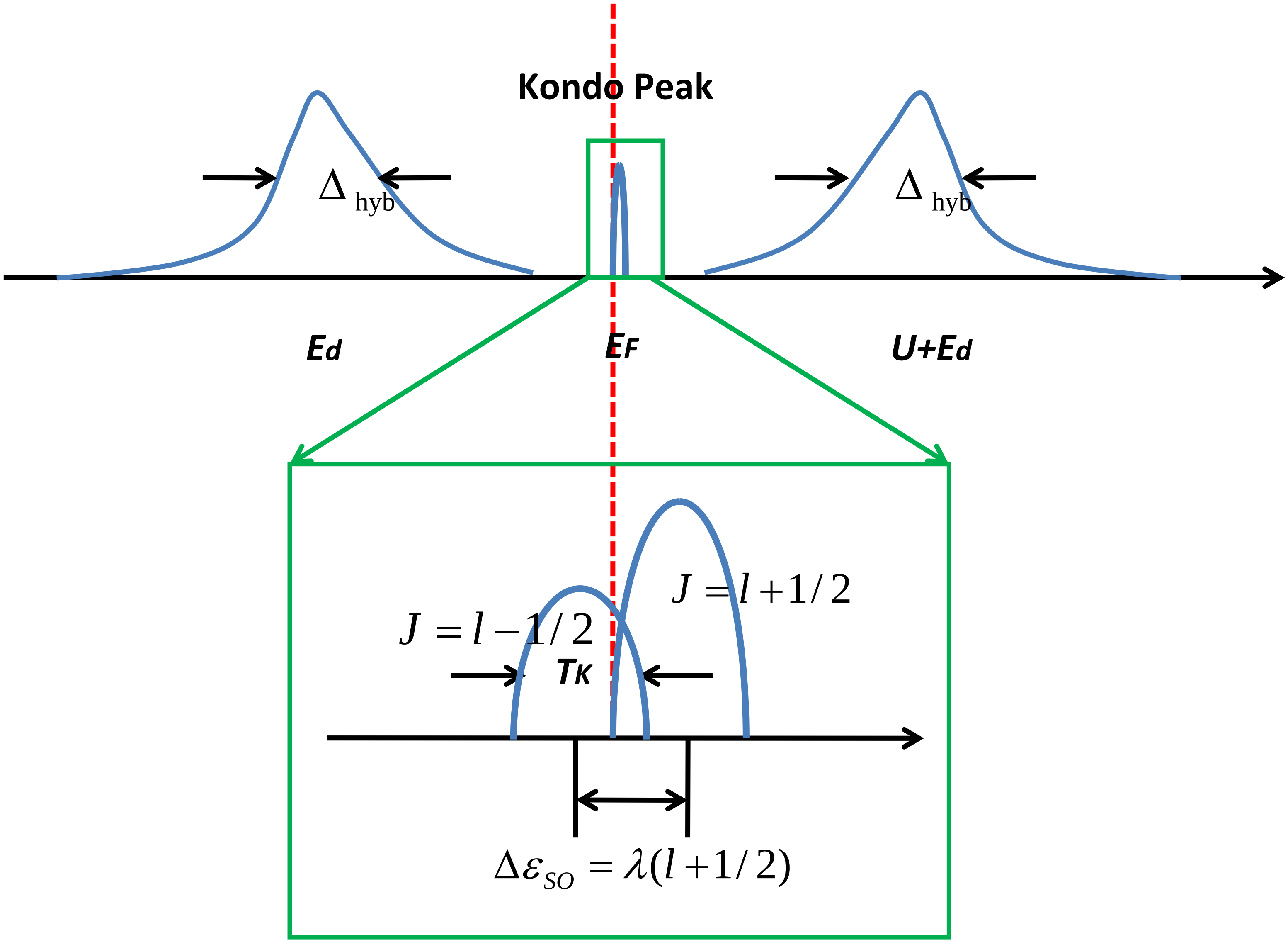
Kondo effect

magnetic impurity

$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow> - |\downarrow\uparrow>)$$

Singlet formation
Quantum entanglement

conduction electrons


Kondo Peak
Δ hyb
Δ hyb
Ed
EF
U+Ed
J = l − 1/2
J = l + 1/2
TK
Δε_SO = λ(l + 1/2)

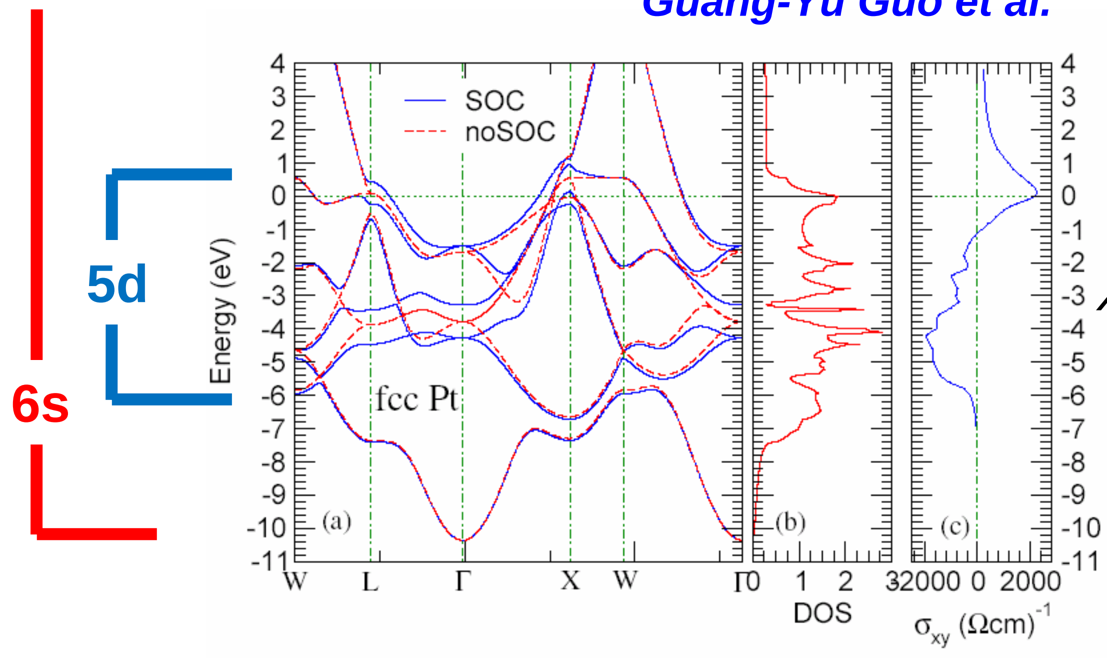
Candidate Materials for Resonant Skew Scattering

Guang-Yu Guo et al.

$\mathrm{Ir}:(5\mathrm{d})^{7}(6\mathrm{s})^{2}$

$\mathrm{Pt}:(5\mathrm{d})^{9}(6\mathrm{s})^{1}$

$\mathrm{Au}:(5\mathrm{d})^{10}(6\mathrm{s})^{1}$



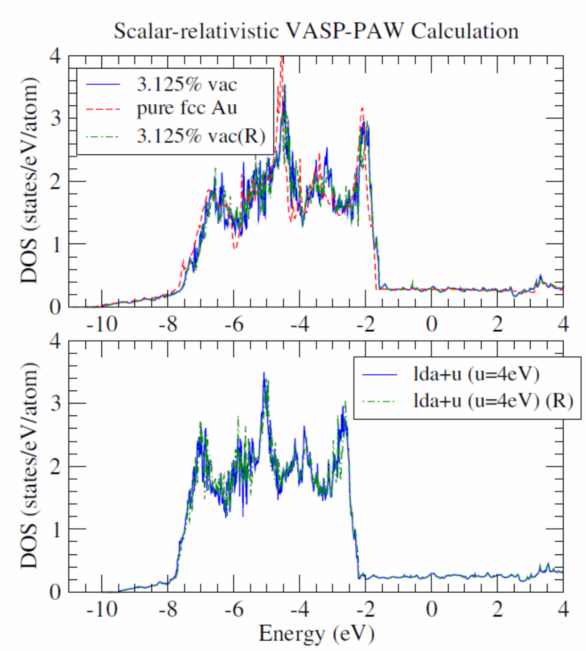
$\lambda \approx 0.5\mathrm{eV}$

vacancy of Au atom
Pt impurity
Fe impurity

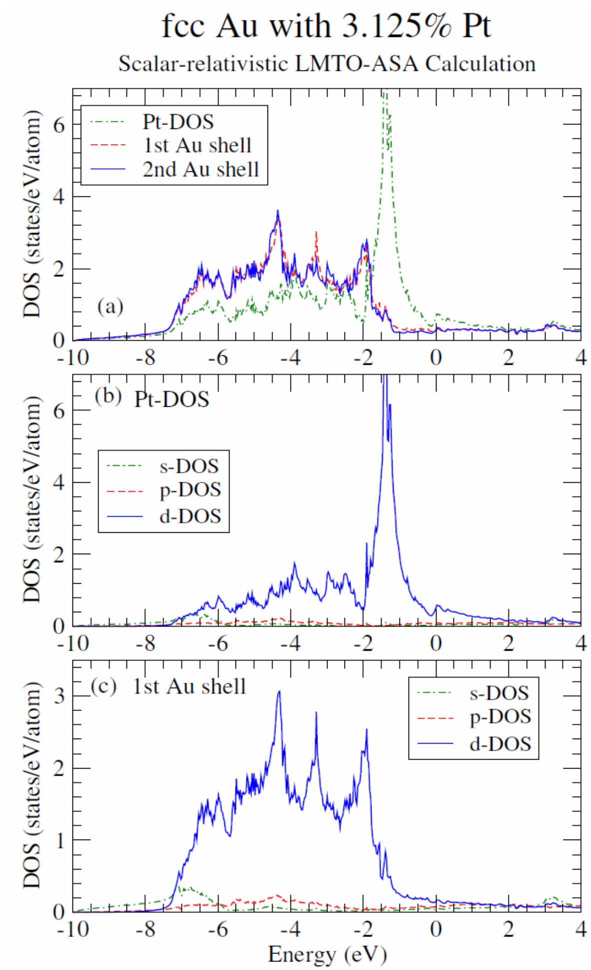
d-orbital character of impurity state at Fermi energy ?

1st principles band calculation of impurity state

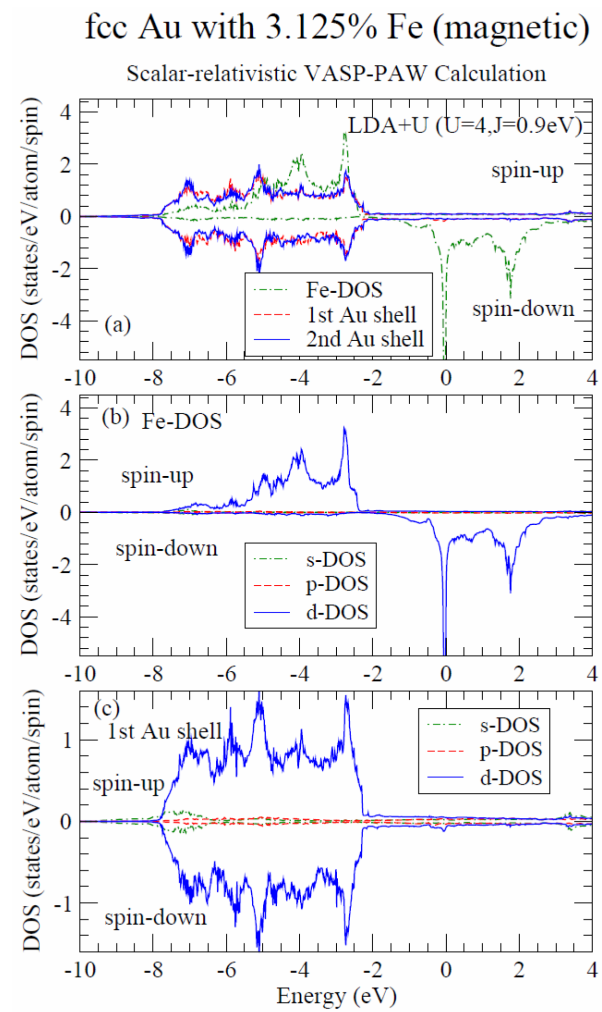
vacancy



Pt



Fe



PHYSICAL REVIEW B VOLUME 32, NUMBER 10 15 NOVEMBER 1985

Pd and Pt impurity-induced changes in noble-metal density of states: Photoelectron spectroscopy and theory

D. van der Marel,* J. A. Jullianus, and G. A. Sawatzky
Physical Chemistry Department of the Material Science Center, University of Groningen, Nijenborgh 16, 9747 AG Groningen, The Netherlands
(Received 25 March 1985)

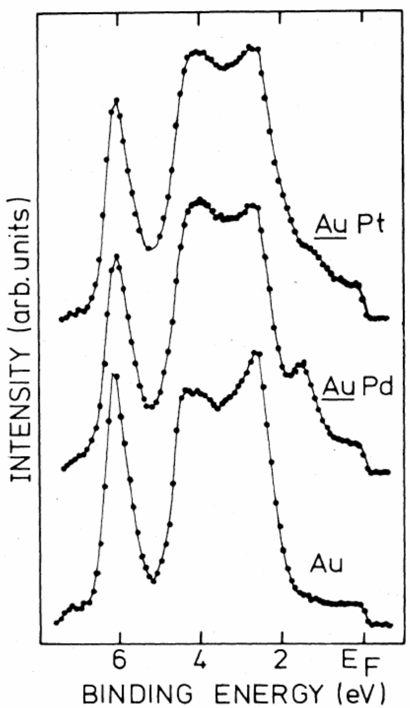


FIG. 6. Corrected UPS spectra of Au, *Au*Pd, and *Au*Pt. The thin solid lines are a guide to the eye.

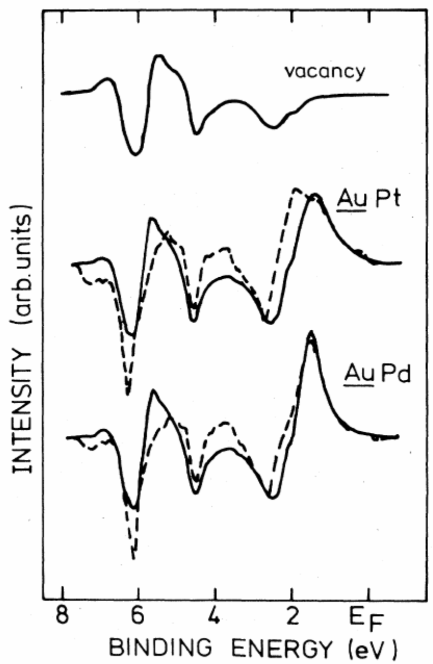


FIG. 14. Theoretical (solid lines) and experimental (dashed lines) UPS difference spectra of a vacancy in Au, *Au*Pt-Au, and *Au*Pd-Au.

$$H=H_{\text{host}}+\frac{1}{\sqrt{N}}\sum_{k}\sum_{\mu,\nu}[V_{k\mu}^{\nu}(C_{k\mu}^{\dagger}C_{0\nu}+C_{0\nu}^{\dagger}C_{k\mu})]$$

$$=H_{\text{host}}+\frac{1}{N}\sum_{k,q}\sum_{\mu,\nu}[(V_{k\mu}^{\nu}+V_{q\nu}^{\mu})C_{k\mu}^{\dagger}C_{q\nu}]\ ,$$

$$H_{\text{imp}}=\frac{1}{N}\sum_{kq}[\Delta_k(d_k^{\dagger}d_q+d_q^{\dagger}d_k)+V_k(c_k^{\dagger}d_q+d_q^{\dagger}c_k)]$$

$$\mathbf{T}_k^q=\frac{1}{N}\begin{bmatrix}\mathbf{D}^{-1}(\mathbf{\Delta}+\sigma_s) & \mathbf{D}^{-1}\mathbf{V}_q\\ \mathbf{V}_k(\mathbf{D}^T)^{-1} & \mathbf{V}_k\mathbf{g}_d^d\mathbf{D}^{-1}\mathbf{V}_q\end{bmatrix}$$

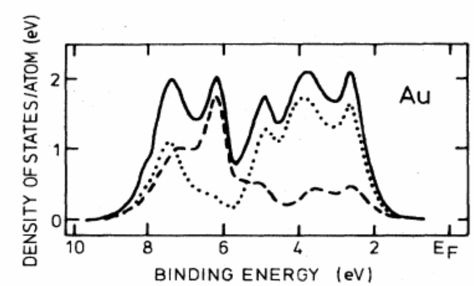


FIG. 20. Density of states of gold. Solid lines: total d density of states. Dashed line: $d_{3/2}$ projected DOS. Dotted line: $d_{5/2}$ projected DOS.

$$\langle \Gamma_7(d_{5/2}) | (\Delta+\sigma_s) | \Gamma_7(d_{5/2}) \rangle = \Delta + \delta\xi_d - 4Dq + \sigma_s ,$$

$$\langle \Gamma_8(d_{5/2}) | (\Delta+\sigma_s) | \Gamma_8(d_{5/2}) \rangle = \Delta + \delta\xi_d + 2Dq + \sigma_s ,$$

$$\langle \Gamma_8(d_{3/2}) | (\Delta+\sigma_s) | \Gamma_8(d_{3/2}) \rangle = \Delta - \tfrac{3}{2}\delta\xi_d + \sigma_s ,$$

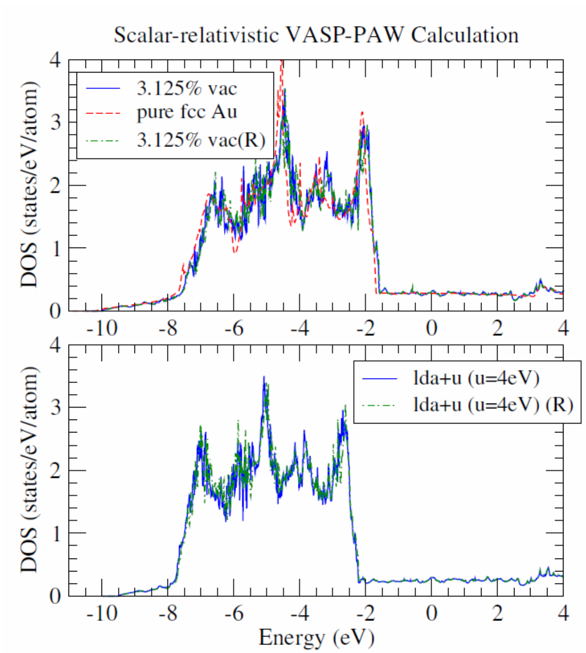
$$\langle \Gamma_8(d_{5/2}) | (\Delta+\sigma_s) | \Gamma_8(d_{3/2}) \rangle = -2\sqrt{6}Dq ,$$

TABLE I. Experimental UPS impurity peak maxima (ϵ_{max}) and half widths at half maximum (Γ): (a) this work and (b) taken from Ref. 23. Parameters that were used in the theoretical spectra: change in impurity d potential (Δ), s-d coupling (σ_s), spin-orbit coupling (ξ_d), cubic crystal field (D_q), and average energy position of the impurity d states $\bar{\epsilon}_d+\Delta$, where $\bar{\epsilon}_d$ is the average host d-band energy.

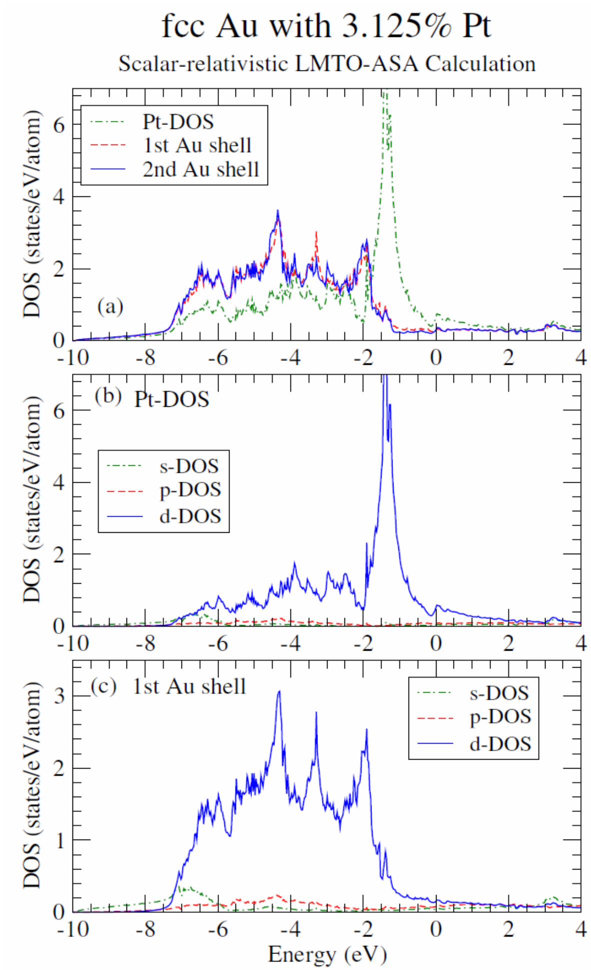
Solid	(a) ϵ_{max} (eV)	(a) Γ (eV)	(b) ϵ_{max} (eV)	(b) Γ (eV)	Δ (eV)	Imσ_s (eV)	ξ_d (eV)	D_q (eV)	$\bar{\epsilon}_d+\Delta$ (eV)
Cu					0	0	0	0	−3.52
*Cu*Pd	1.8	0.30±0.07	1.75	0.28	1.0	0.30±0.07	0.12	0	−2.52
*Cu*Pt	1.65/2.0	0.35±0.07			1.18	0.35±0.07	0.31	0	−2.34
Ag					0	0	0	0	−5.68
*Ag*Pd	1.8/2.2	0.40±0.05	1.95	0.35	3.4	0.40±0.05	0.18	0	−2.28
*Ag*Pt	1.5/2.6	0.28±0.07	1.95	0.47	3.23	0.28±0.07	0.44	0.043	−2.45
Au					0	0	0.45	0	−5.02
*Au*Pd	1.6	0.40±0.10	1.55	0.18	2.1	0.40±0.10	0.18	0	−2.92
*Au*Pt	1.3/1.9	0.50±0.10			2.1	0.50±0.10	0.44	0	−2.92

1st principles band calculation of impurity state

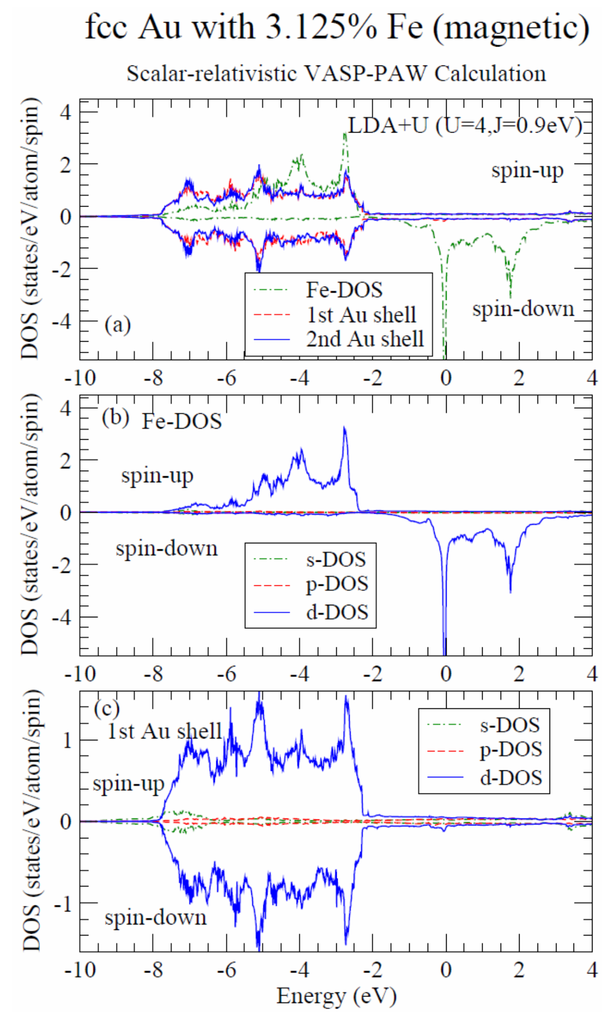
vacancy



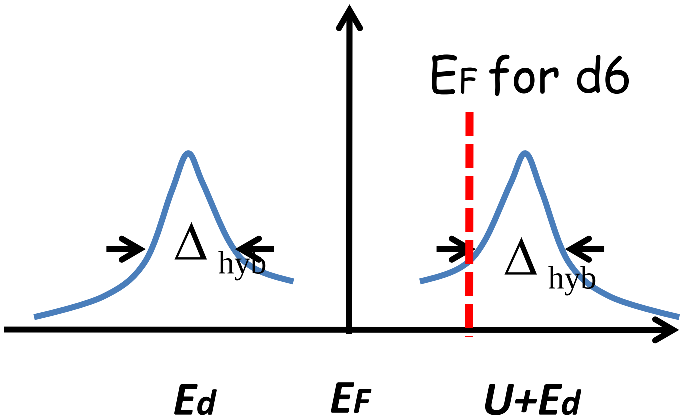
Pt



Fe



Conventional wisdom on Kondo effect of Fe in Au



$U = 3eV$

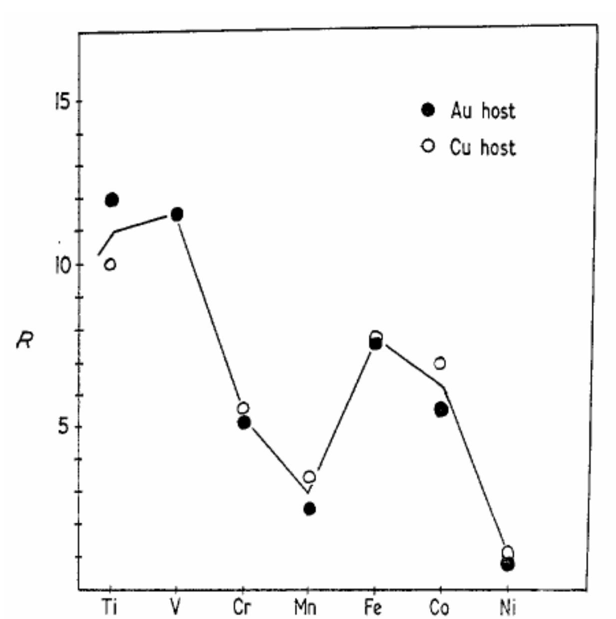
$\Delta = 1.4eV$

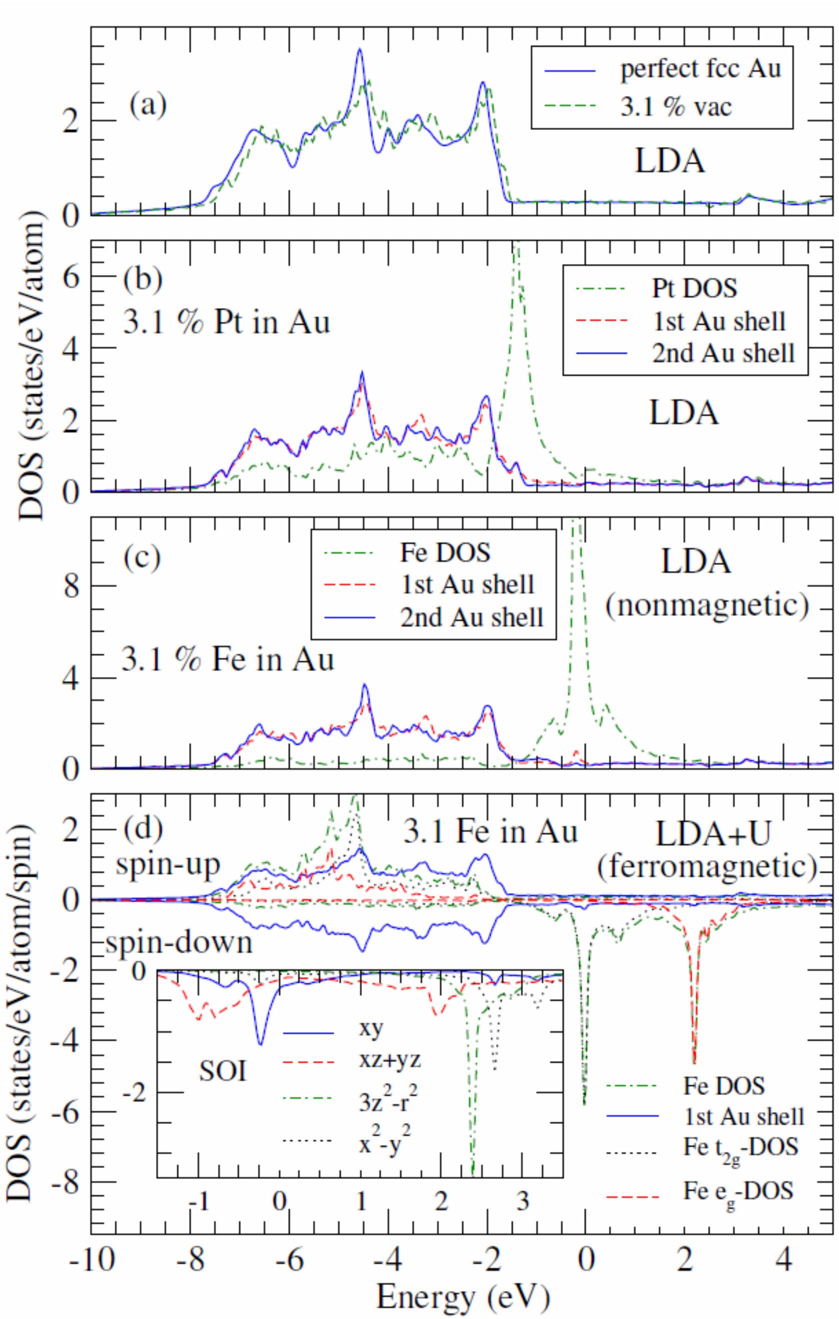
$10Dq = 0.1eV$

$\lambda = 0.03eV$

mixed valence

Kondo limit with 5 orbital degeneracy with Kondo temperature $T_K \approx 0.4K$





with G.Y. Guo and S. Maekawa

Spin Hall Effect by Kondo singlet state

Orbital selective Kondo

eg Kondo limit → $T_K \approx 0.4K$

t2g Mixed valence d^6 and d^7

hybridization with Au s- and d-orbitals

Renormalization effect due to electron correlation

$$\Delta = 1.4eV \Rightarrow \Delta = 0.3eV$$

$$10Dq = 0.1eV \Rightarrow 10Dq = 2.0eV$$

$$\lambda = 0.03eV \Rightarrow \lambda = 1eV$$

TABLE I: Down-spin occupation numbers of the $3d$-suborbitals of the Fe impurity in Au from LDA+U calculations without SOI and with SOI. The calculated magnetic moments are: $m_s^{Fe} = 3.39\ \mu_B$ and $m_s^{tot} = 3.32\ \mu_B$ without SOI, as well as $m_s^{Fe} = 3.19\ \mu_B$, $m_o^{Fe} = 1.54\ \mu_B$ and $m_s^{tot} = 3.27\ \mu_B$ with SOI. The muffin-tin sphere radius $R_{mt} = 2.65 a_0$ (a_0 is Bohr radius) is used for both Fe and Au atoms.

(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

Physics

Physics **2**, 6 (2009)

Viewpoint

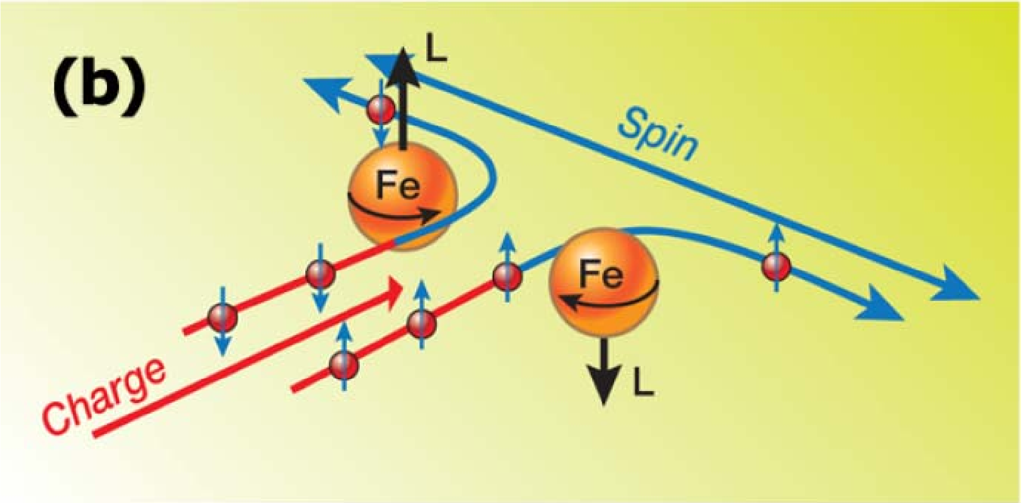
Lending an iron hand to spintronics

Piers Coleman
Department of Physics and Astronomy, Rutgers University, 136 Frelinghuysen Road, Piscataway, NJ 08854-8019, USA

Published January 20, 2009

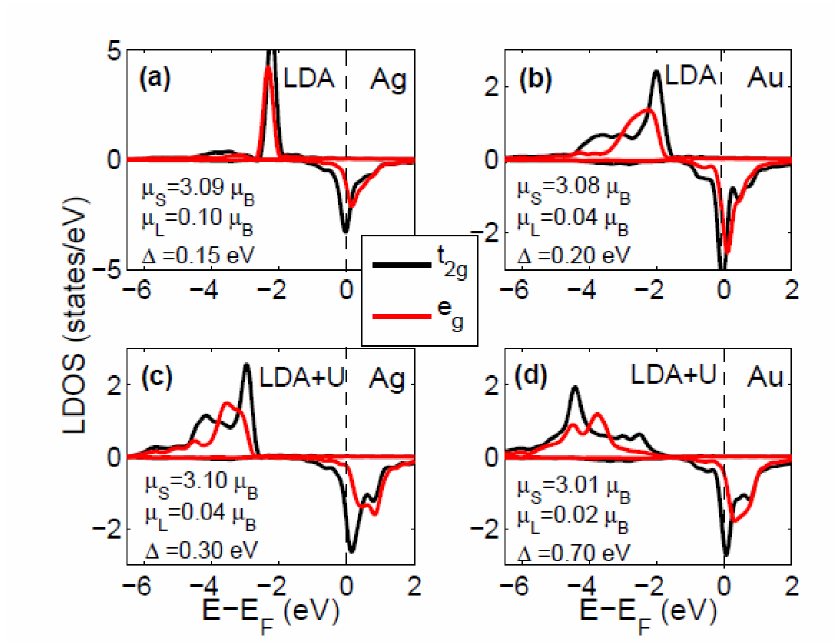
Subject Areas: Spintronics

A Viewpoint on:
Enhanced Spin Hall Effect by Resonant Skew Scattering in the Orbital-Dependent Kondo Effect
Guang-Yu Guo, Sadamichi Maekawa and Naoto Nagaosa
Phys. Rev. Lett. **102**, 036401 (2009) – Published January 20, 2009

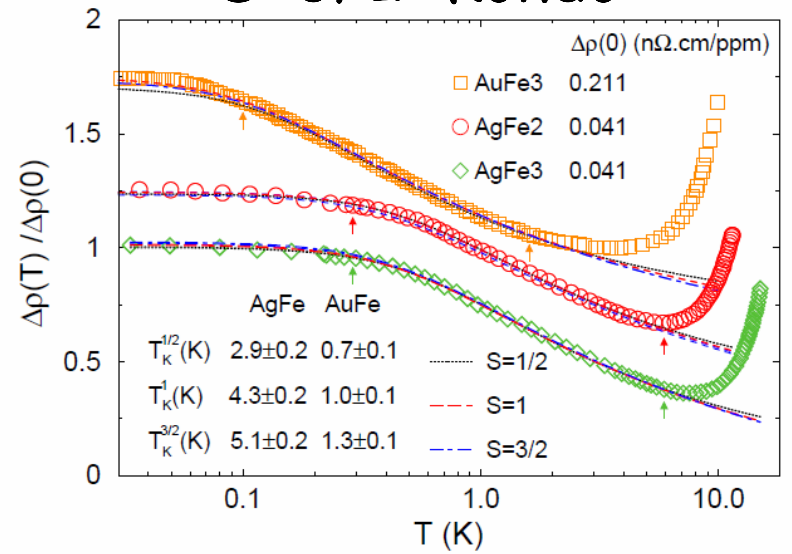


Kondo decoherence: finding the right spin model for iron impurities in gold and silver

T. A. Costi[1,2], L. Bergqvist[1], A. Weichselbaum[3], J. von Delft[3], T. Micklitz[4,7], A. Rosch[4], P. Mavropoulos[1,2], P. H. Dederichs[1], F. Mallet[5], L. Saminadayar[5,6], and C. Bäuerle[5]



S=3/2 Kondo



	method	picture
ours	all-electron full-potential linearized Augmented plane wave (FLAPW) method	S=3/2 large orbital moment Mixed valence and Kondo
Costi	ultra-soft pseudopotential-like projector augmented wave (PAW) method	S=3/2 small orbital moment Kondo limit

Conclusions

Anomalous Hall effect v.s. Spin Hall effect (Skew scattering)

Resonance due to virtual bound state ⇒ $\alpha_{AHE} \leq 0.01$

Spin fluctuation and Kondo effect further enhances SHE ⇒ $\alpha_{SHE} \approx 0.1$

$\sigma_{SHE} \approx 10^{5}\,\Omega^{-1}\mathrm{cm}^{-1}$

Fe impurity in Au

Orbital selective Kondo effect eg v.s. t2g
Renormalization of spin-orbit, hybridization energies due to electron correlation

Material design for SHE

5d impurity ⇒ $\alpha_{SHE} \approx 0.2 \sin 2\delta_1 \approx 0.04$