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Funsilab

UNIVERSITÄT DUISBURG ESSEN

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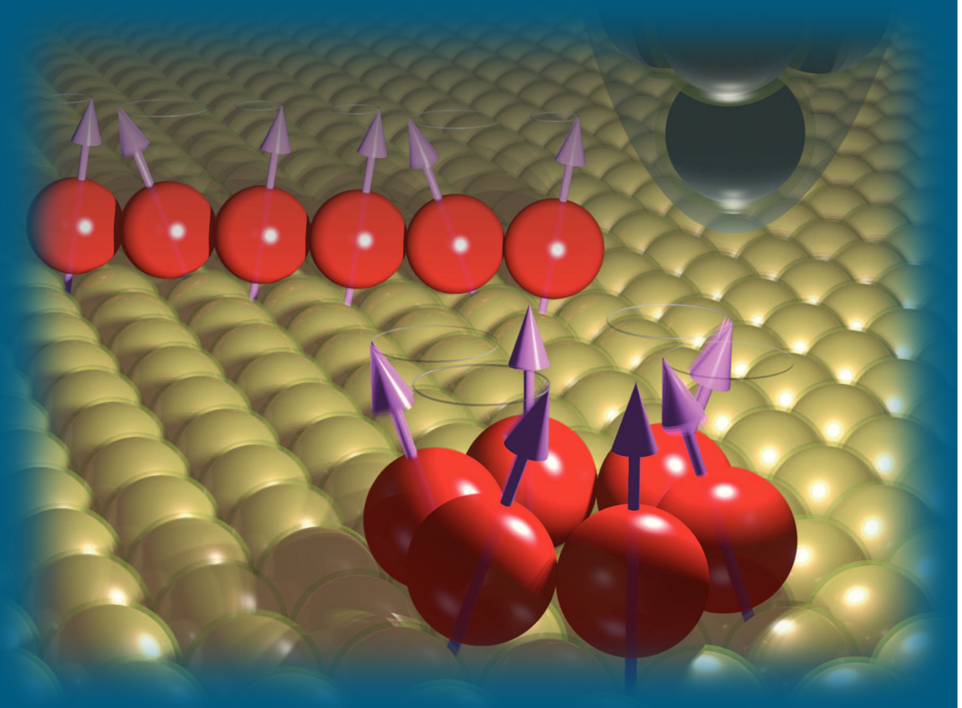
JÜLICH FORSCHUNGSZENTRUM

A new view on the origin of zero-bias anomalies of Co atoms atop noble metal surfaces

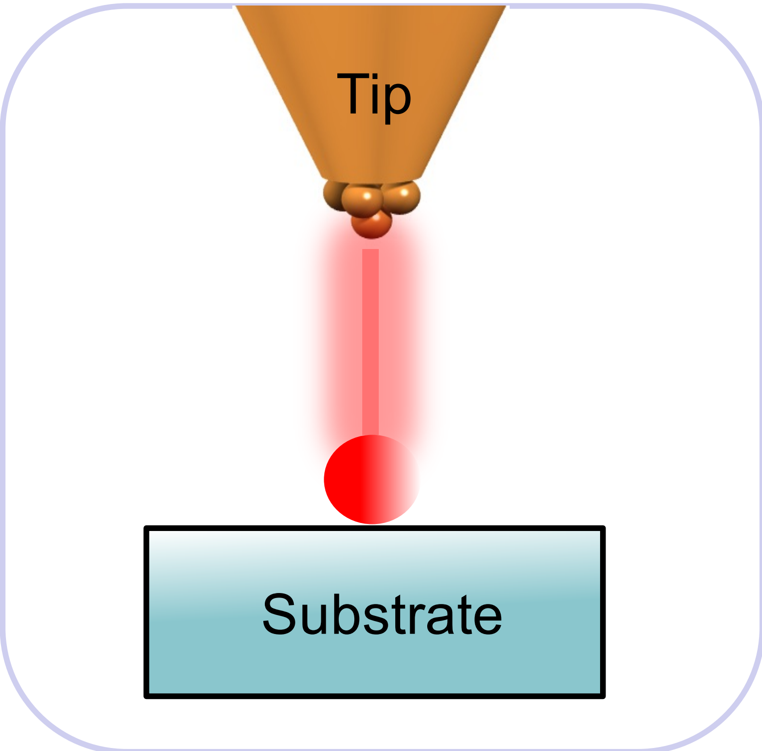
Samir Lounis

Faculty of Physics @UDE
Peter Grünberg Institut &
Institute for Advanced Simulation

18. Februar 2021



Scanning tunneling microscopy



Binnig and Rohrer,
1986 Nobel Prize

Tunneling current

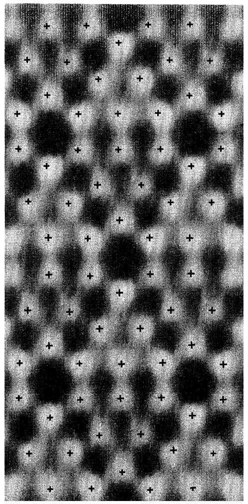
(Tersoff-Hamman, Fermi's golden rule)

$$\frac{\mathrm{d}I}{\mathrm{d}V}(\mathrm{V},\boldsymbol{r}_T)\sim n_T(E_F)\cdot n_S(E_F+\mathrm{eV},\boldsymbol{r}_T)$$

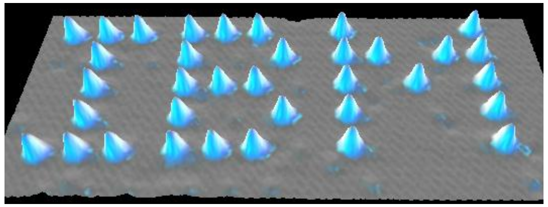
Tersoff and Hamann, Phys. Rev. Lett. 50, 1998 '83

Milestones

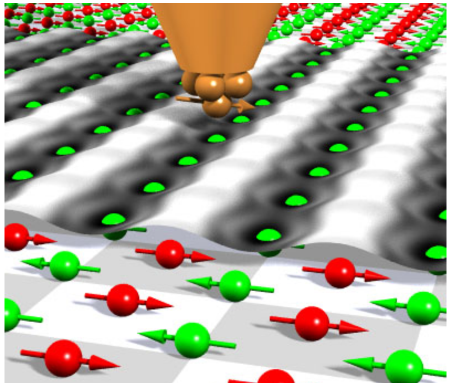
Binning et al.
PRL 50, 120 ‘83



D. Eigler & E.K. Schweizer,
Nature 344, 524 ‘90

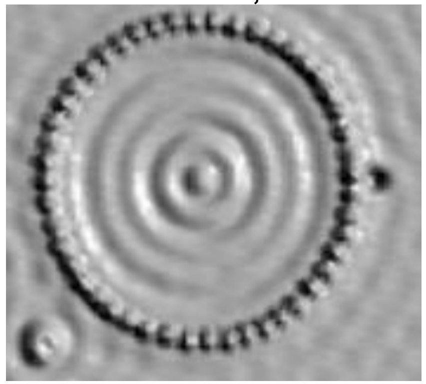


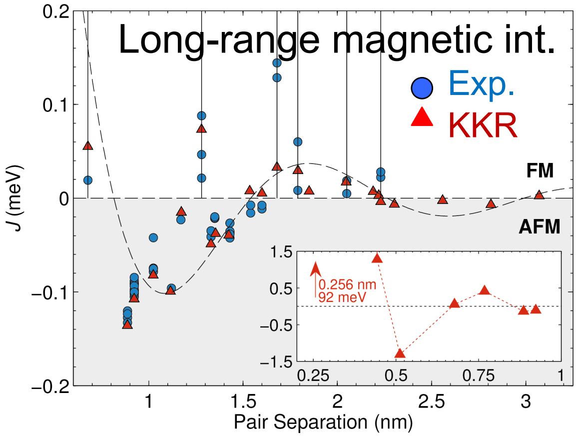
Heinze et al.
Science 288, 1805 ‘00



Wiesendanger et al.
PRL 65, 247 ’90

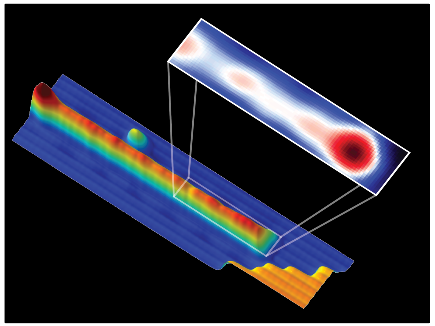
Crommie et al.
Science 262, 218 ‘93





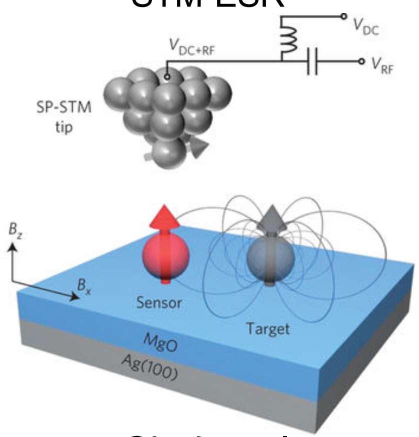
Zhou et al. Nat.Phys. 6, 187 ‘10
Khajetoorians et al. Nat.Phys. 8 497 ‘12

Superconductors & Majorana



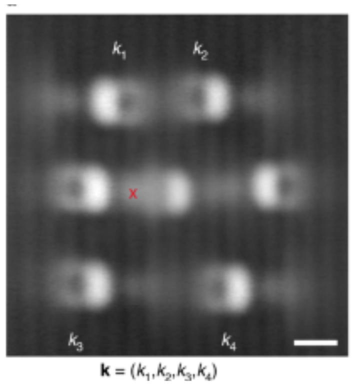
Nadj-Perge et al.
Science 346, 6209‘14

STM-ESR



Choi et al.
Nat. Nano. 12, 420 ‘17

Adatom-synapses

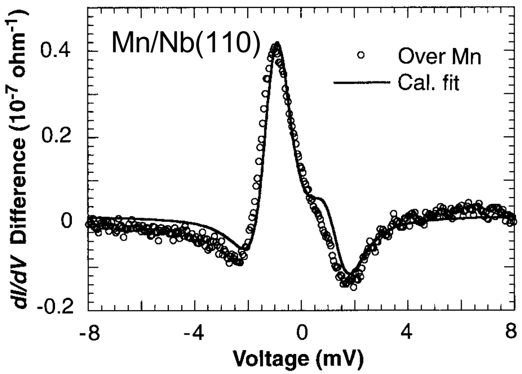


Kiraly et al.
Nat. Nano. ‘21

Low-energy anomalies

Probing the Local Effects of Magnetic Impurities on Superconductivity

Ali Yazdani,* B. A. Jones, C. P. Lutz, M. F. Crommie,†
D. M. Eigler



Science **275**, 1767 ‘97

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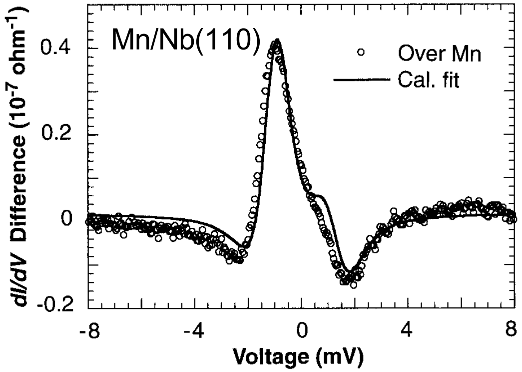
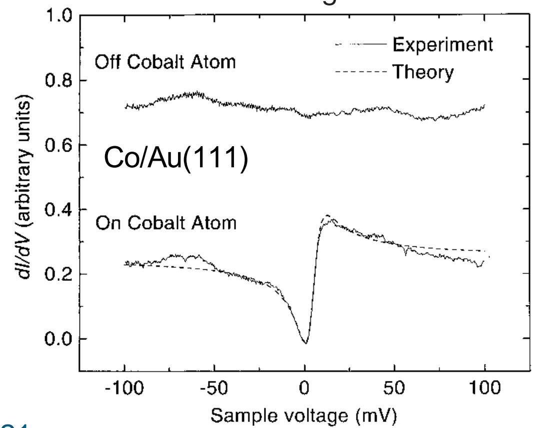


Science **275**, 1767 ‘97

Tunneling into a Single Magnetic Atom: Spectroscopic Evidence of the Kondo Resonance

V. Madhavan, W. Chen, T. Jamneala, M. F. Crommie, N. S. Wingreen



Science **280**, 567 ‘98

Low-energy anomalies

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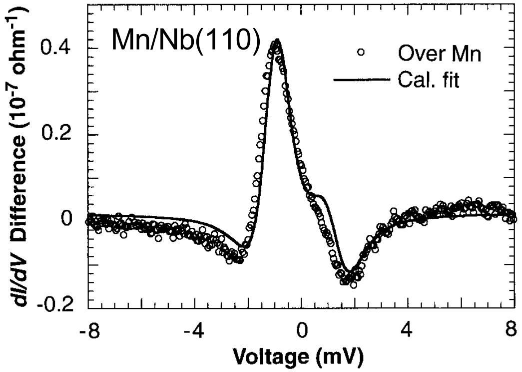

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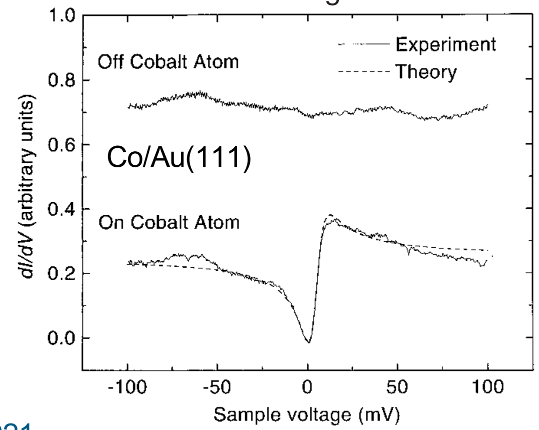
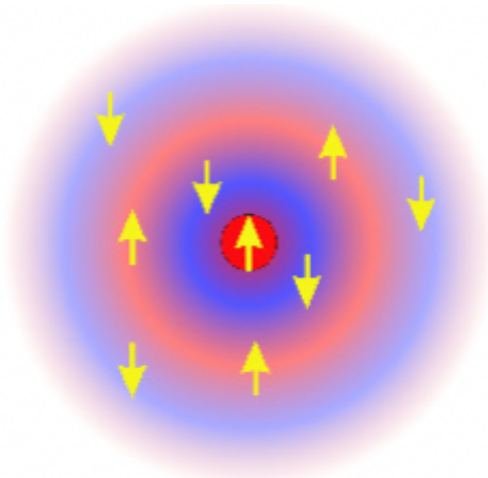
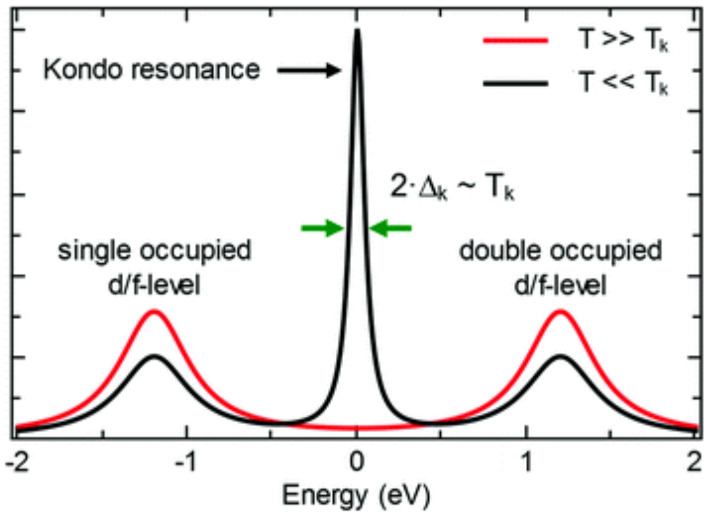


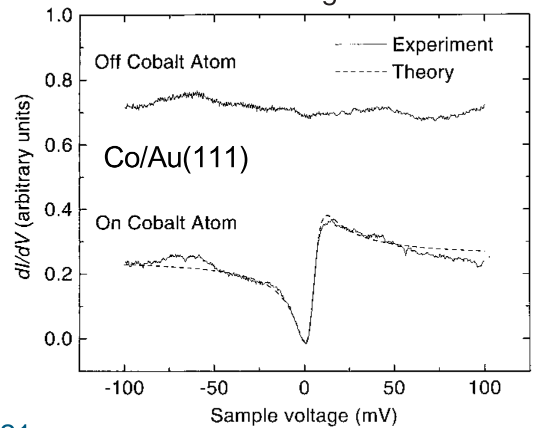
Science **280**, 567 ‘98



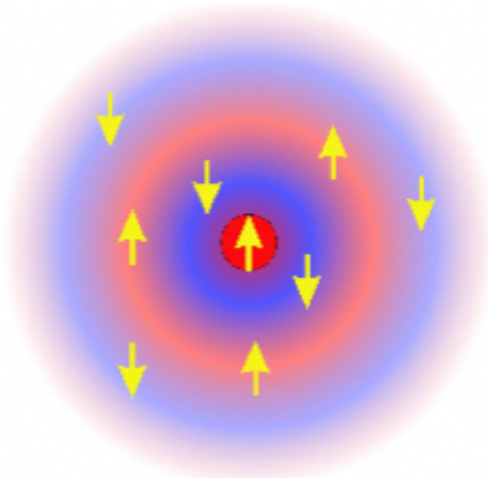
Low-energy anomalies



Courtesy of H. Prüser



Science **280**, 567 ‘98



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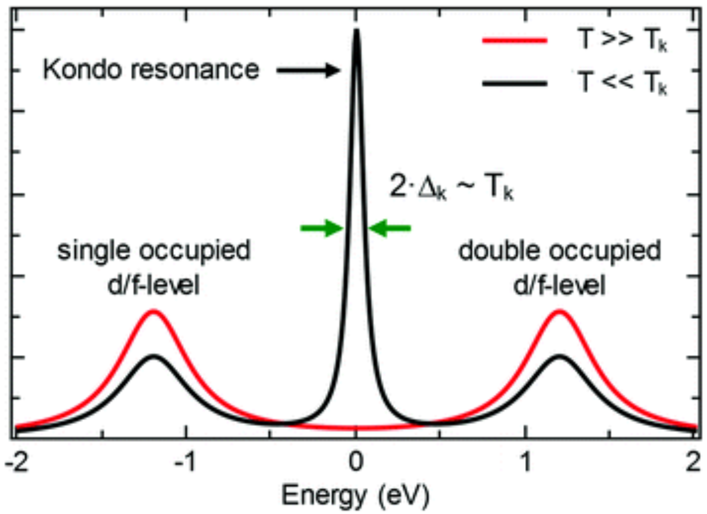

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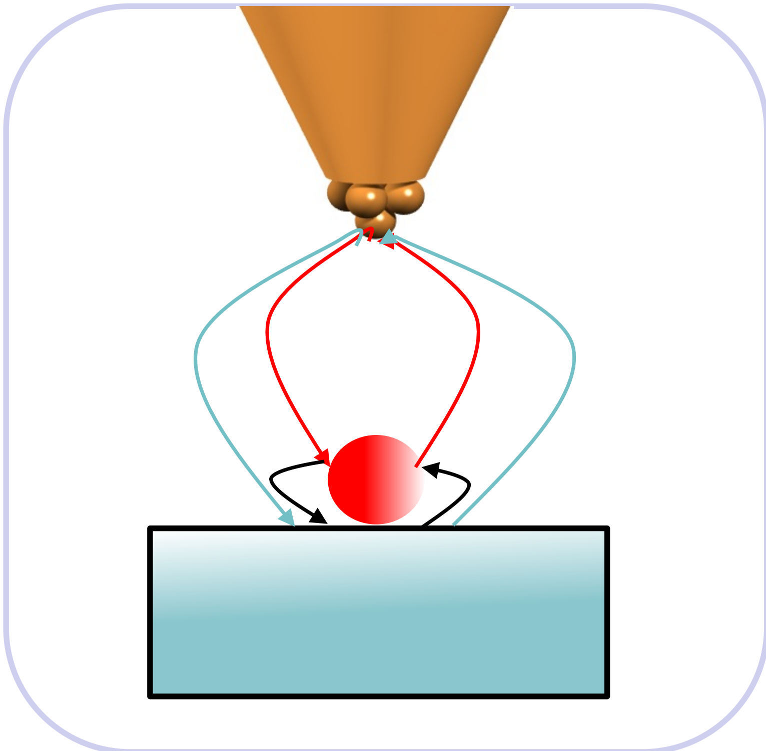

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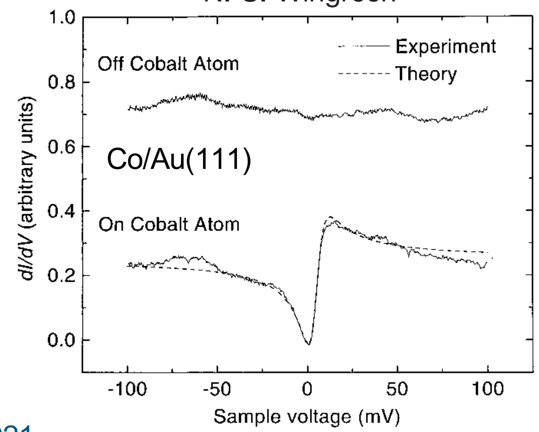
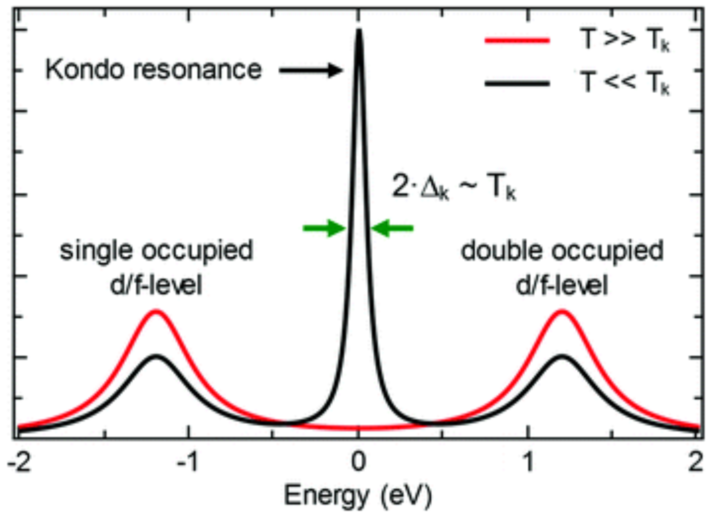


Science **280**, 567 ‘98

Low-energy anomalies



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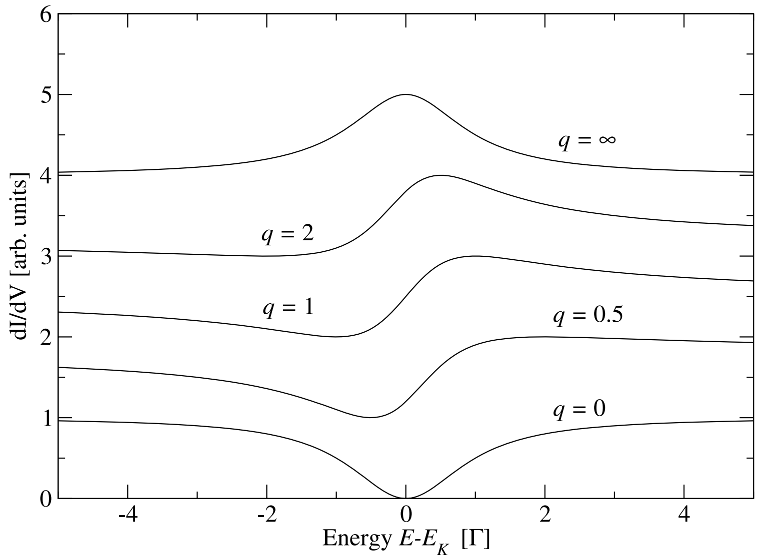

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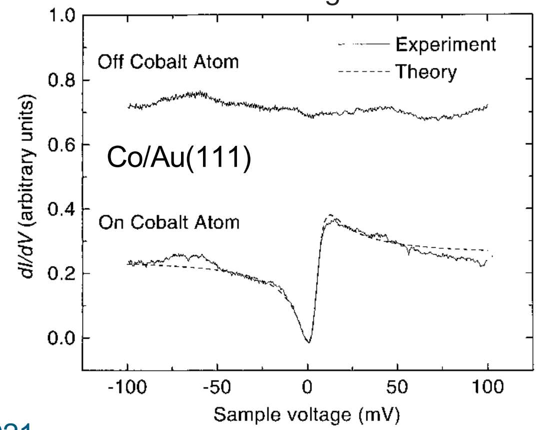

Science **280**, 567 '98

Fano-resonance:

$$n_v(\varepsilon) = A\frac{(\varepsilon + q)^2}{\varepsilon^2 + 1}$$

$$\varepsilon = \frac{\mathrm{eV} - E_0}{k_B T_K}$$

$k_B T_K \approx 5.8\ \mathrm{meV}$ $\quad E_0 \approx 6.5\ \mathrm{meV}$ $\quad q \approx 0.6$

$T_K \approx 70\ \mathrm{K}$

Low-energy anomalies

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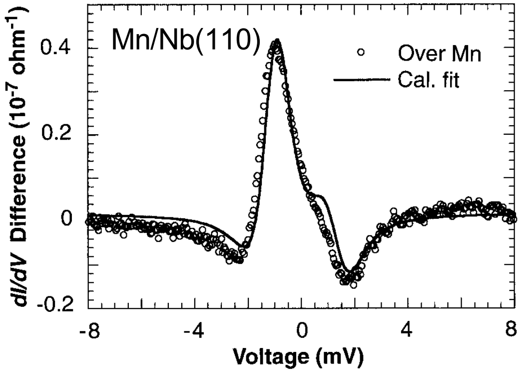
Ali Yazdani,* B. A. Jones, C. P. Lutz, M. F. Crommie,† D. M. Eigler



Science **275**, 1767 '97

Tunneling into a Single Magnetic Atom: Spectroscopic Evidence of the Kondo Resonance

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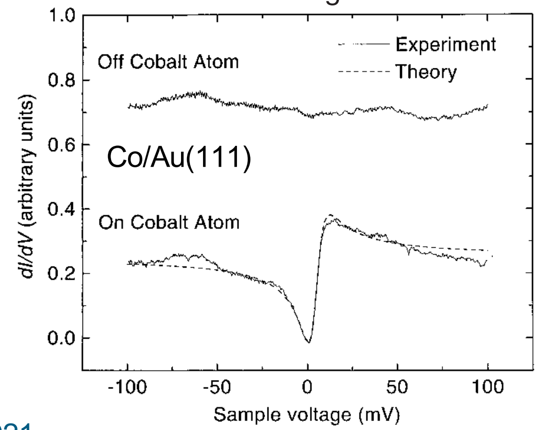

Science **280**, 567 '98

An alternative explanation for the resonance shown in Fig. 2 is that it is not a Kondo resonance but is due to tunneling into a "bare" *d* resonance that happens to lie at E_F. We believe that this is not the case for two reasons. (i) Photoemission results imply that the 3*d* state of Co deposited onto Au(111) does not lie right at E_F, but rather 0.8 eV below it (*23*). (ii) The width of the resonance observed here (only 11 meV) is much narrower than the typical width of a bare *d* resonance. A *d* resonance usually measures hundreds of millielectron volts in width (*3*, *24–26*) [even for an adsorbate (*17*, *27*)], whereas the Kondo resonance, a collective effect, is expected to have a much narrower width (on the order of $k_B T_K$).

Low-energy anomalies

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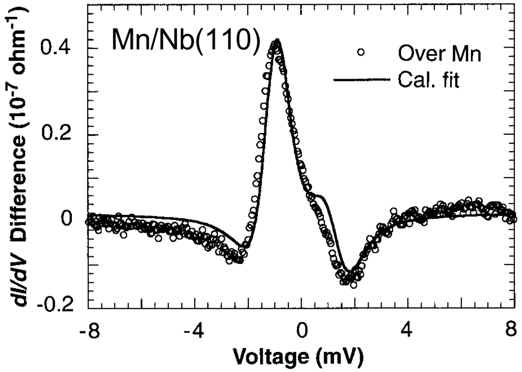
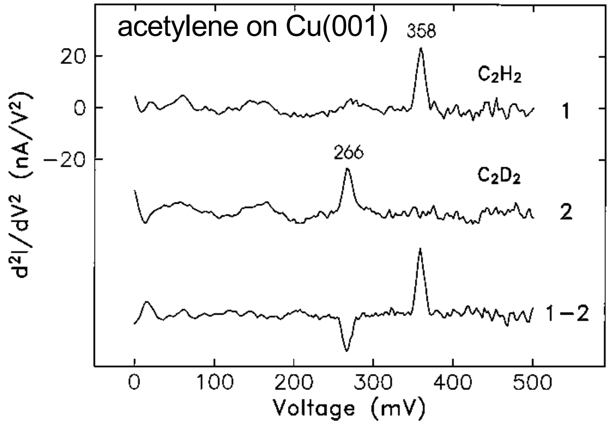


Science **275**, 1767 ‘97

Single-Molecule Vibrational Spectroscopy and Microscopy

B. C. Stipe, M. A. Rezaei, W. Ho*



Science **280**, 1732 ‘98

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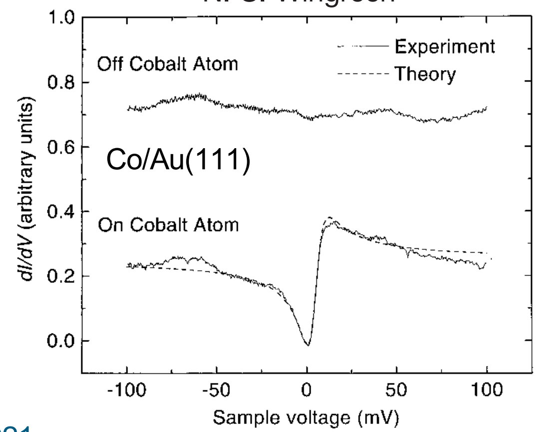
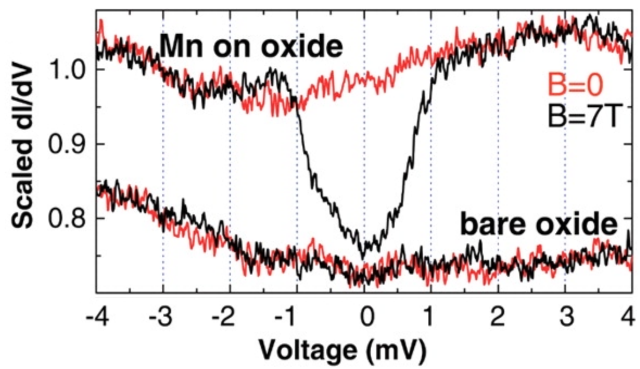
V. Madhavan, W. Chen, T. Jamneala, M. F. Crommie, N. S. Wingreen



Science **280**, 567 ‘98

Single-Atom Spin-Flip Spectroscopy

A. J. Heinrich,* J. A. Gupta, C. P. Lutz, D. M. Eigler



Science **306**, 446 ‘04

Low-energy anomalies

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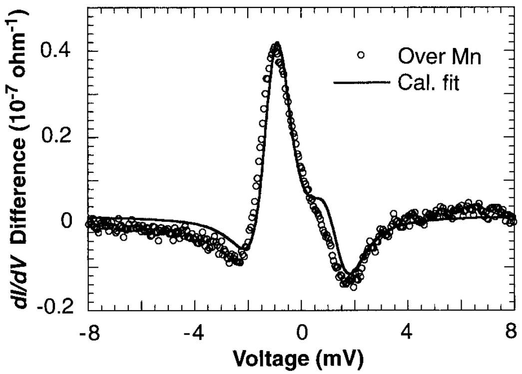

Science **275**, 1767 ‘97

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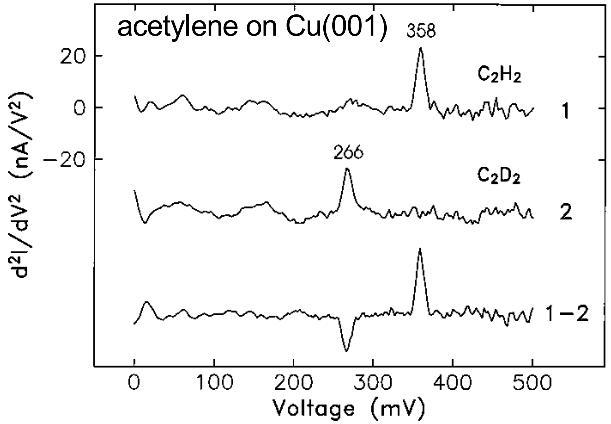

Science **280**, 1732 ‘98

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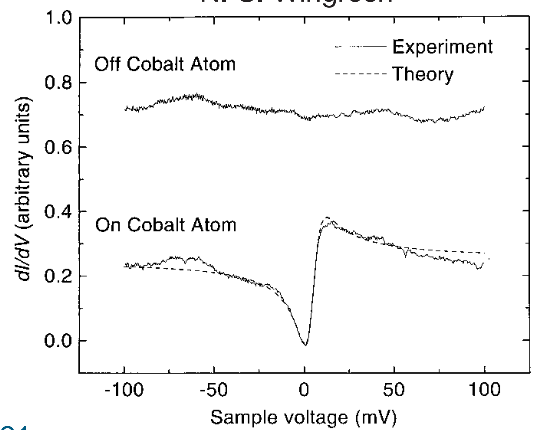
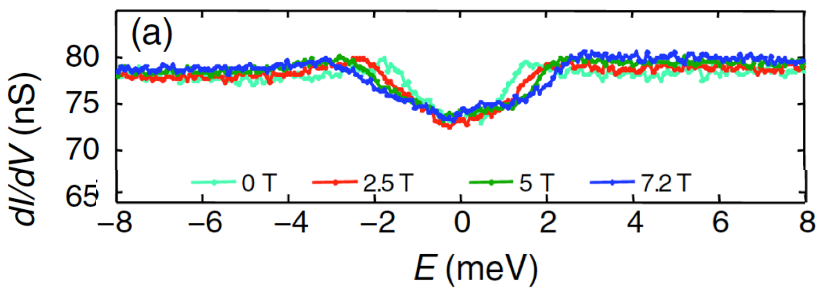


Science **280**, 567 ‘98

ISTS for Fe adatom on Cu(111)

A. A. Khajetoorians, S. Lounis, B. Chilian, A. T. Costa,
B. L. Zhou, D. L. Mills, J. Wiebe, and R. Wiesendanger



PRL **106**, 037205 ‘11

Gapped spin-excitations instead of Kondo

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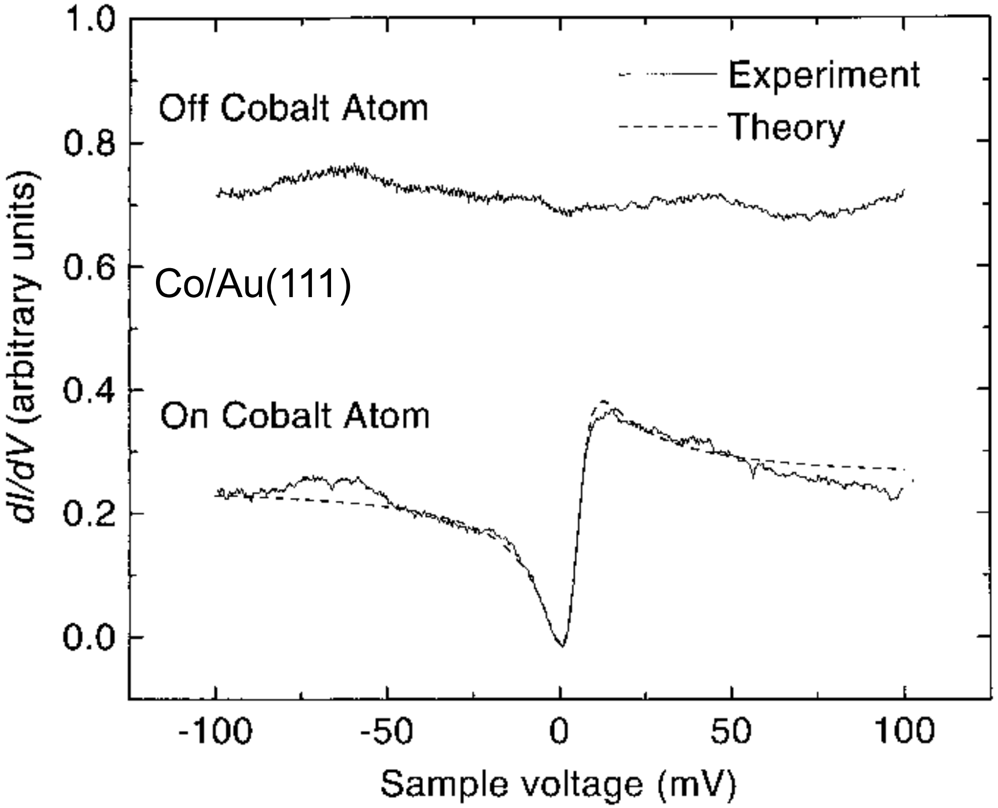
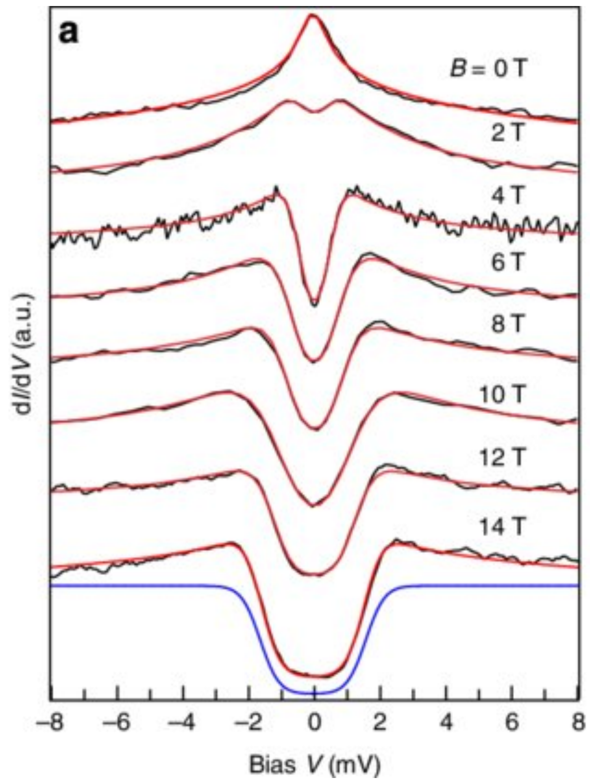


Science **280**, 567 ‘98

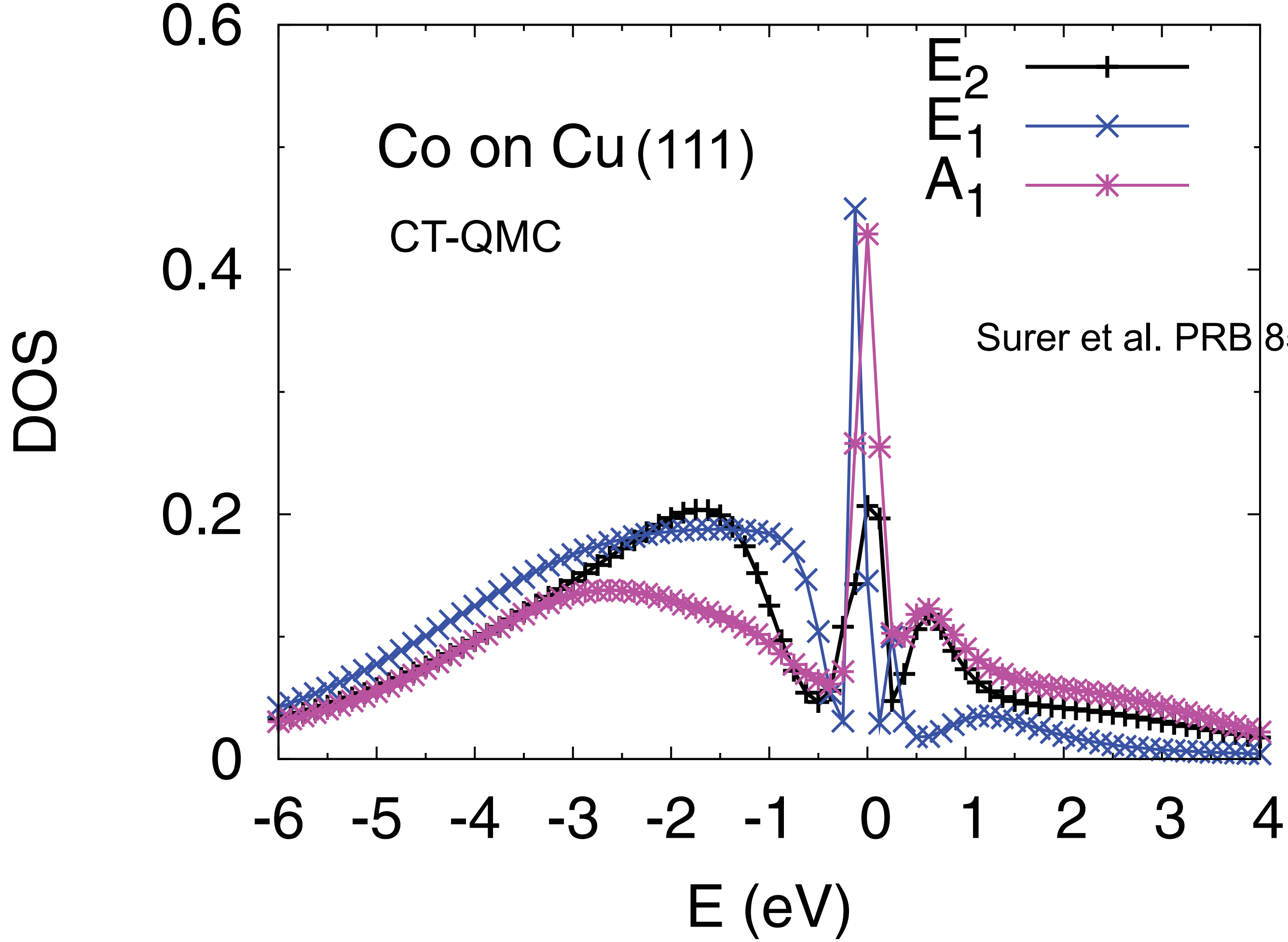
Molecule on Au(111)

$C_{28}H_{25}O_2N_4$



Zhang et al.
Nat. Commun. **4**, 2110 ‘13

Ab-initio treatment



Surer et al. PRB 85, 085114 ‘12

Baruselli et al. PRB 92, 045119 ‘15

Jacob, J. Phys. Cond. Matt. 27, 245606 ‘15

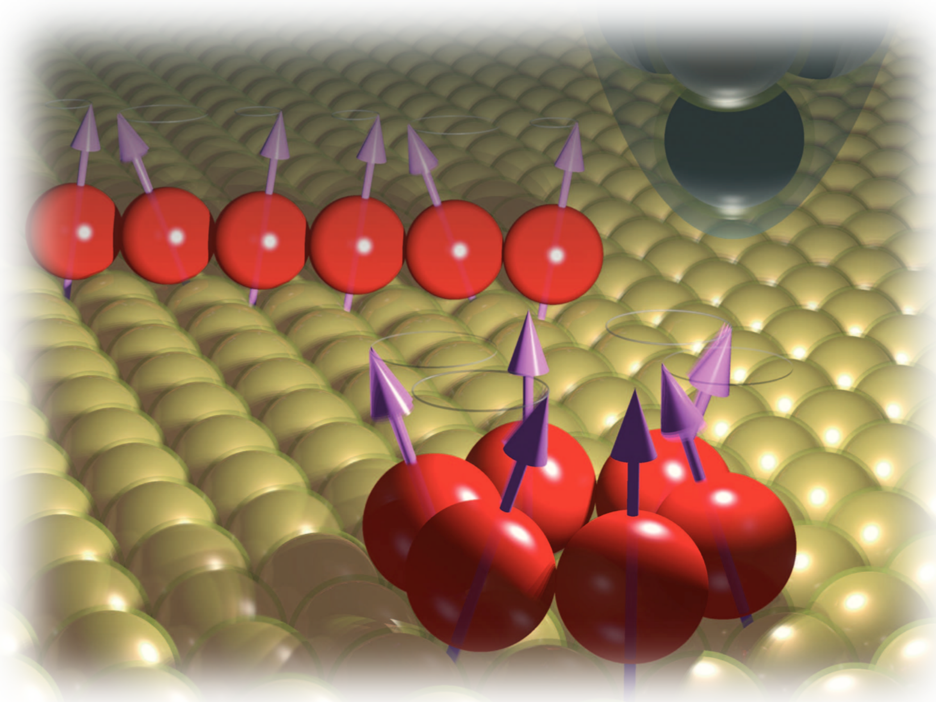
Dang et al. PRB 93, 115123 ‘16

Valli et al. PRR 2, 033432 ‘20

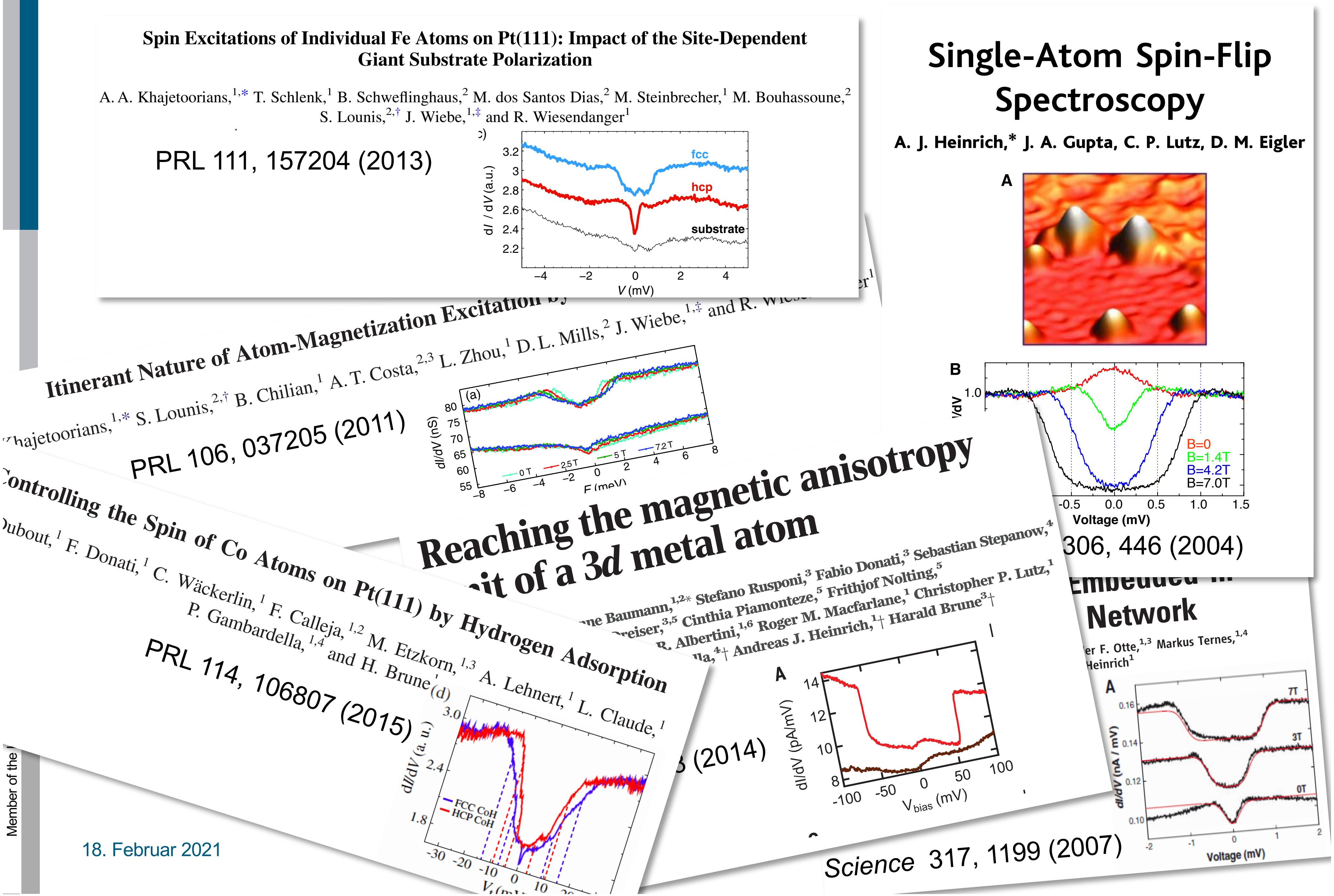
Outline

- Introduction
- Description of formalism for conventional spin-excitations
- Zero-bias anomalies
- Conclusions

Formalism for description of spin-excitations & Basics



Experimental access of spin-excitations



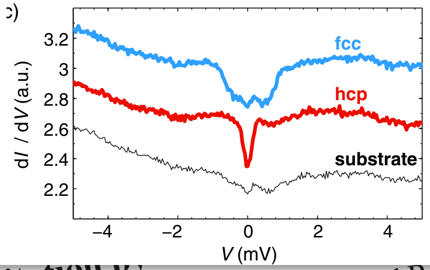
Experimental access of spin-excitations

JÜLICH
FORSCHUNGSZENTRUM

Spin Excitations of Individual Fe Atoms on Pt(111): Impact of the Site-Dependent Giant Substrate Polarization

A. A. Khajetoorians,[1,*] T. Schlenk,[1] B. Schweflinghaus,[2] M. dos Santos Dias,[2] M. Steinbrecher,[1] M. Bouhassoune,[2] S. Lounis,[2,†] J. Wiebe,[1,‡] and R. Wiesendanger[1]

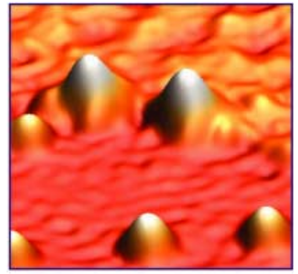
PRL 111, 157204 (2013)



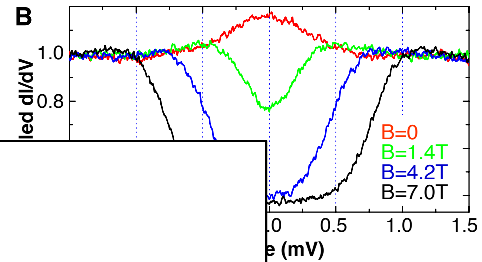
Single-Atom Spin-Flip Spectroscopy

A. J. Heinrich,* J. A. Gupta, C. P. Lutz, D. M. Eigler

A



B

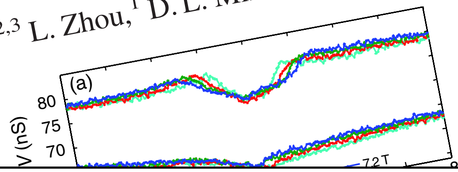


446 (2004)

Itinerant Nature of Atom-Magnetization Excitation by ...

...hajetoorians,[1,*] S. Lounis,[2,†] B. Chilian,[1] A. T. Costa,[2,3] L. Zhou,[1] D. L. Mills,[2] J. Wiebe,[1,‡] and R. Wie...

PRL ... 037205 (2011)



Controlling the Spi...

...ubout,[1] F. Donati,[1] C. ...

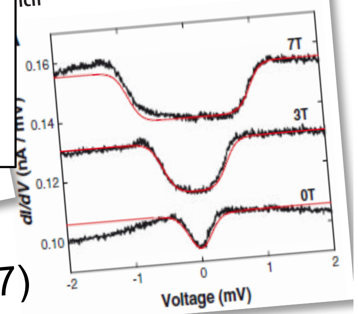
PR...

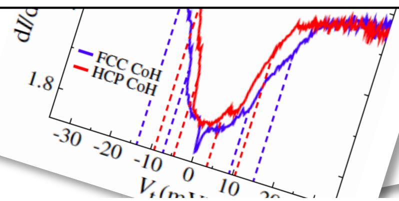
Theory

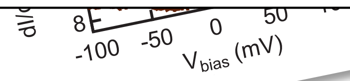
- Fernandez-Rossier, PRL 102, 256802 '09
- Lorente, Gauyacq, PRL 103, 176601 '09
- Fransson, Nanoletters 9, 2414 '09
- Sothmann, König, New J. Phys. 12 083028 '10

...etwork

...Otte,[1,3] Markus Ternes,[1,4] ...ich[1]



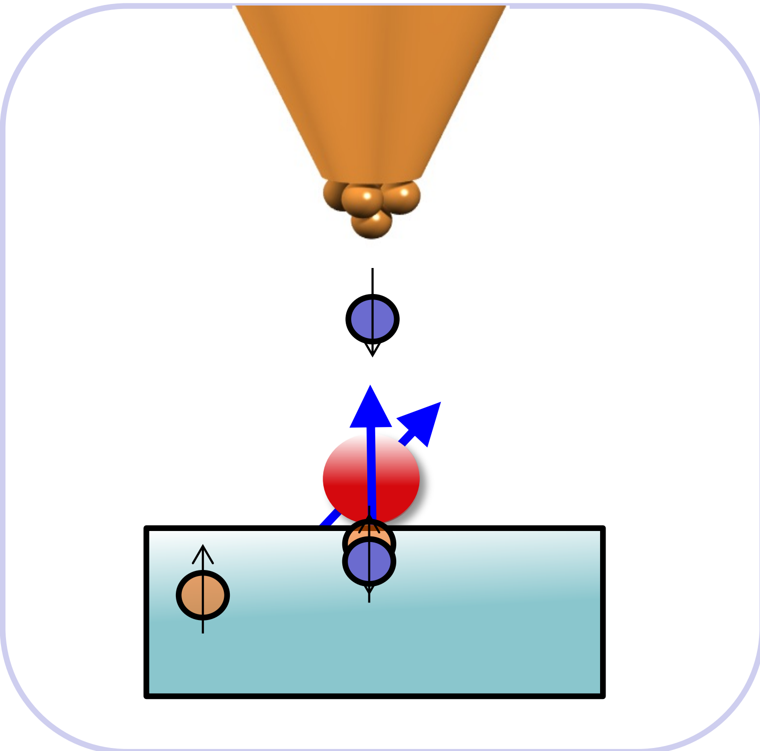


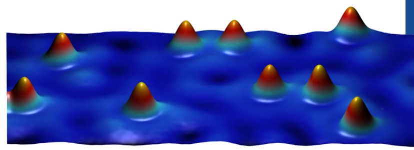


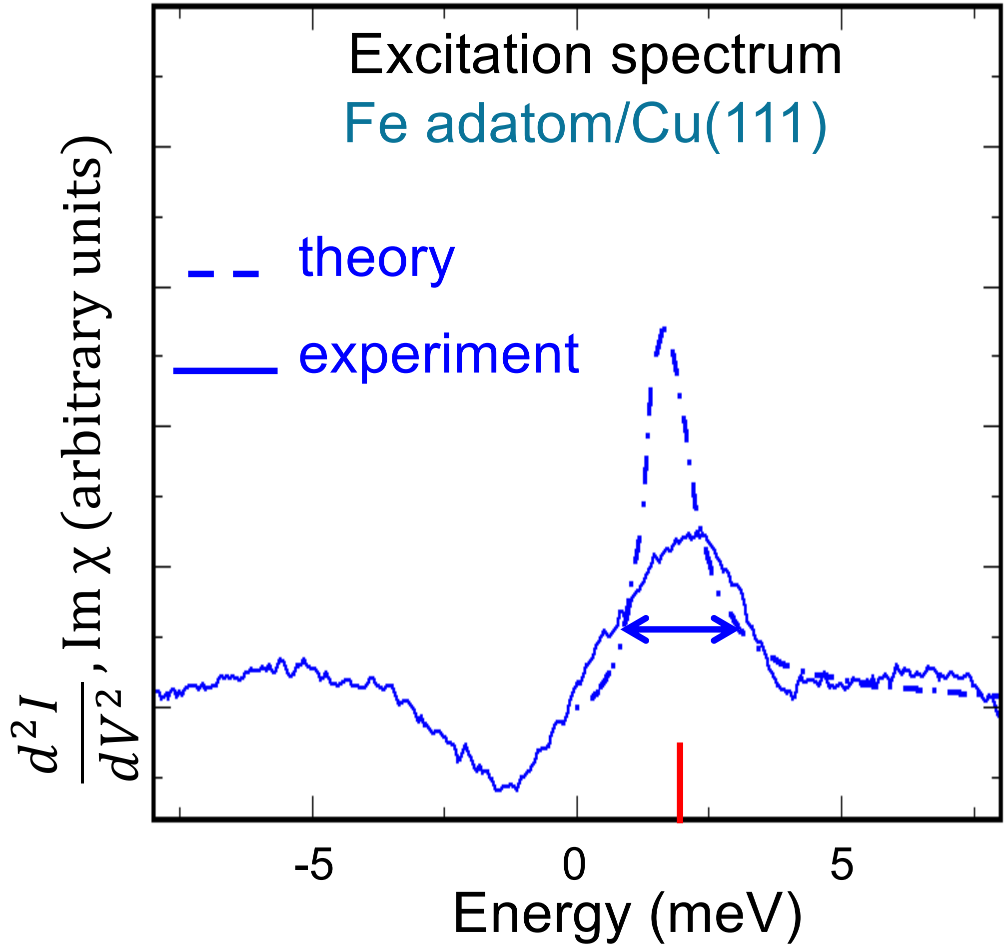
Science 317, 1199 (2007)

Lifetime limitation–Interactions by conduction electrons

Inelastic Scanning Tunneling Microscopy







Lifetime = couple of hundred femtosec

- Lounis et al., PRL '10 & PRB '11 & '14
- Khajetoorians, Lounis, et al. PRL '11

Theoretical framework I

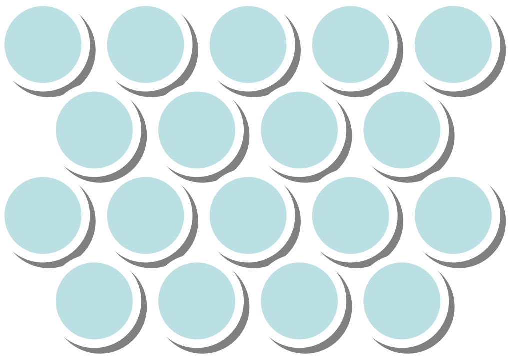
JÜLICH FORSCHUNGSZENTRUM

UNIVERSITÄT DUISBURG ESSEN

Offen im Denken

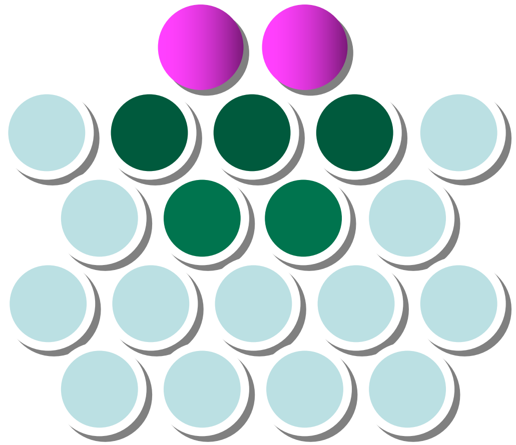
Ground state properties

G_0



Crystal surface

G



Cluster on surface

Dyson eq.: Reference system → New system

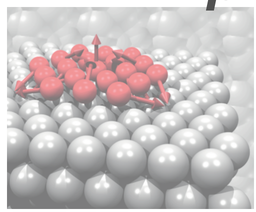
$$G(E) = G_0(E) + G_0(E)V\,G(E)$$

$$n(E) = -1/\pi \,\mathrm{Im}\, G(E)$$

No periodic supercell needed

Takes into account the infinite system

KKRimp



Korringa-Kohn-Rostoker Green function method / DFT

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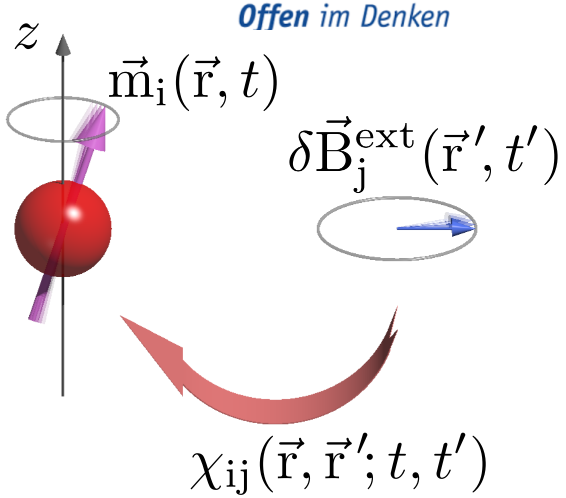
Theoretical framework II

Intrinsic spin-excitations



- Probe response functions: Output = χ * Input
- Information on spin-excitations encoded in $\mathrm{Im}\,\chi$:
  Density of Spin Excitation States

TT sector [meV]

TL sector

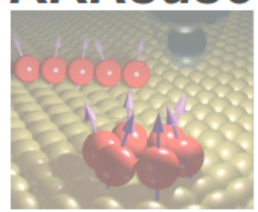
[eV] LL sector

$$\chi = \begin{bmatrix} \boxed{\begin{matrix} \chi_{xx} & \chi_{xy} \\ \chi_{yx} & \chi_{yy} \end{matrix}} & \boxed{\begin{matrix} \chi_{xz} & \chi_{x0} \\ \chi_{yz} & \chi_{y0} \end{matrix}} \\ \boxed{\begin{matrix} \chi_{zx} & \chi_{zy} \\ \chi_{0x} & \chi_{0y} \end{matrix}} & \boxed{\begin{matrix} \chi_{zz} & \chi_{z0} \\ \chi_{0z} & \chi_{00} \end{matrix}} \end{bmatrix}$$

- Lounis et al., PRL '10
- Lounis et al., PRB '11
- Lounis et al., Surf. Sc. '14
- Lounis et al., PRB. '15
- dS Dias et al., PRB '15

Challenges:
SOC + non-col.

KKRsusc



Korringa-Kohn-Rostoker Green function method / TD-DFT

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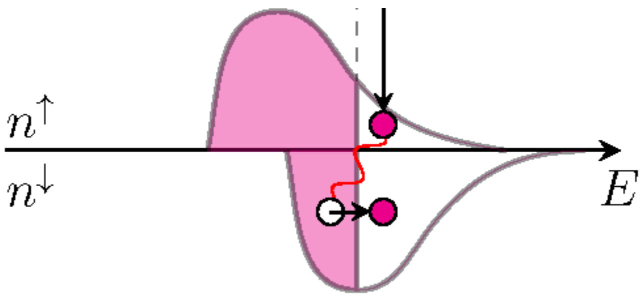
Theoretical framework II

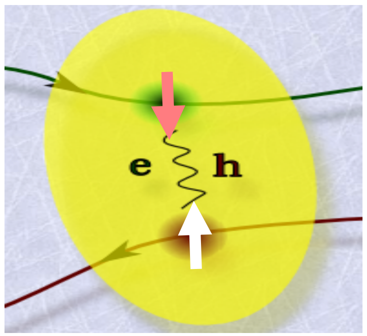
Intrinsic spin-excitations

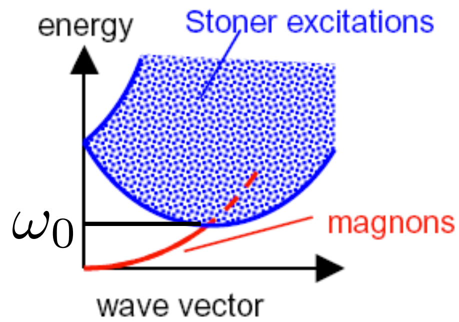
In practice use of Dyson-like equation

$$\chi(\omega) = \frac{\chi_{KS}(\omega)}{1 - K_{xc}(\omega)\chi_{KS}(\omega)} \qquad \mathrm{Im}\,\chi(\omega) = \frac{\mathrm{Im}\,\chi_{KS}(\omega)}{(1 - K_{xc}\,\mathrm{Re}\,\chi_{KS}(\omega))^2 + (K_{xc}\,\mathrm{Im}\,\chi_{KS}(\omega))^2}$$

$$\chi_{KS}^{ij,\alpha\beta}(\vec{r},\vec{r}';\omega) = -\frac{1}{\pi}\int dz f(z)\mathrm{Tr}(\sigma^\alpha G_{ij}(\vec{r},\vec{r}';z+\omega)\sigma^\beta\,\mathrm{Im}\,G_{ji}(\vec{r}',\vec{r};z)$$
$$+\sigma^\alpha\,\mathrm{Im}\,G_{ij}(\vec{r},\vec{r}';z)\sigma^\beta G_{ji}^{-}(\vec{r}',\vec{r};z-\omega))$$



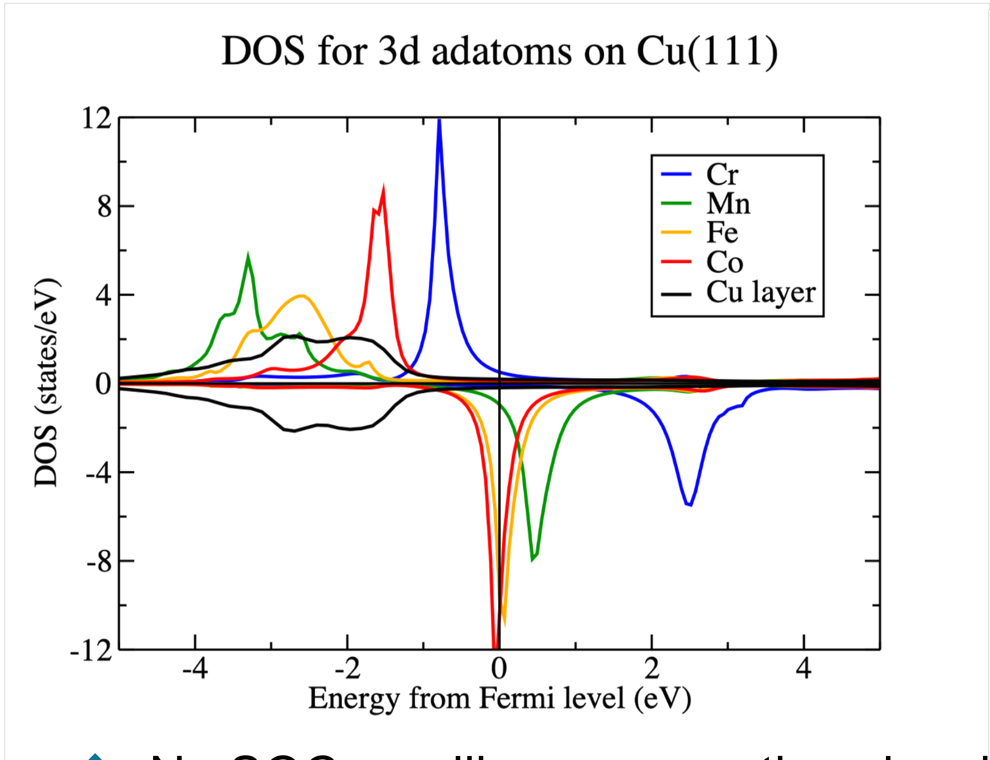


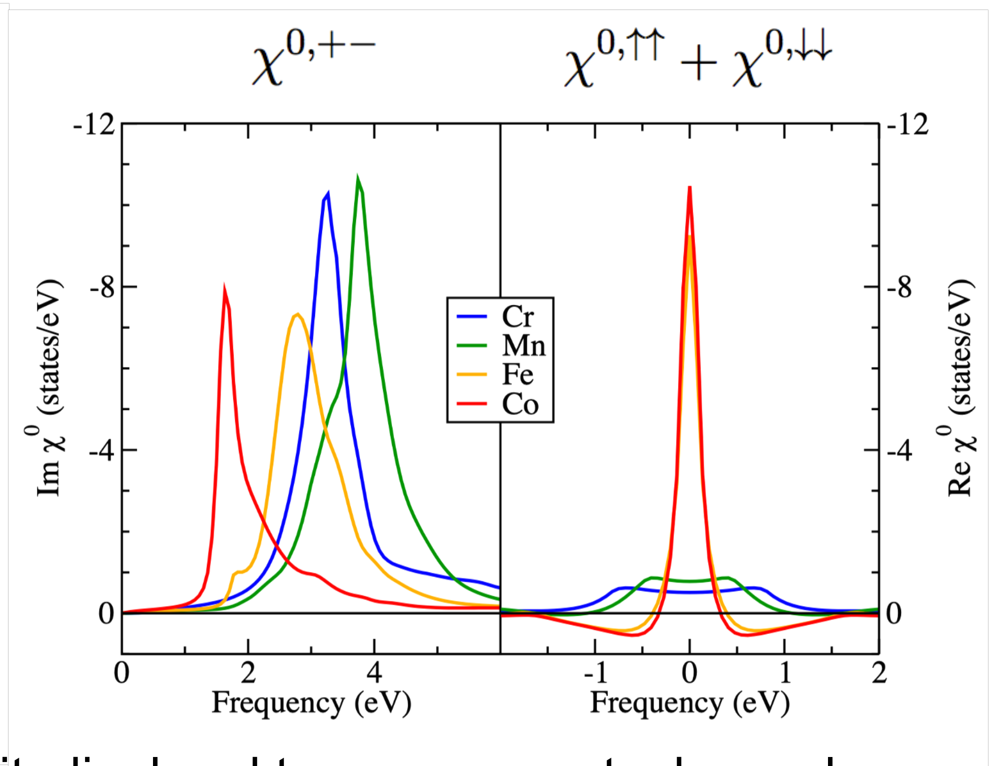


Theoretical framework II

Intrinsic spin-excitations

Kohn-Sham susceptibility without SOC





- No SOC + collinear magnetism: longitudinal and transverse parts decouple

$$\chi^0 \equiv \begin{pmatrix} 0 & \chi^{0,+-} & 0 & 0 \\ \chi^{0,-+} & 0 & 0 & 0 \\ 0 & 0 & \chi^{0,\uparrow\uparrow} & 0 \\ 0 & 0 & 0 & \chi^{0,\downarrow\downarrow} \end{pmatrix}, \quad \mathcal{K} \equiv \begin{pmatrix} 0 & \mathcal{K}^{\mathrm{T}} & 0 & 0 \\ \mathcal{K}^{\mathrm{T}} & 0 & 0 & 0 \\ 0 & 0 & \mathcal{K}^{\mathrm{H}} + \mathcal{K}^{\mathrm{xc},\uparrow\uparrow} & \mathcal{K}^{\mathrm{xc},\uparrow\downarrow} \\ 0 & 0 & \mathcal{K}^{\mathrm{xc},\downarrow\uparrow} & \mathcal{K}^{\mathrm{H}} + \mathcal{K}^{\mathrm{xc},\downarrow\downarrow} \end{pmatrix}$$

Dynamical transverse magnetic susceptibility

KKRsusc

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Challenge:

- Energies of interest (meV) vs Error in well converged calculation (meV)

$$\begin{pmatrix} G^{\uparrow\uparrow} & \cancel{G^{\uparrow\downarrow}} \\ \cancel{G^{\downarrow\uparrow}} & G^{\downarrow\downarrow} \end{pmatrix}$$

Solution: Key relation: spin density sum rule

- No SOC: magnetization sum rule ➔ existence of Goldstone mode

$$\boxed{m_z^i(\vec{r}) = \int d\vec{r}\,'\chi_{KS}^{ij}(\vec{r},\vec{r}\,';0)B_{xc}^j(\vec{r}\,')} \equiv \frac{2}{\pi}\,\mathrm{Im}\int^{E_F} dE\; G^{\downarrow\downarrow}(\vec{r},\vec{r}\,';E)\underline{B_{xc}^j(\vec{r}\,')}G^{\uparrow\uparrow}(\vec{r}\,',\vec{r};E)$$

- Mathematically true for the ALDA kernel – has to be enforced numerically

Lounis, Costa, Muniz, Mills, PRL 2010 & PRB 2011

- With SOC: magnetization sum rule ➔ No Goldstone mode

New:

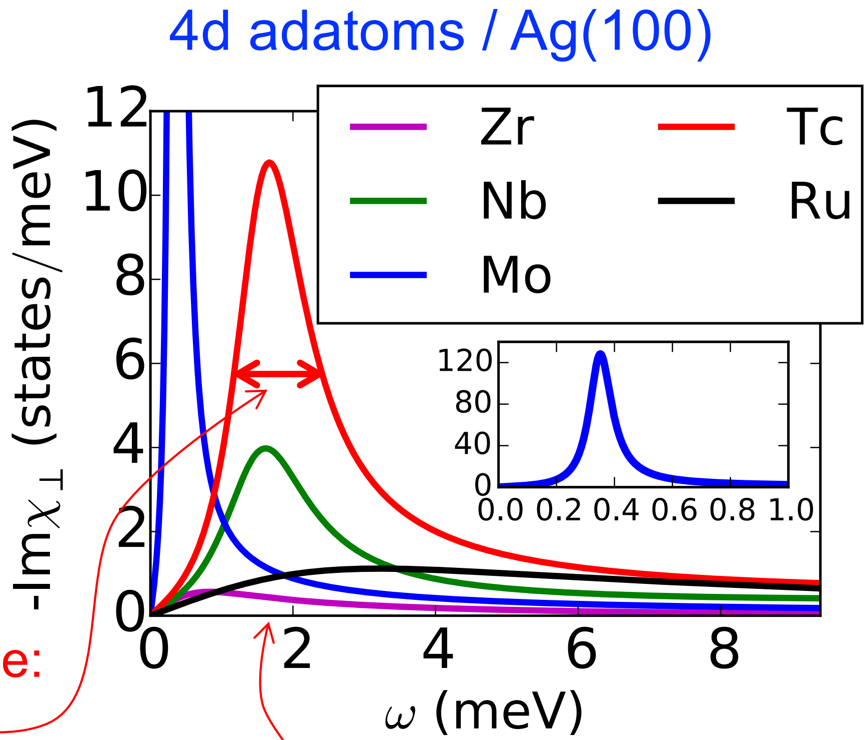
$$G^{\uparrow\uparrow}(\vec{r},\vec{r}\,';E) - G^{\downarrow\downarrow}(\vec{r},\vec{r}\,';E) = \int\!\!\int d\vec{r}_1\, d\vec{r}_2\, G^{\downarrow\downarrow}(\vec{r},\vec{r}_1;E)\underline{\Delta(\vec{r}_1,\vec{r}_2;E)}G^{\uparrow\uparrow}(\vec{r}_2,\vec{r}\,';E)$$

$$\Delta(\vec{r}_1,\vec{r}_2;E) = 2\left(B_{xc}(\vec{r}_1) + \xi(\vec{r}_1)L^z\right)\delta(\vec{r}_1 - \vec{r}_2)$$
$$+\xi(\vec{r}_1)L^-\tilde{G}^{\downarrow}(\vec{r}_1,\vec{r}_2;E)L^+\xi(\vec{r}_2) - \xi(\vec{r}_1)L^+\tilde{G}^{\uparrow}(\vec{r}_1,\vec{r}_2;E)L^-\xi(\vec{r}_2)$$

dos Santos Dias, Schweflinghaus, Blügel, Lounis, PRB (2015)

s.lounis@fz-juelich.de

Density of Spin Excitation States: Dissection



Linewidth / lifetime:
e-h excitations

Resonance energy:
Magnetic anisotropy energy ~ $2\gamma \frac{\mathrm{MAE}}{M_s}$

Azpiroz, dos Santos Dias, Blügel, Lounis, Nanoletters (2016)

Density of Spin Excitation States: Dissection

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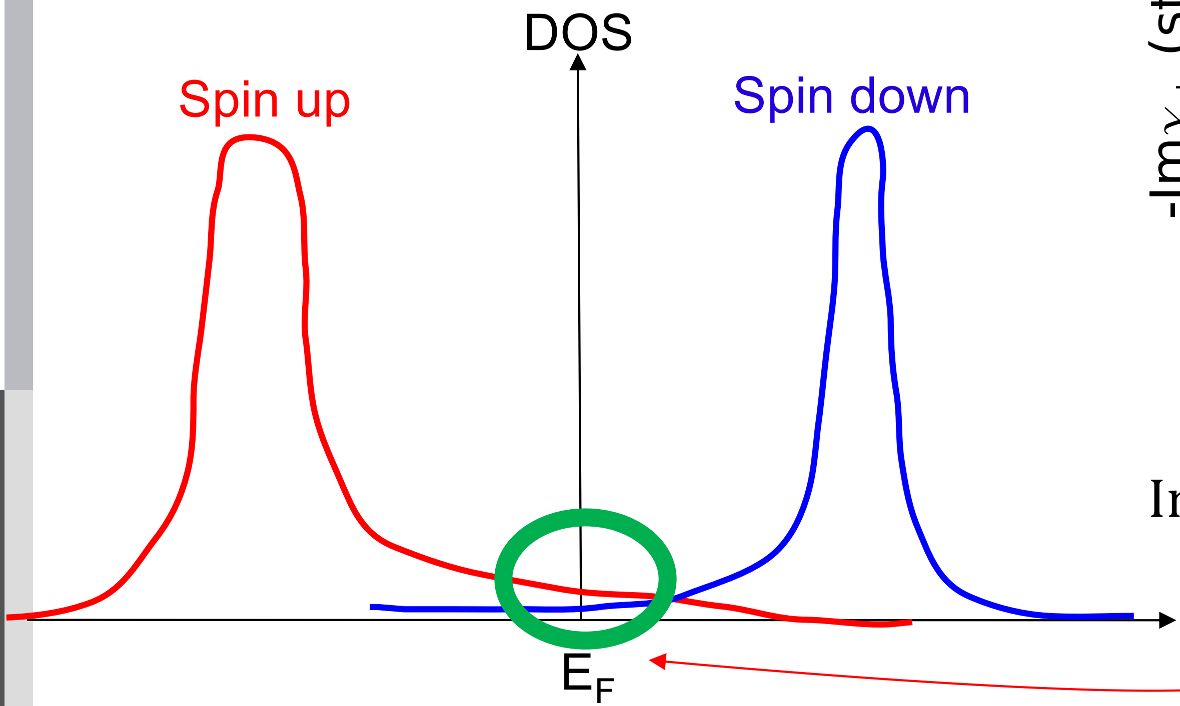
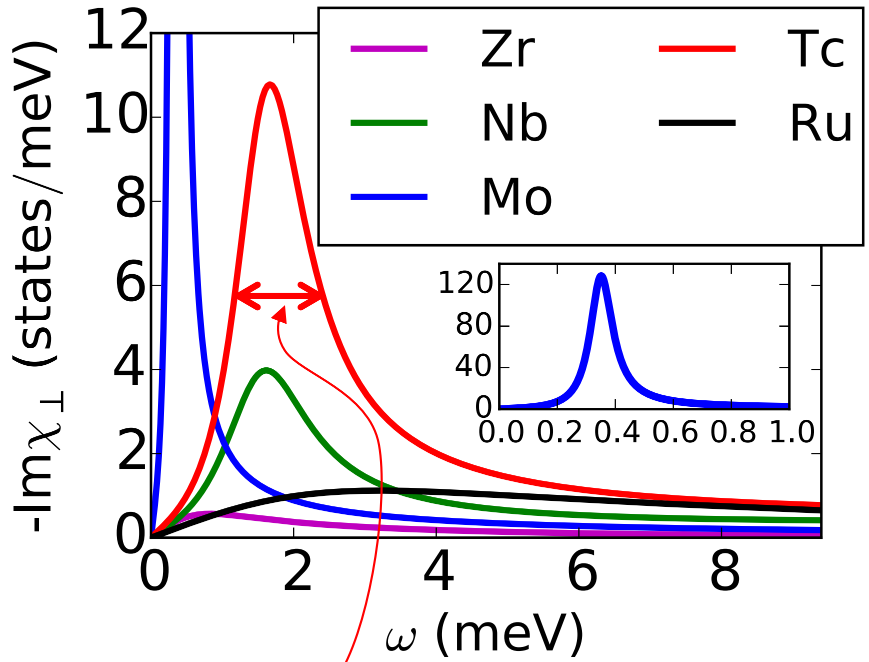
Link to electronic structure



4d adatoms / Ag(100)



$$\mathrm{Im}\,\chi_{KS}(\omega) \sim -\pi\, n_{\uparrow}(E_F)\, n_{\downarrow}(E_F)\,\omega$$

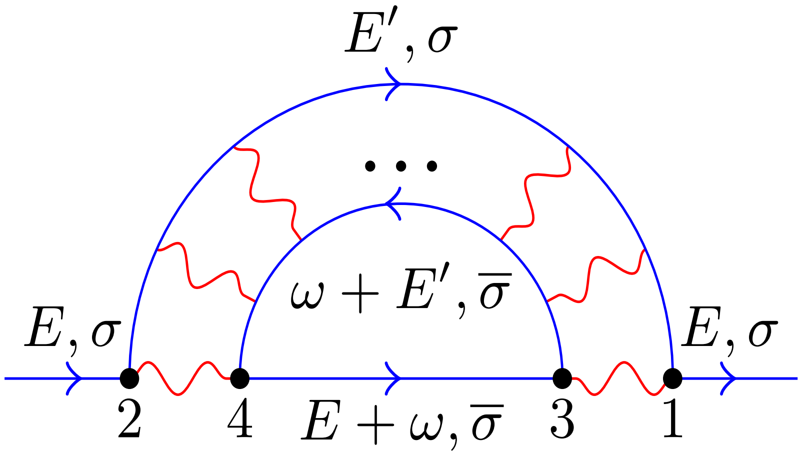
- Lounis et al., PRL. (2010)
- Lounis et al., PRB (2011)
- Lounis et al. PRB (2015)
- Guimaraes et al. JPCM (2019)

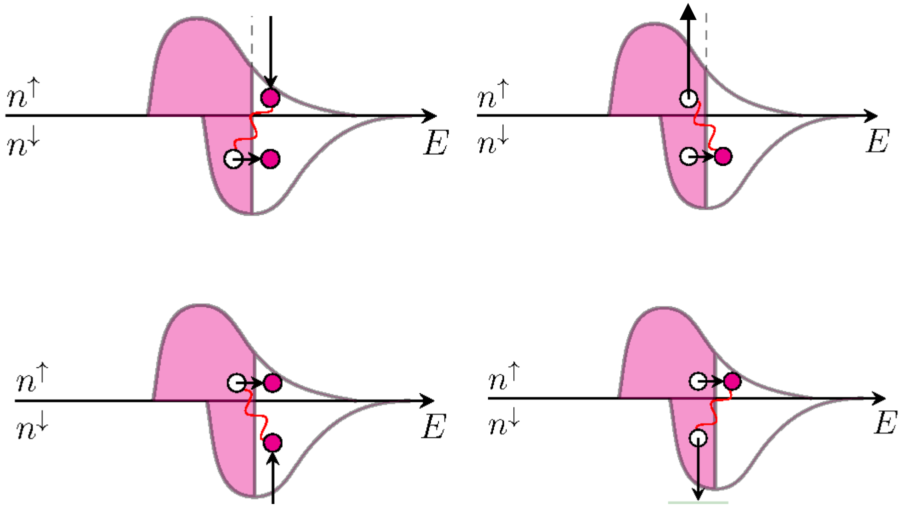
- Azpiroz, dos Santos Dias, Blügel, Lounis, Nanoletters (2016)

Theoretical framework III

Interaction of electrons & spin-excitations

- Doniach, Engelsberg, PRL **17**, 750 ‘66
- Hertz, Edwards, J. Phys. F: Metal Phys. **3**, 2174 ‘73
- Hong, Mills, PRB **59**, 13840 ‘99
- Zhukov, Chulkov, Echenique, PRL **93**, 096401 ‘04

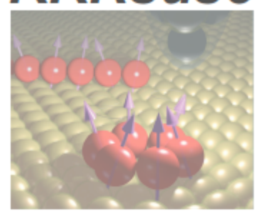




$$\Sigma \propto G\chi$$

$$\mathrm{Im}\Sigma_{ij}^{\uparrow\uparrow}(\varepsilon_F + \mathrm{V}) = -\frac{U_i U_j}{\pi}\int_0^{\mathrm{V}} d\omega \,\mathrm{Im}\,\chi_{ij}^{+-}(\omega)\mathrm{Im}\,G_{ij}^{\downarrow\downarrow}(\varepsilon_F + \mathrm{V} - \omega)$$

KKRsusc



- Bouaziz et al. Nat. Commun **11**, 6112 (2020)
- Schweflinghaus et al. Phys. Rev. B **89**, 235439 (2014)

Korringa-Kohn-Rostoker Green function method / MBPT

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Theoretical framework III

Interaction of electrons & spin-excitations

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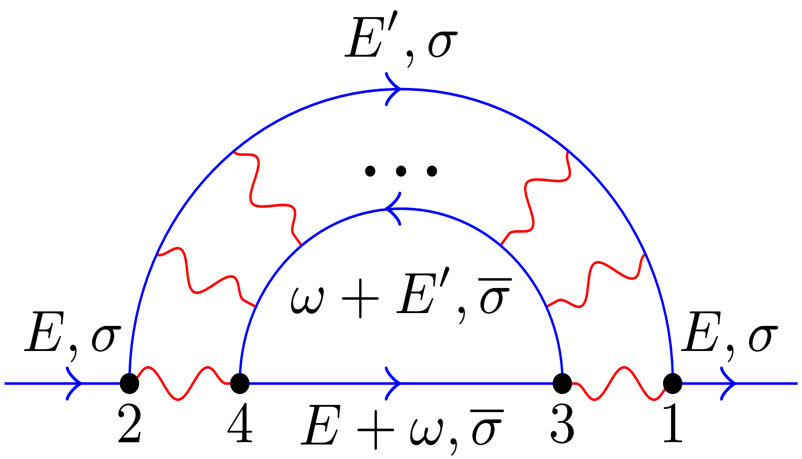
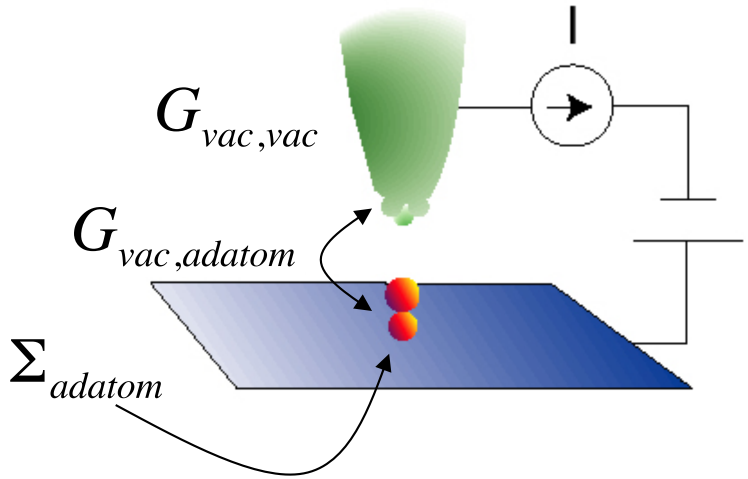
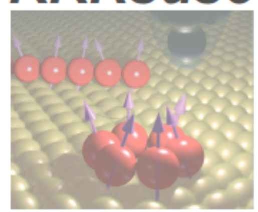


$$\Sigma \propto G\chi$$



$$g_{\mathrm{vac,vac}} = G_{\mathrm{vac,vac}} + G_{\mathrm{vac,adatom}}\, \Sigma_{\mathrm{adatom}}\, G_{\mathrm{adatom,vac}}$$

KKRsusc



- Bouaziz et al. Nat. Commun **11**, 6112 (2020)
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Korringa-Kohn-Rostoker Green function method / MBPT

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Theoretical framework III

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Offen im Denken

Interaction of electrons & spin-excitations

- Doniach, Engelsberg, PRL **17**, 750 '66
- Hertz, Edwards, J. Phys. F: Metal Phys. **3**, 2174 '73
- Hong, Mills, PRB **59**, 13840 '99
- Zhukov, Chulkov, Echenique, PRL **93**, 096401 '04

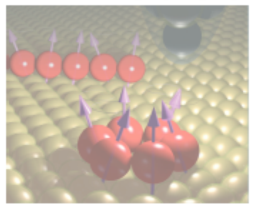
Connection to the GT approach

$$T = U + U\chi_0 T = U + U\chi\, U \quad \text{with} \quad \chi = \frac{\chi_0}{I - U\chi_0}$$

$$GT = GU + GU\chi_0 T = GU + GU\chi\, U$$

See e.g.: Essenberger et al. PRB **90**, 214504 (2014)

KKRsusc



- Bouaziz et al. Nat. Commun **11**, 6112 (2020)
- Schweflinghaus et al. Phys. Rev. B **89**, 235439 (2014)

Korringa-Kohn-Rostoker Green function method / MBPT

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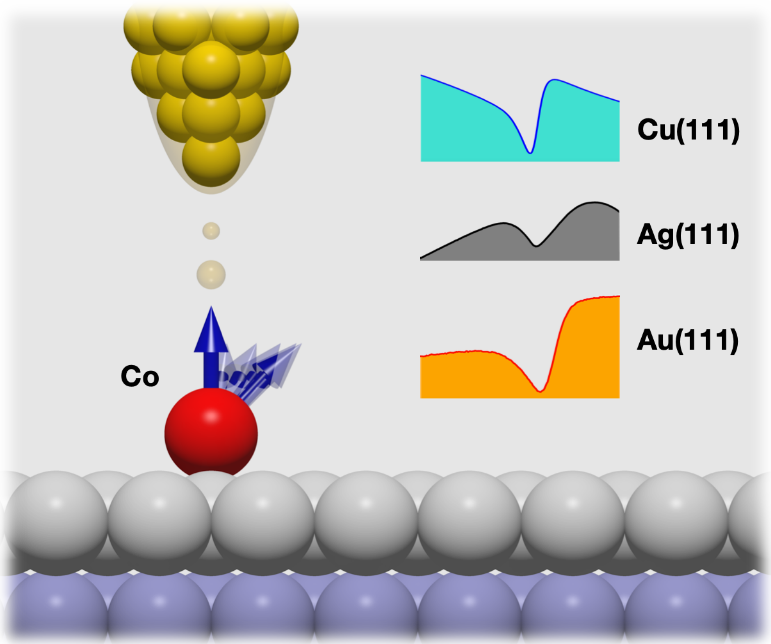
Fe atom on various surfaces

	Cu(111)	Ag(111)	Pt(111)-fcc	Pt(111)-hcp
magnetic moment	~3.3 μ_B	~3.5 μ_B	~3.5 μ_B	~3.5 μ_B
Resonance position	~1 meV	~1 meV	~1 meV	2.5 meV
g-factor	1.97 (exp: 2.1)	3.3 (exp: 3.1)	2.24 (exp: 2.4)	2.18 (exp: 2.0)
lifetime τ (B=0)	440 fsec (exp: 200 fsec)	200 fsec (exp: 400 fsec)	4.8 ps (exp: 2.5 ps)	1.2 ps (exp: 0.7 ps)
source	Phys. Rev. Lett. 106, 037205 (2011) Science 339, 55 (2013)	Phys. Rev. B 84, 212401, (2011)	Phys. Rev. Lett. 111, 157204 (2013)	Phys. Rev. Lett. 111, 157204 (2013)

Zero-bias anomalies: Co-adatom/noble metals



Bouaziz, Guimaraes, Lounis, Nature Comm. 11, 6112 (2020)

Ground state properties

Co adatoms on Cu, Ag, Au(111)

Surface	MAE (meV)	$M_{spin}(\mu_B)$	$M_{orb}(\mu_B)$
Cu(111)	4.29	2.02	0.47
Ag(111)	3.27	2.21	0.70
Au(111)	4.46	2.22	0.44

→ Out of plane easy axis

→ Large spin moment

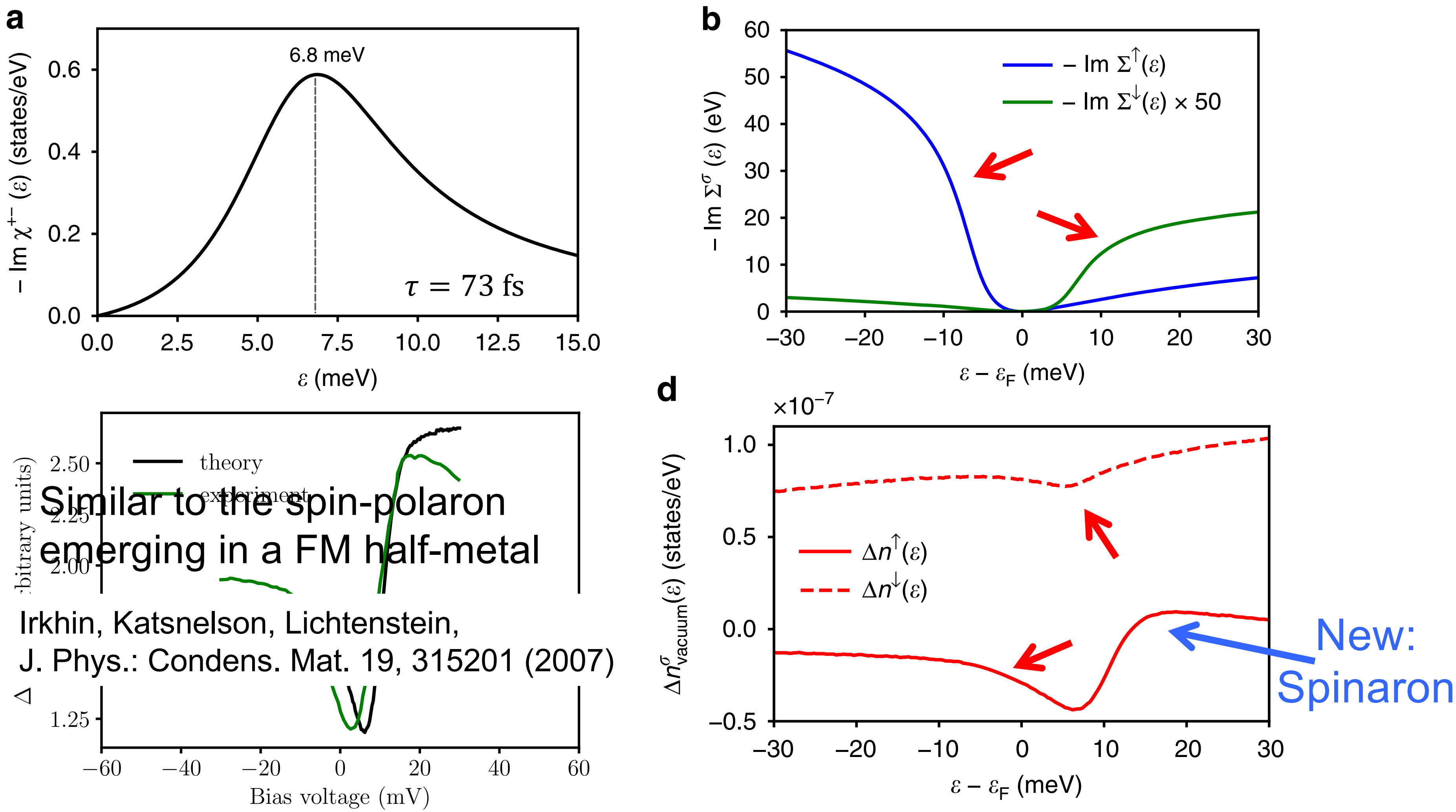
The role of magnetic anisotropy in the Kondo effect

ALEXANDER F. OTTE[1,2], MARKUS TERNES[1], KIRSTEN VON BERGMANN[1,3], SEBASTIAN LOTH[1,4], HARALD BRUNE[1,5], CHRISTOPHER P. LUTZ[1], CYRUS F. HIRJIBEHEDIN[1,6] AND ANDREAS J. HEINRICH[1]*

Nature Phy. 4, 847 ‘08

- Bouaziz, Guimaraes, Lounis, Nature Commun. 11, 6112 (2020)

ISTS for Co adatom on Au(111)



Similar to the spin-polaron emerging in a FM half-metal

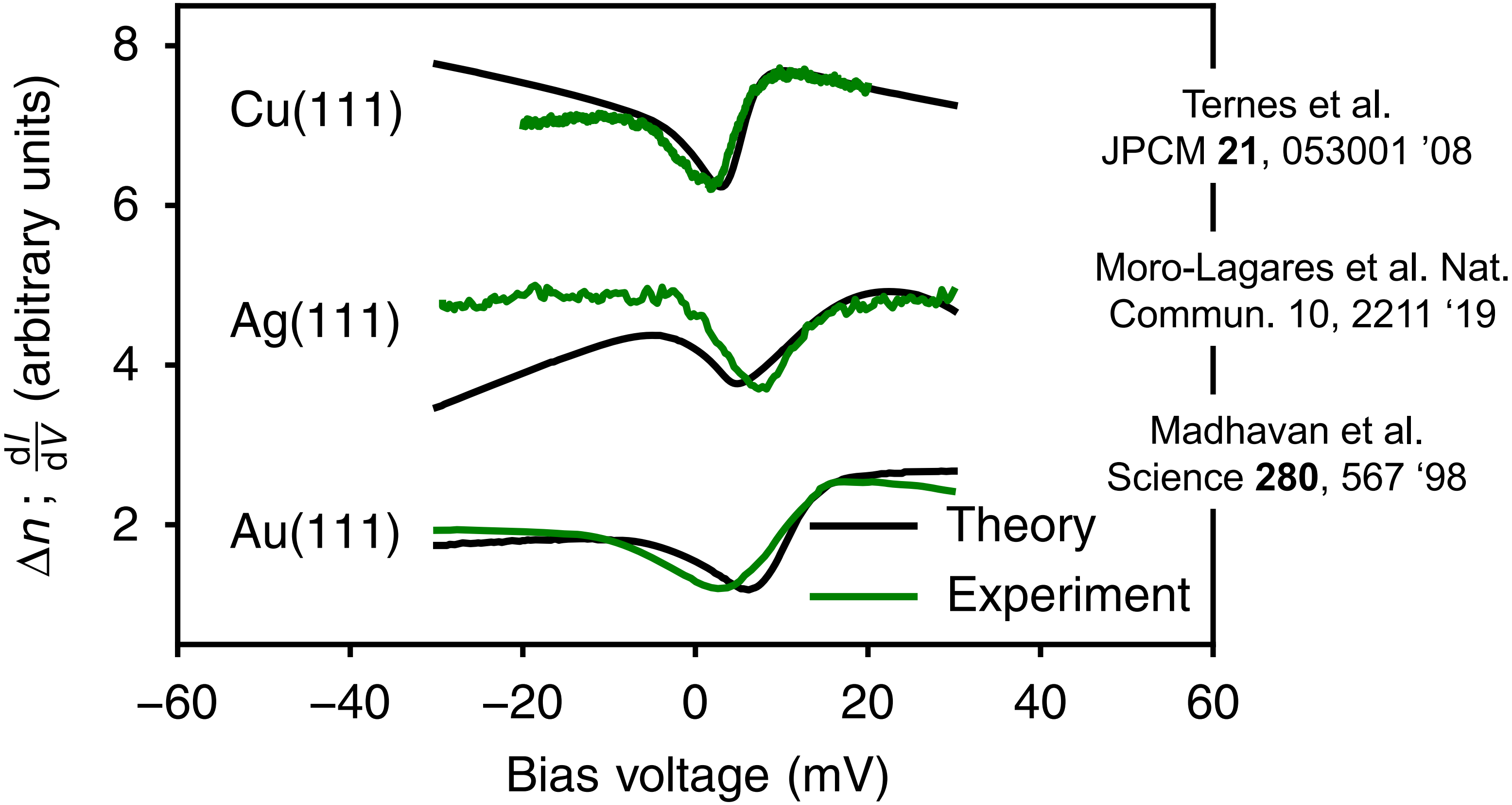
Irkhin, Katsnelson, Lichtenstein,
J. Phys.: Condens. Mat. 19, 315201 (2007)

Spinaron: Many-body state resulting from interaction of electron and spin-excitations

$$g = \frac{G}{1 - G\Sigma}$$

- Bouaziz, Guimaraes, Lounis, Nature Commun. 11, 6112 (2020)

ISTS for Co adatom on metals



Fano-resonance formula

$$n(\varepsilon) = \mathcal{A}\,\frac{(\varepsilon + q)^2}{\varepsilon^2 + 1}$$

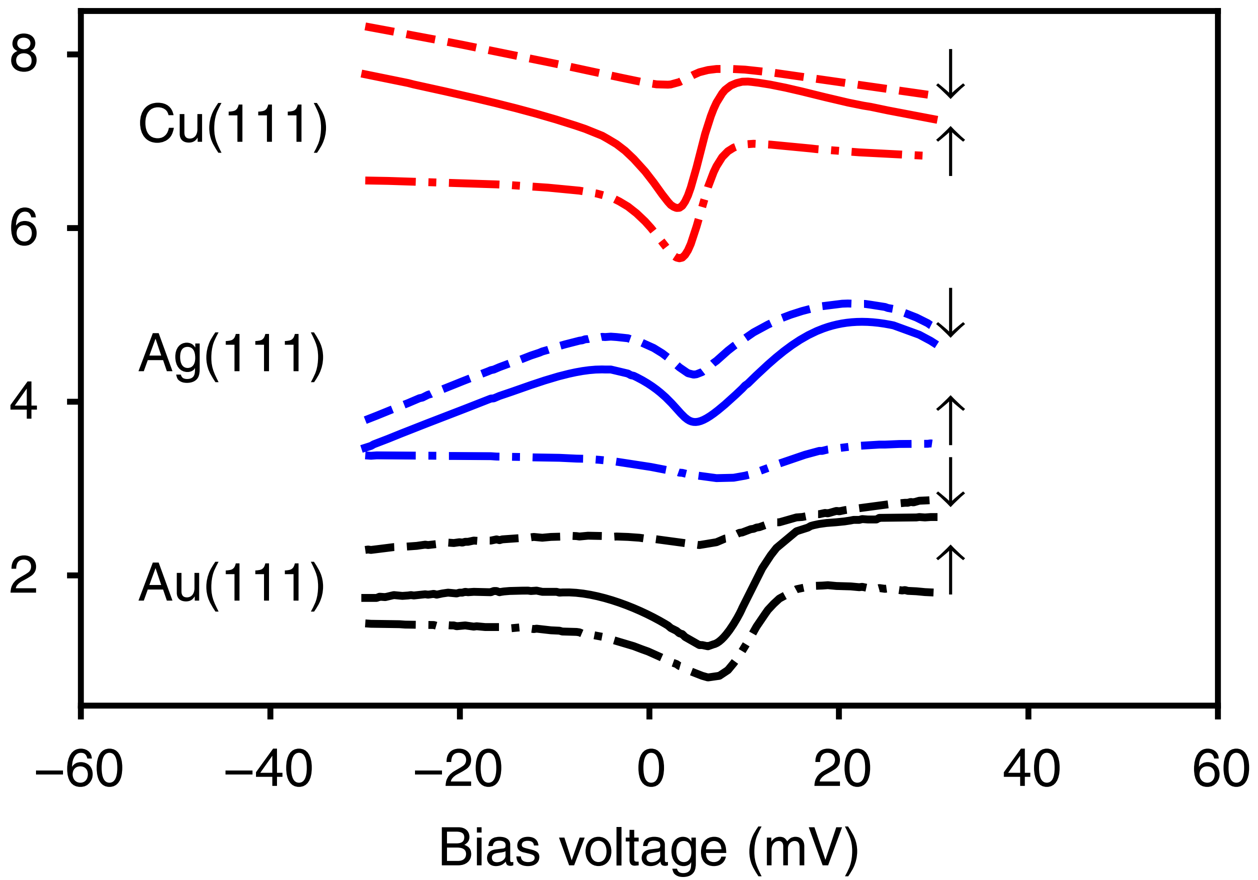
$$\varepsilon = (eV - E_0)/k_\mathrm{B}T_\mathrm{K}^\mathrm{eff}$$

Surface	E_0(meV)	$T_\mathrm{K}^\mathrm{eff}$(K)	$T_\mathrm{K}^\mathrm{exp}$(K)	q	q^exp
Cu(111)	3.74	37.3	44.9 [57 [17]]	0.42	0.38 [0.5 [13]]
Ag(111)	4.71	89.4	73 [56 [41,45]]	-0.05	-0.004 [0.02±0.02 [41,45]]
Au(111)	10.61	67.5	91 [76±8 [17]]	0.55	0.45 [0.7 [17]]

- Bouaziz, Guimaraes, Lounis, Nature Commun. 11, 6112 (2020)

ISTS for Co adatom on metals

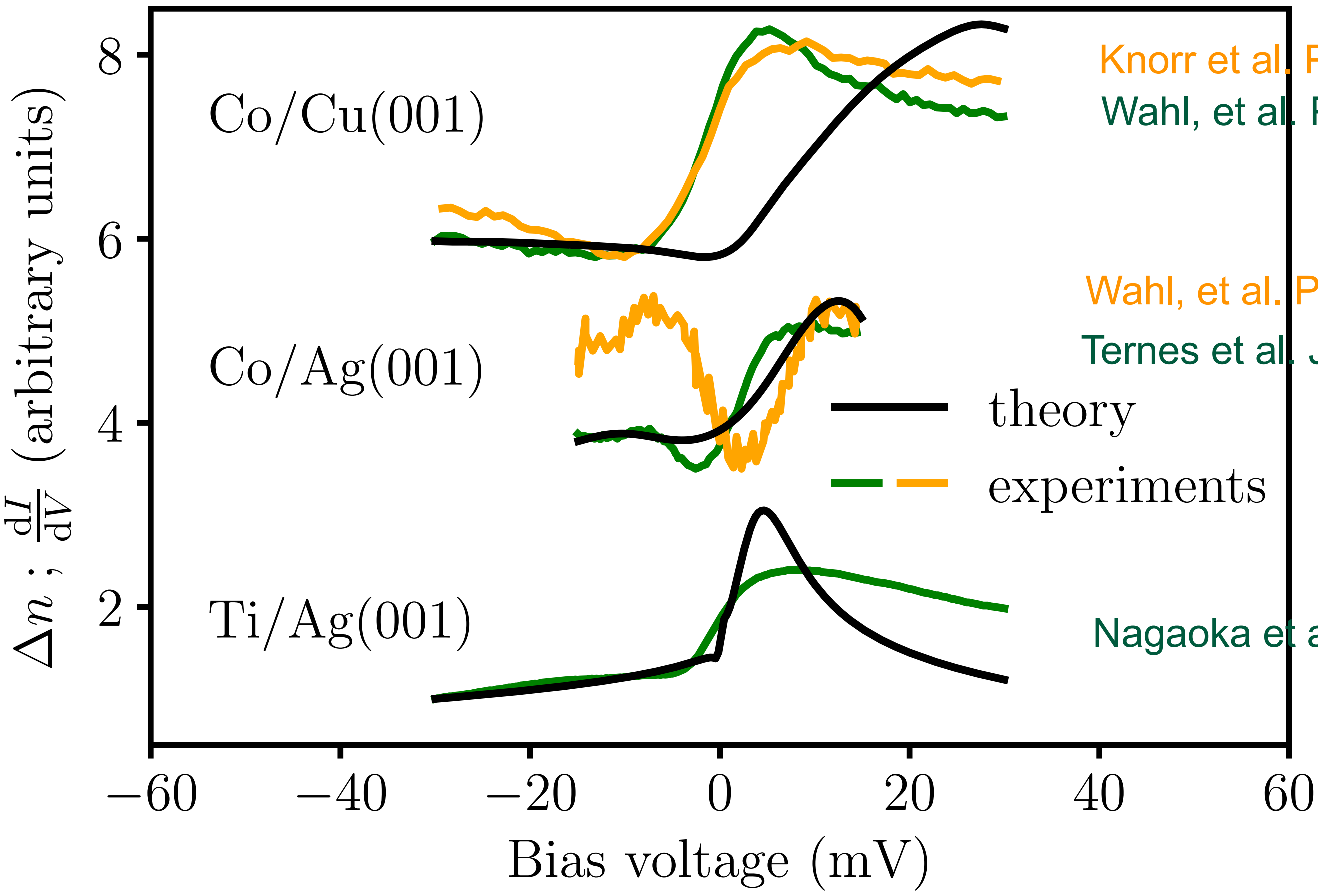
Co adatoms on Cu, Ag, Au(111)



- Bouaziz, Guimaraes, Lounis, Nature Commun. 11, 6112 (2020)

ISTS for adatoms on metals

Co adatoms on Cu, Ag(001) and Ti on Ag(001)



Knorr et al. PRL 88, 096804 ‘02

Wahl, et al. PRL.98, 056601 ‘07

Wahl, et al. PRL 93, 176603 ‘04

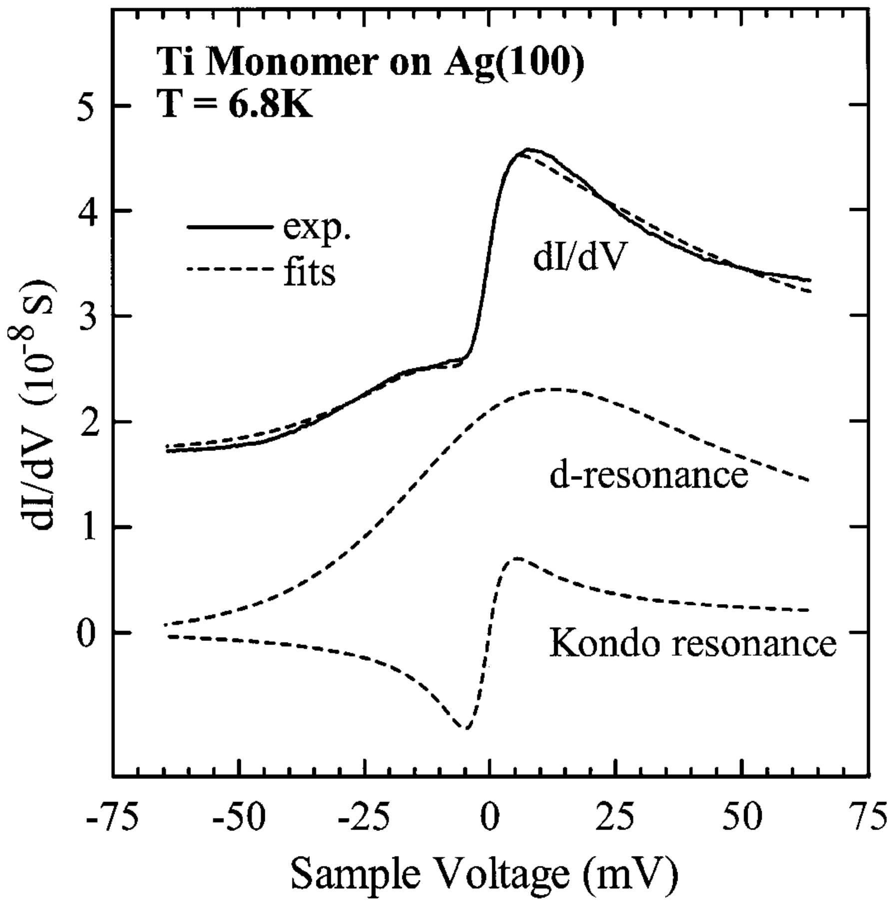
Ternes et al. JPCM 21, 053001 ‘08

Nagaoka et al. PRL 88, 077205 ‘02

Bouaziz, Guimaraes, Lounis, Nature Commun. 11, 6112 (2020)

Impact of a magnetic field

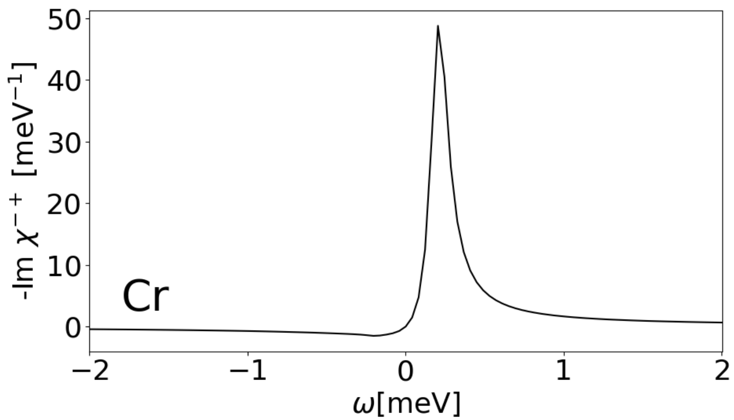
Nagaoka et al. PRL 88, 077205 '02



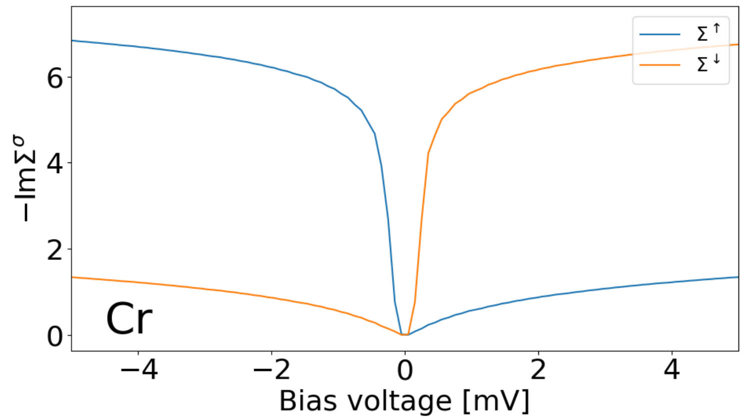
- Bouaziz, Guimaraes, Lounis, Nature Commun. 11, 6112 (2020)

Example of adatoms on Nb(110)

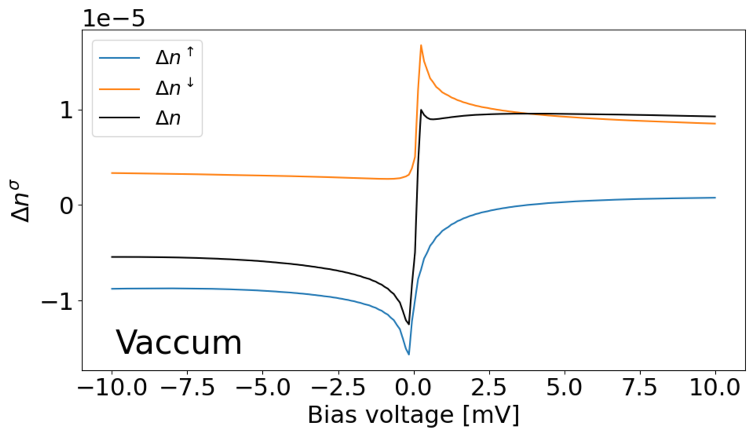
Magnetic susceptibility



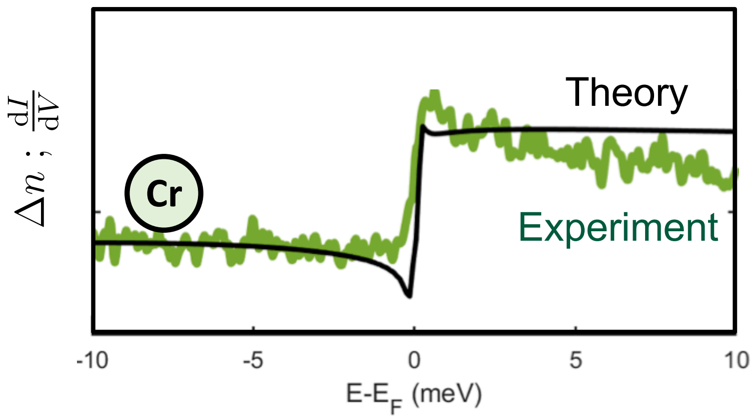
Self-energy



Spin-excitation



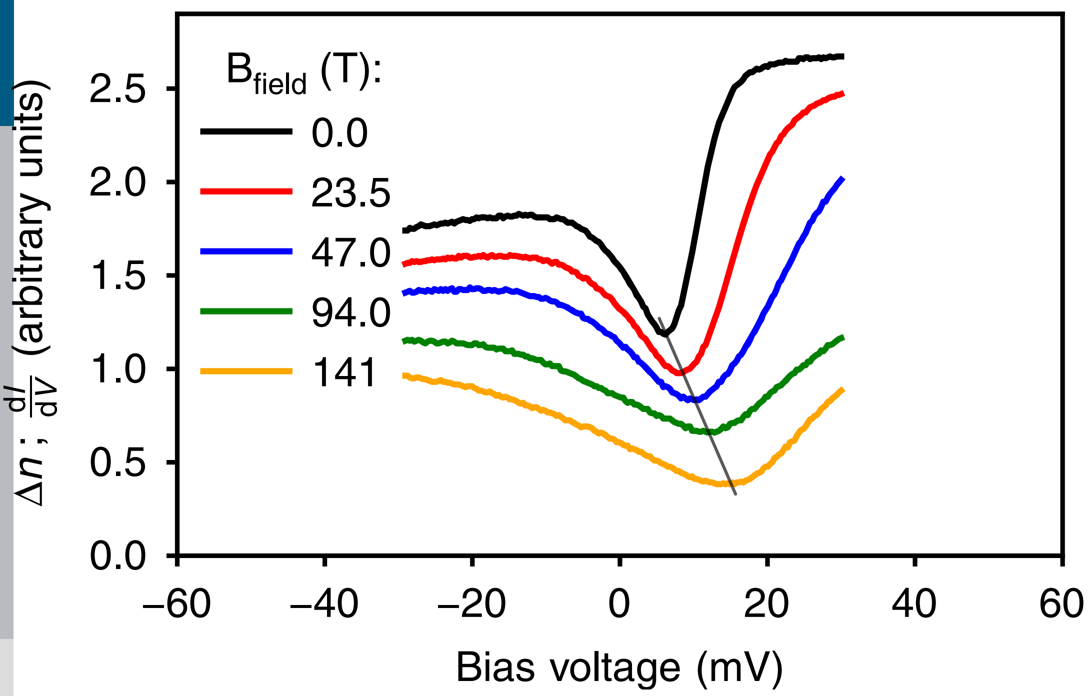
ISTS



Küster, Montero, Guimaraes, Brinker, Lounis, Parkin, Sessi. Nature Commun. 12, 1108 '21

Impact of a magnetic field

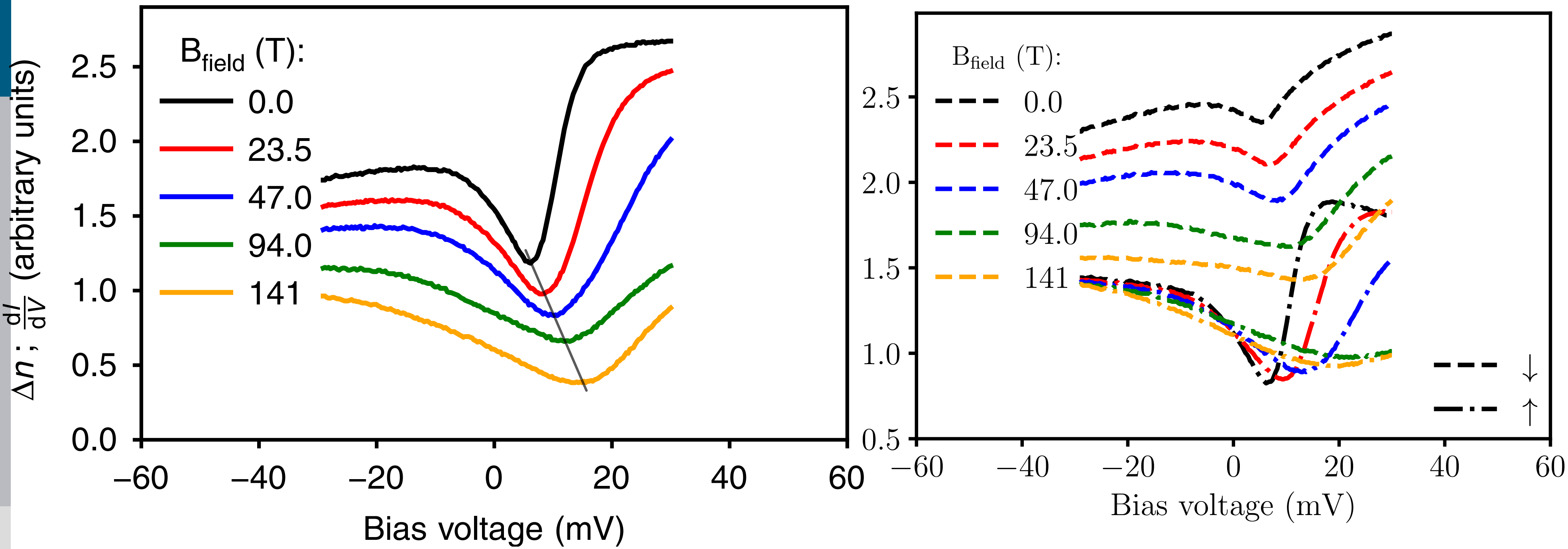
Co adatom on Au(111)



Bouaziz, Guimaraes, Lounis, Nature Commun. 11, 6112 (2020)

Impact of a magnetic field

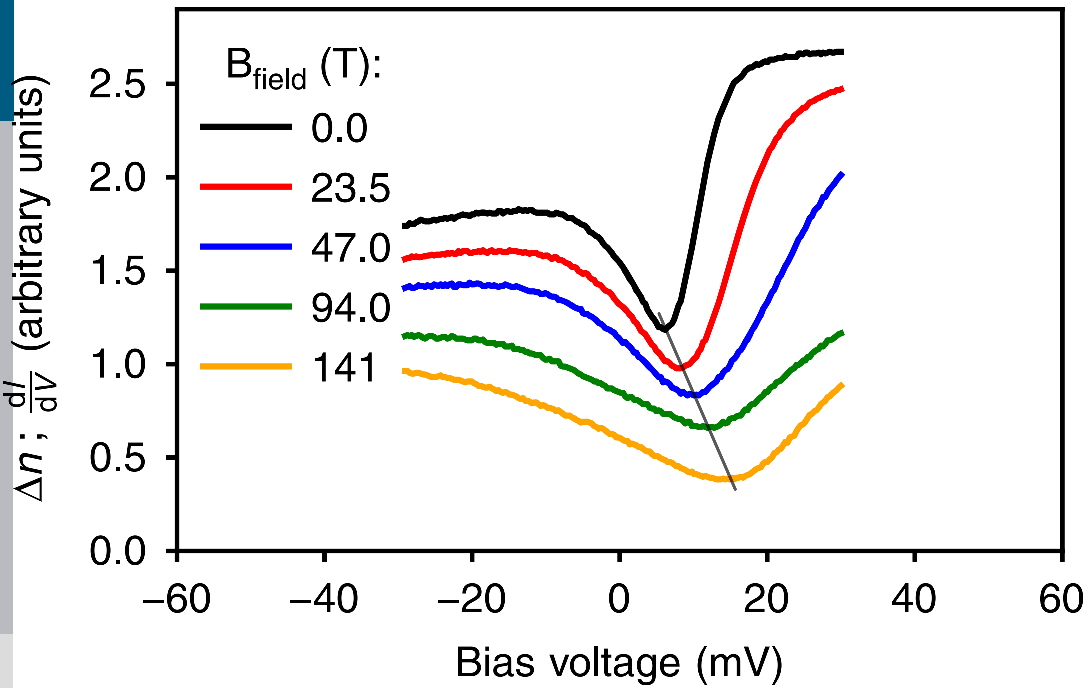
Co adatom on Au(111)

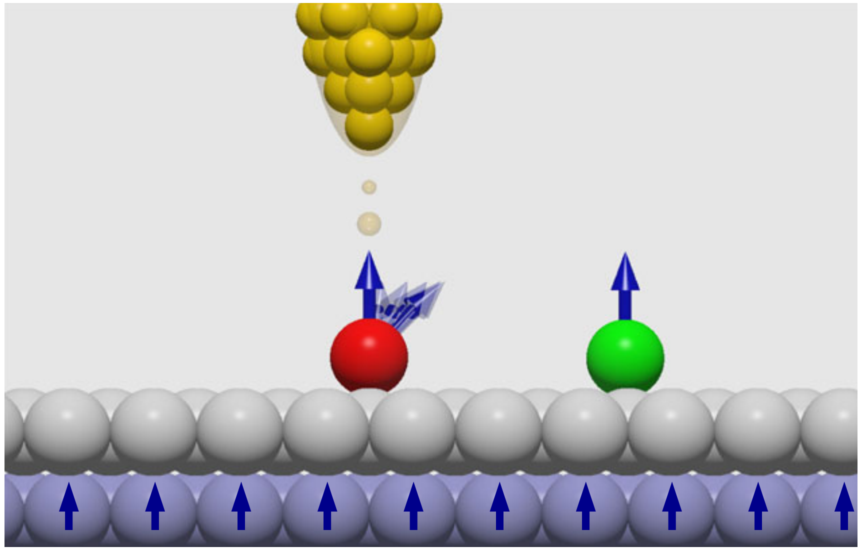


Bouaziz, Guimaraes, Lounis, Nature Commun. 11, 6112 (2020)

Impact of a magnetic field

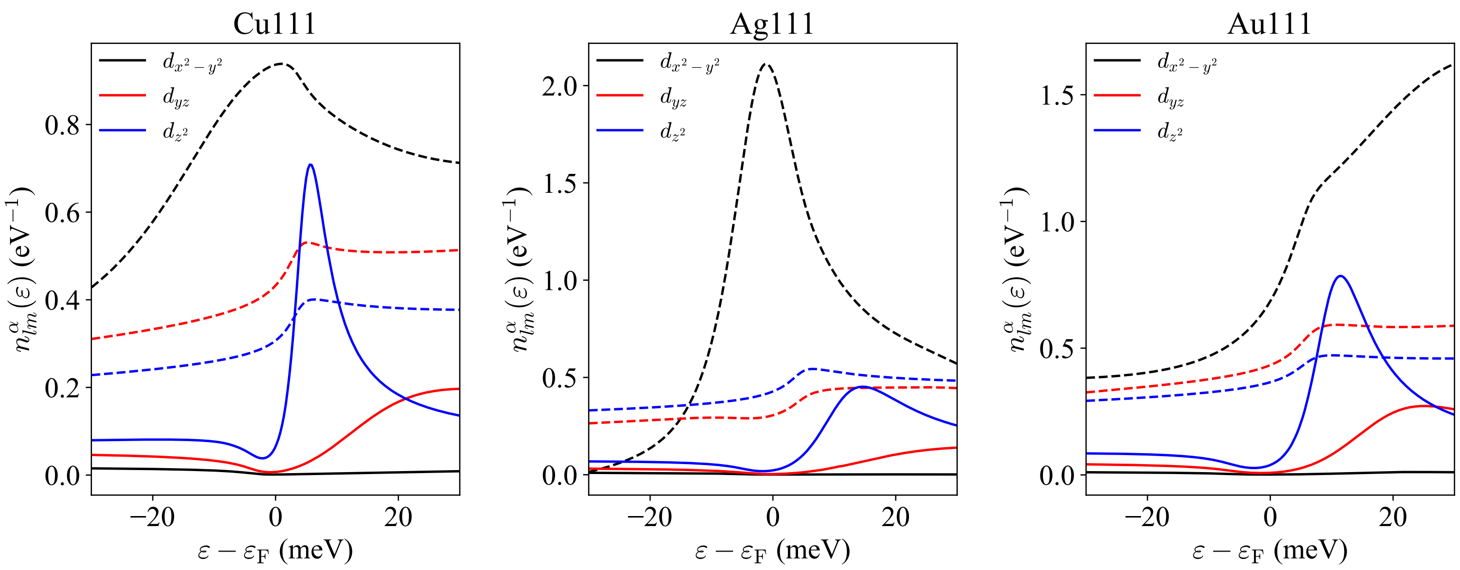
Co adatom on Au(111)





- Bouaziz, Guimaraes, Lounis, Nature Commun. 11, 6112 (2020)

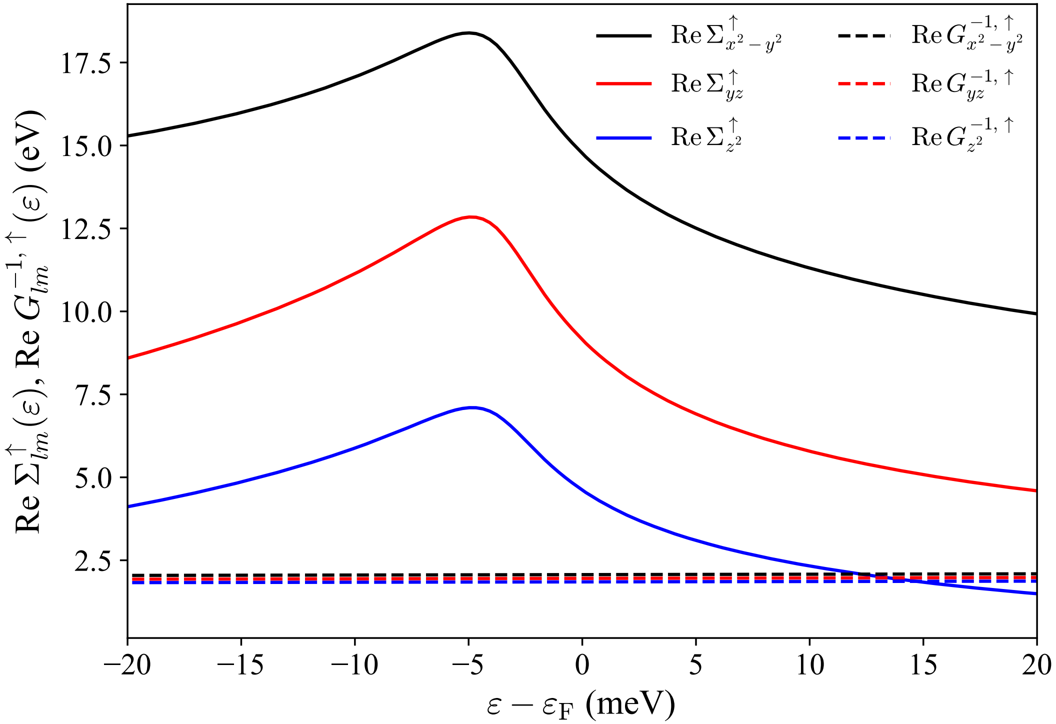
Supplement



Supplementary Figure 5: Orbital-resolved renormalized local density of states of Co adatoms on the three surfaces Cu, Ag, Au(111). Full (dashed) lines correspond to the majority-spin (minority-spin) channel. The spinaron emerges from the majority-spin d_{z^2} orbital (full blue line).

Bouaziz, Guimaraes, Lounis, Nature Commun. 11, 6112 (2020)

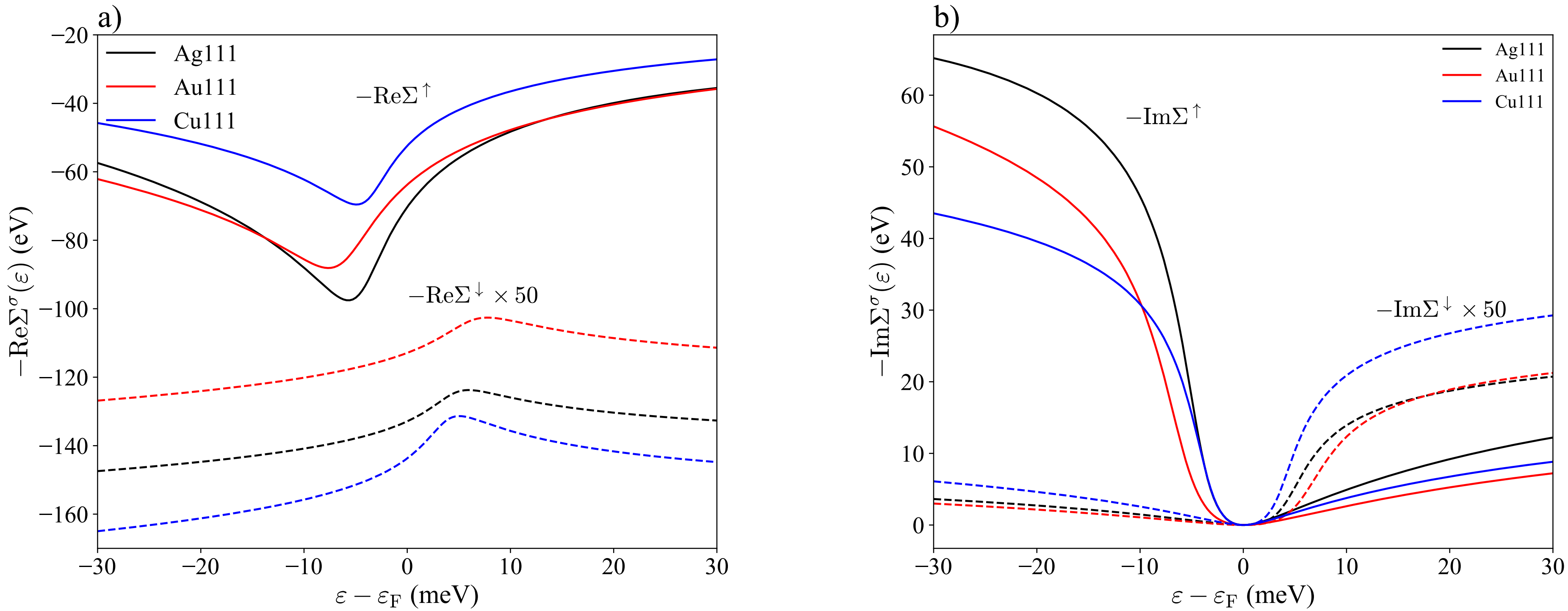
Supplement



Supplementary Figure 6: Orbital-resolved real part of inverse Green function and self-energy of the majority spin channel of Co adatoms on Cu(111) surface. The intersection occurring in the d_{z^2}-orbital leads to a vanishing denominator of the Eq 1 of the main text and, therefore, to the spinaron. The contribution of $\mathrm{Im}[\underline{G}(\varepsilon)]\mathrm{Im}[\underline{\Sigma}(\varepsilon)]$ (and other interference effects) shifts the spinaron to lower energies.

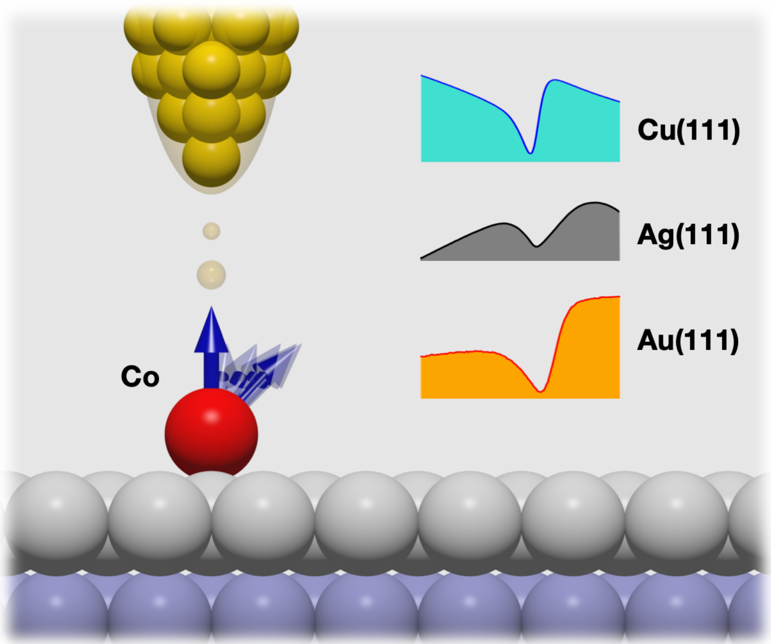
Bouaziz, Guimaraes, Lounis, Nature Commun. 11, 6112 (2020)

Supplement



- Bouaziz, Guimaraes, Lounis, Nature Commun. 11, 6112 (2020)

Zero-bias anomalies: Manipulation of MAE



Noei, Weismann, Berndt,
Mozara, Lichtenstein,
Montero, Brinker, Guimaraes, Lounis
(in preparation)

Conclusions

- Zero-bias anomalies of Co adatoms not Kondo features

  but gapped spin-excitations (importance of spin-orbit int.)

+ Spinaron

- Strategies to manipulate spin-excitations gap: magnetic field or magnetic anisotropy energy

- Co@Cu-chains reduces magnetic anisotropy energy, observation of spin-excitation of a non-collinear mag. moment

- Unconventional signature of spin-excitations (adatoms on Nb)

Collaborations on presented work

Funsilab


J. Bouaziz

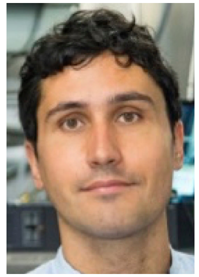

F. Guimaraes


A. Martinez


S. Brinker

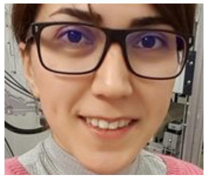
MPI Halle


F. Küster


P. Sessi


S.S. Parkin

Kiel


N. Noei


A. Weismann

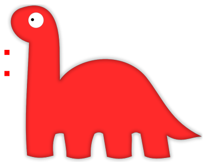

R. Berndt

Hamburg


R. Mozara


A. Lichtenstein

Dynasore:
ERC
consolidator grant



- Discussions on zero-bias anomalies:

  M. Ternes@RWTH Aachen Uni.; A. Weismann@Kiel Uni.; W.D. Schneider@EPFL;

  M. Crommie@Berkley; L. Diekhöner@Aalborg Uni.

Theoretical framework II

Intrinsic spin-excitations

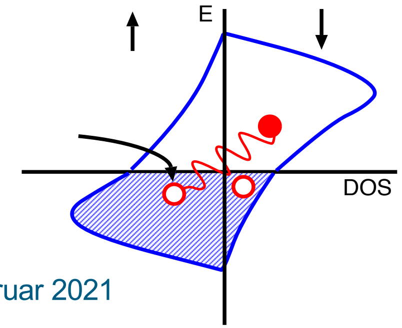
$$\delta m^i_{x,y}(\vec{r}t) = \int\int d\vec{r}'dt'\chi^{ij}(\vec{r}t,\vec{r}'t')\delta B^j_{ext}(\vec{r}'t')$$

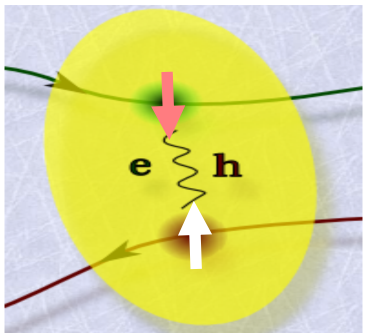
$$\delta m^i_{x,y}(\vec{r}t) = \int\int d\vec{r}'\,dt'\chi^{ij}_{KS}(\vec{r}t,\vec{r}'t')\left(\delta B^j_{xc}(\vec{r}'t') + \delta B^j_{ext}(\vec{r}'t')\right)$$

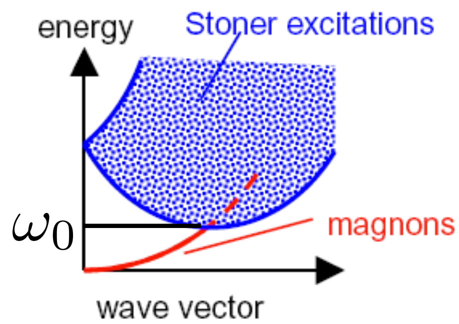
$$\chi^{ij}(\vec{r},\vec{r}';\omega) = \chi^{ij}_{KS}(\vec{r},\vec{r}';\omega) + \sum_{kl}\int\int d\vec{r}''d\vec{r}'''\chi^{ik}_{KS}(\vec{r},\vec{r}'';\omega)K^{kl}_{xc}(\vec{r}'',\vec{r}''';\omega)\chi^{lj}(\vec{r}''',\vec{r}';\omega)$$

Adiabatic LDA: $K^{ij}_{xc}(\vec{r},\vec{r}';\omega) \approx K^{ij}_{xc}(\vec{r},\vec{r}';0)\,\delta_{ij}\delta_{\vec{r}\vec{r}'}$

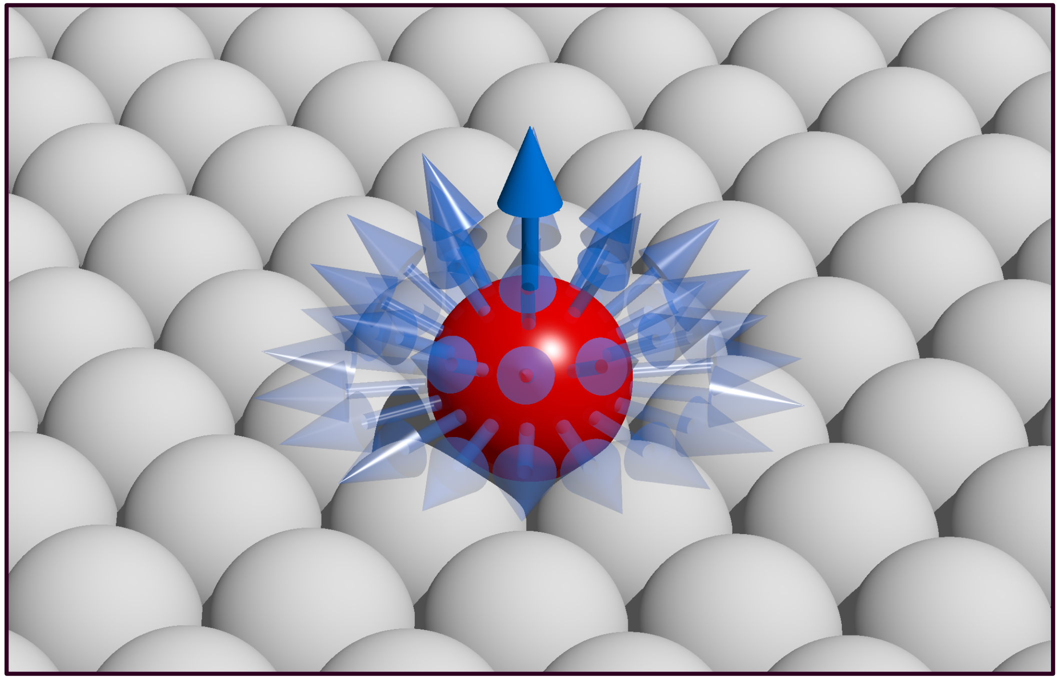
$$\chi^{ij,\alpha\beta}_{KS}(\vec{r},\vec{r}';\omega) = -\frac{1}{\pi}\int dz f(z)\mathrm{Tr}(\sigma^\alpha G_{ij}(\vec{r},\vec{r}';z+\omega)\sigma^\beta \operatorname{Im} G_{ji}(\vec{r}',\vec{r};z)$$
$$+\sigma^\alpha \operatorname{Im} G_{ij}(\vec{r},\vec{r}';z)\sigma^\beta G^-_{ji}(\vec{r}',\vec{r};z-\omega))$$





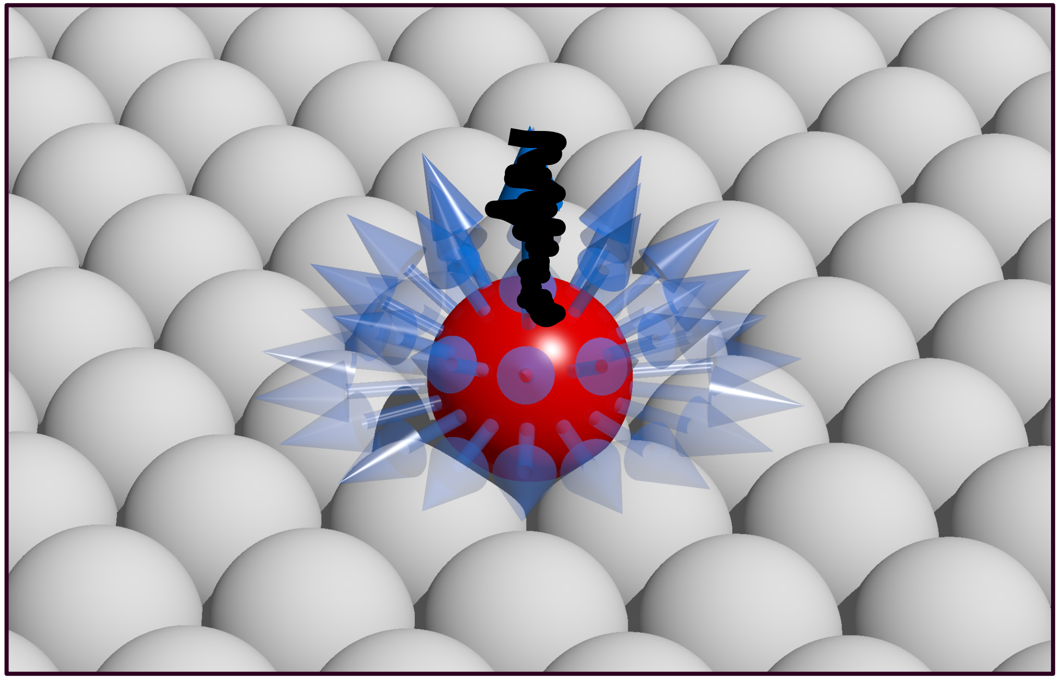


Magnetic fluctuations even without a moment?



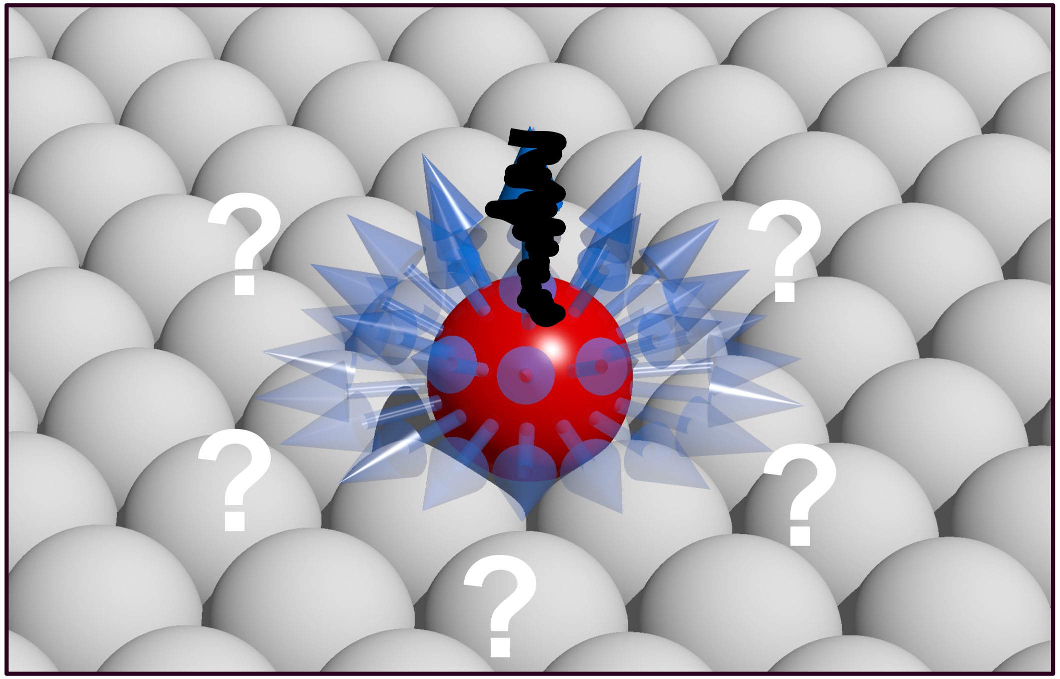
- Azpiroz, dos Santos Dias, Schweflinghaus, Blügel, Lounis, PRL (2017); Editor's suggestion

Magnetic fluctuations even without a moment?



- Azpiroz, dos Santos Dias, Schweflinghaus, Blügel, Lounis, PRL (2017); Editor’s suggestion

Magnetic fluctuations even without a moment?



Azpiroz, dos Santos Dias, Schweflinghaus, Blügel, Lounis, PRL (2017); Editor's suggestion

Stoner criterion

Transition to a magnetic state if $I_s n(E_F) > 1$

$$\delta m = \chi \delta B$$

$$\delta m = \frac{\chi_{KS}(\omega)}{1 - K_{xc}\chi_{KS}(\omega)} \delta B$$

$$\delta m = \frac{n(E_F)}{1 - I_s n(E_F)} \delta B$$

Stoner parameter

Azpiroz, dos Santos Dias, Schweflinghaus, Blügel, Lounis, PRL (2017); Editor's suggestion

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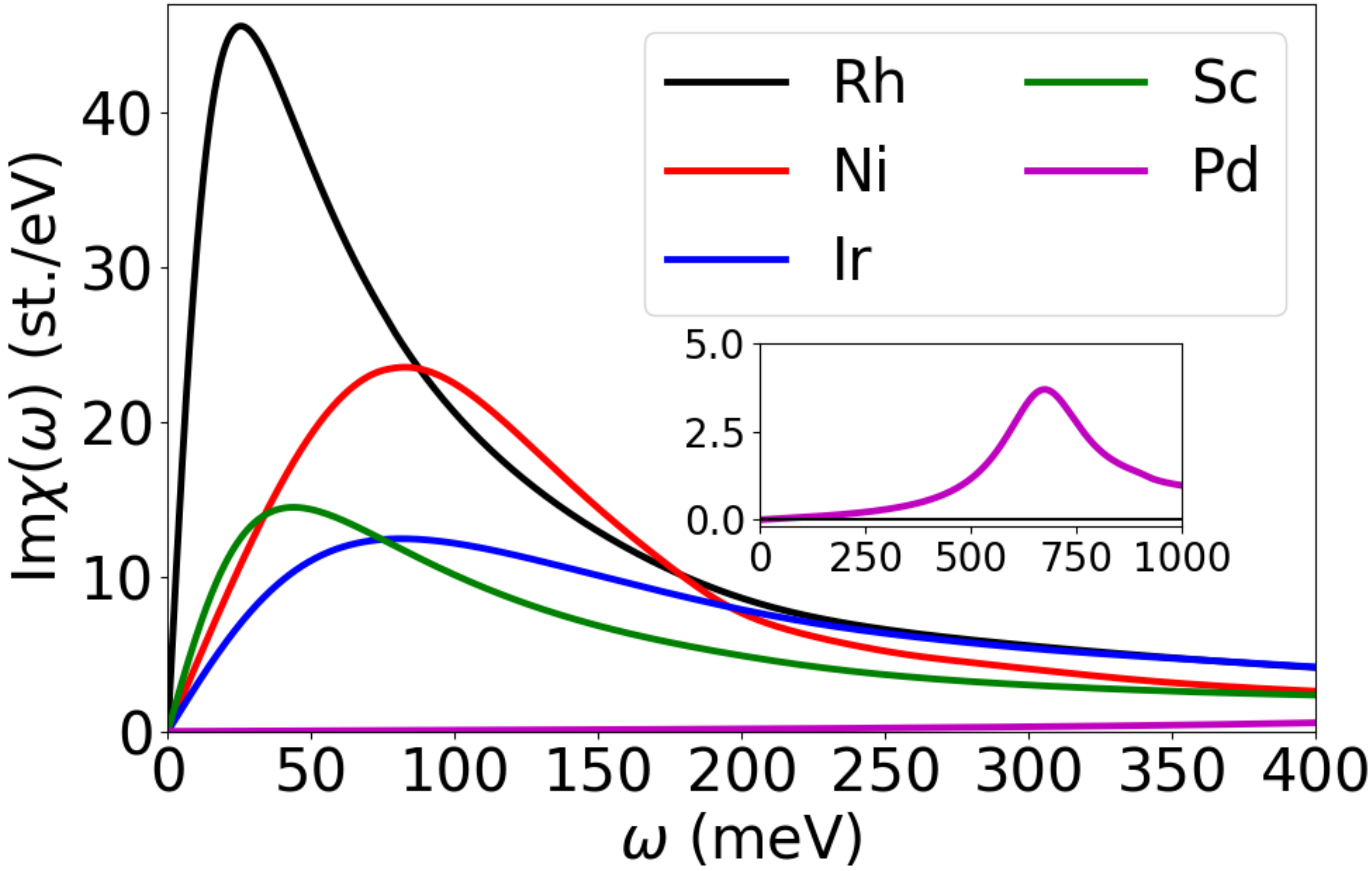
Stoner parameter

But what happens in the dynamical regime?

Azpiroz, dos Santos Dias, Schweflinghaus, Blügel, Lounis, PRL (2017); Editor's suggestion

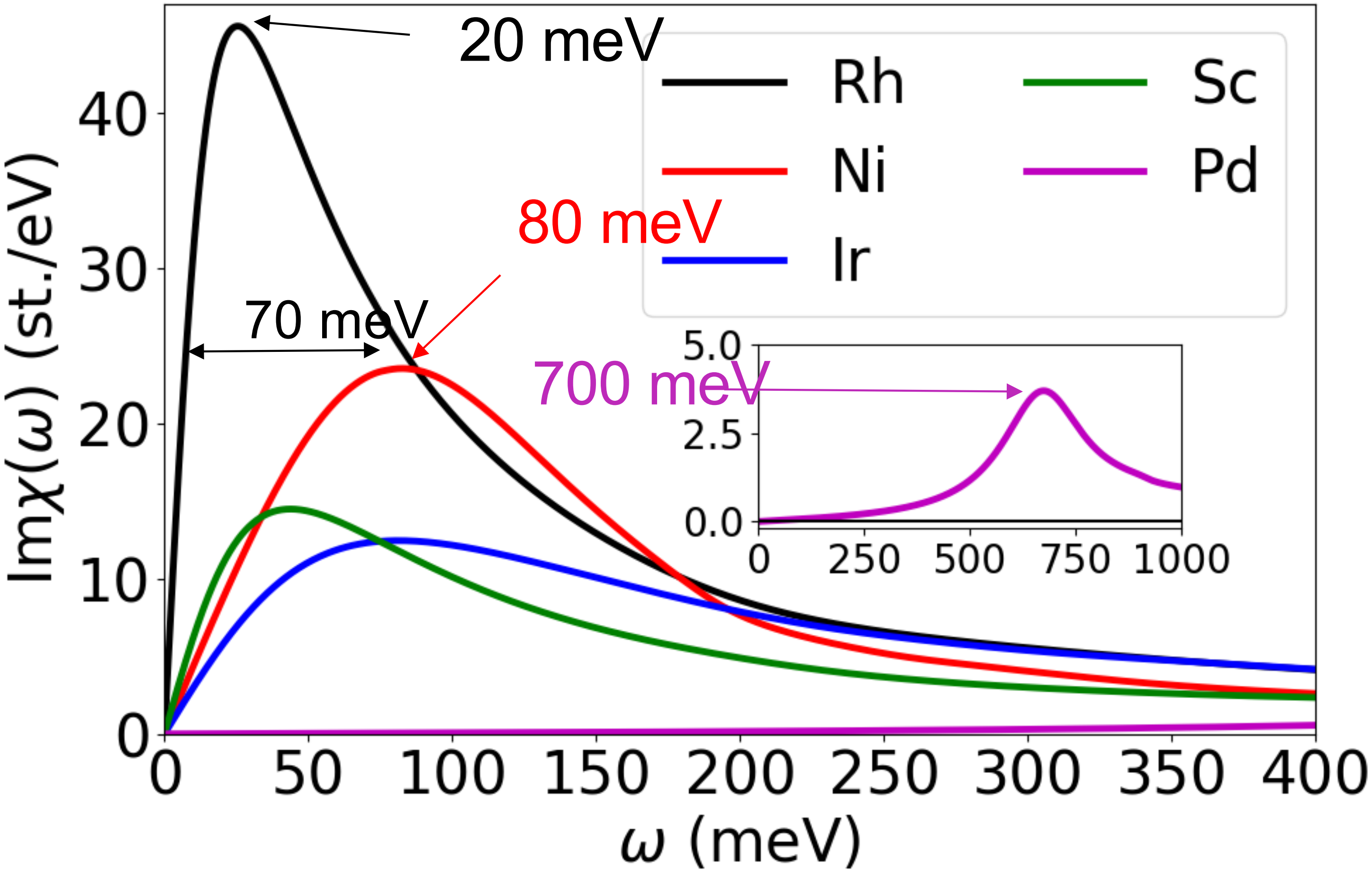
Spin-fluctuation modes:
non-magnetic adatoms on Ag(100)



Azpiroz, dos Santos Dias, Schweflinghaus, Blügel, Lounis, PRL (2017); Editor’s suggestion

Spin-fluctuation modes: **non-magnetic** adatoms on Ag(100)

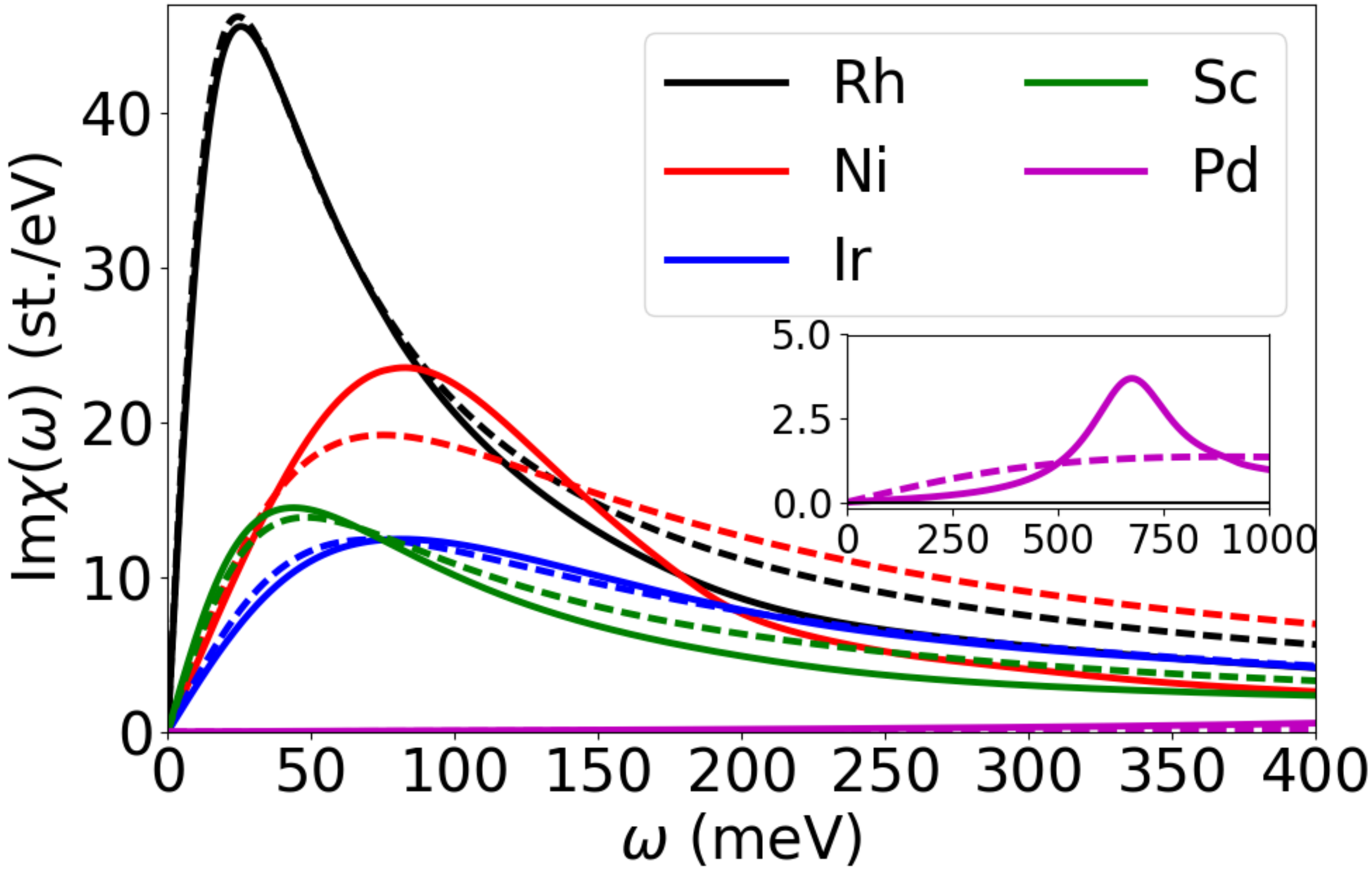
Can exhibit well-defined peaks



Azpiroz, dos Santos Dias, Schweflinghaus, Blügel, Lounis, PRL (2017); Editor's suggestion

Physics: Stoner criterion

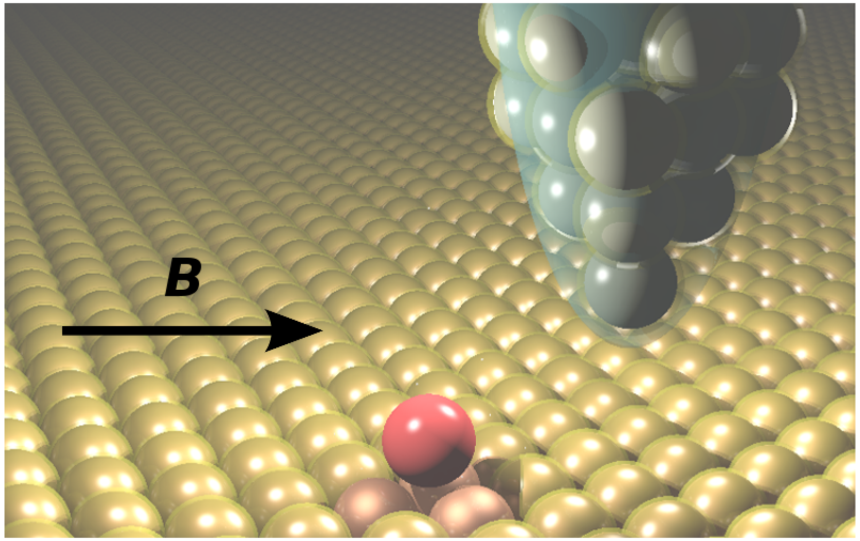
dashed lines: $$\mathrm{Im}\,\chi(\omega) = \frac{\pi}{2}\frac{n^2(E_F)\omega}{(1 - I_{xc}n(E_F))^2 + \left(\frac{\pi}{2}I_{xc}n^2(E_F)\omega\right)^2}$$

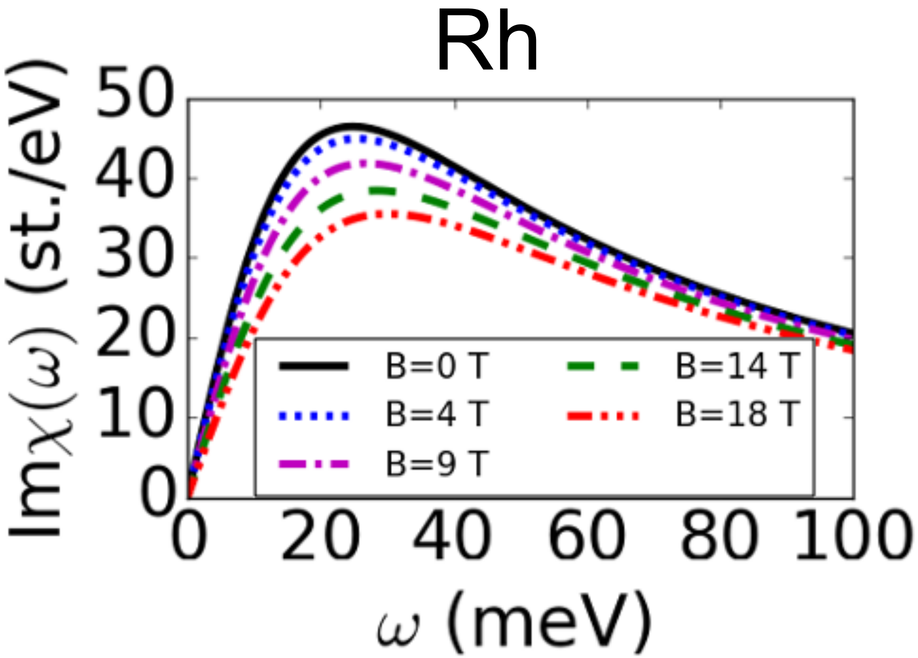


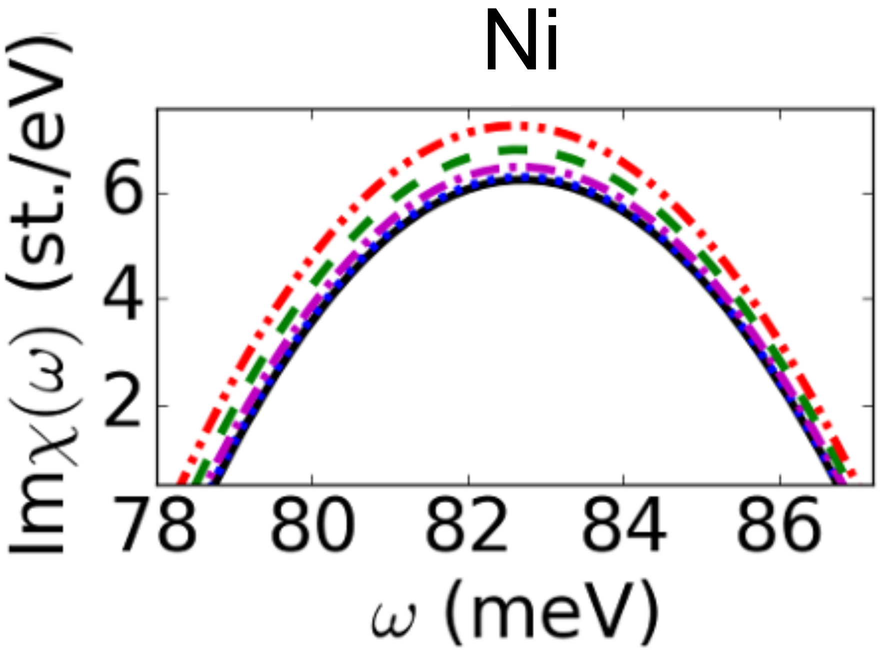
Means of extracting Stoner Exchange experimentally

Azpiroz, dos Santos Dias, Schweflinghaus, Blügel, Lounis, PRL (2017); Editor’s suggestion

Manipulation with external mag. field

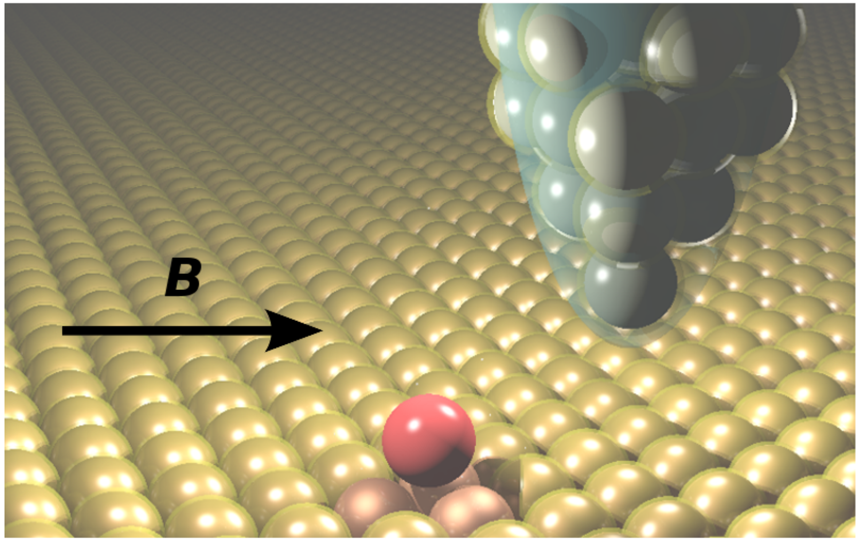


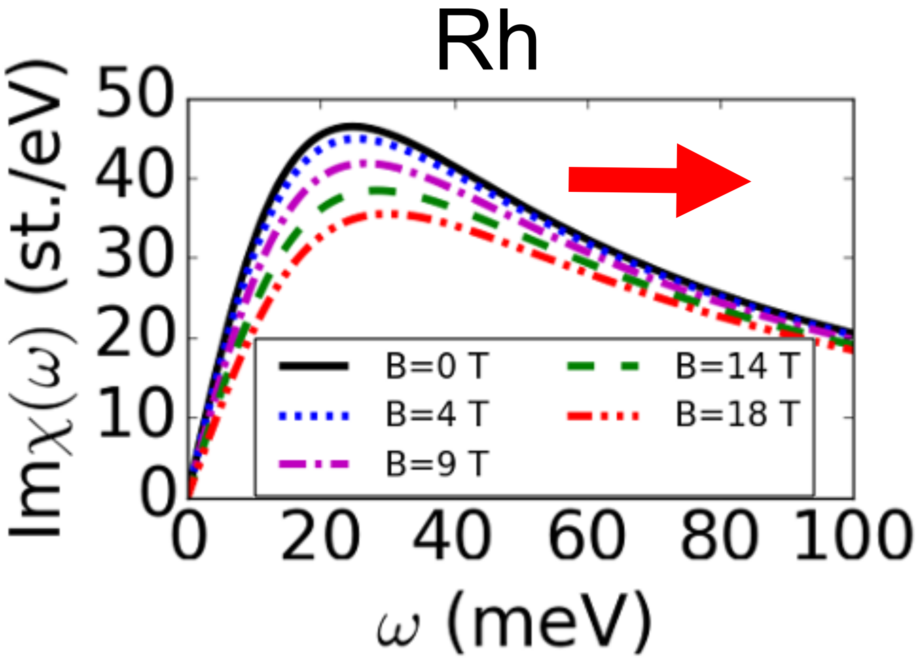


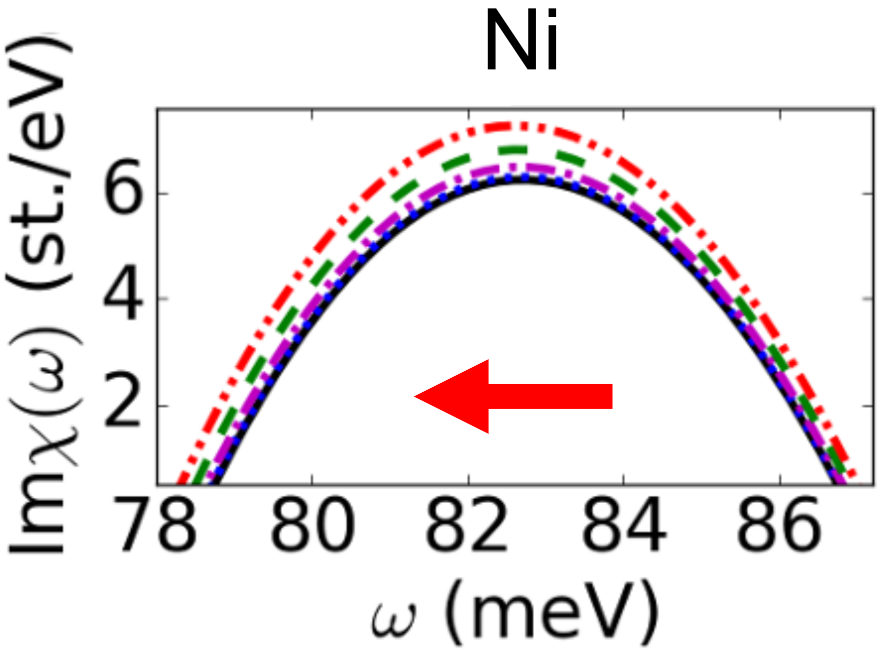


Azpiroz, dos Santos Dias, Schweflinghaus, Blügel, Lounis, PRL (2017); Editor’s suggestion

Manipulation with external mag. field

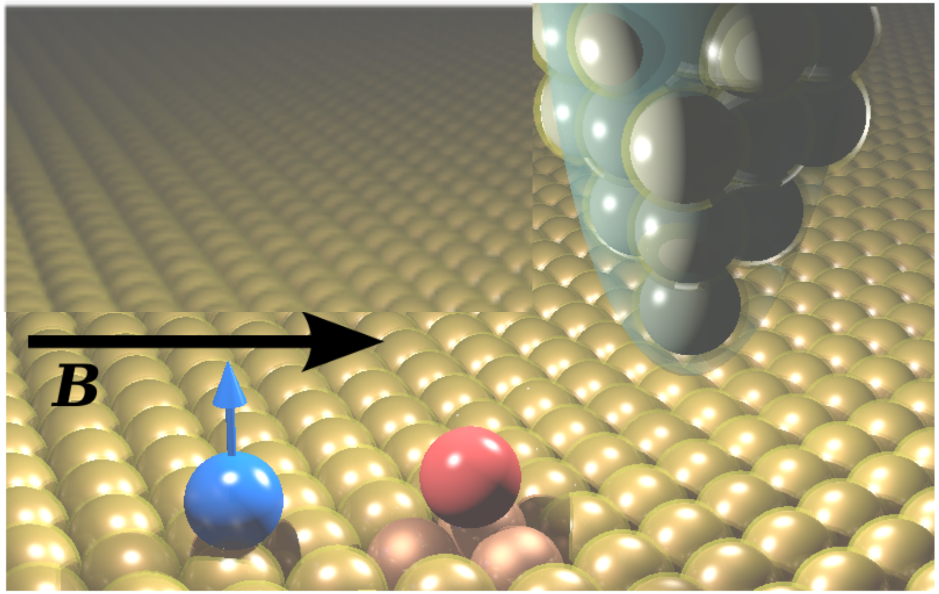






Peaks shift in opposite direction

Magnetic transition from a proximity-effect



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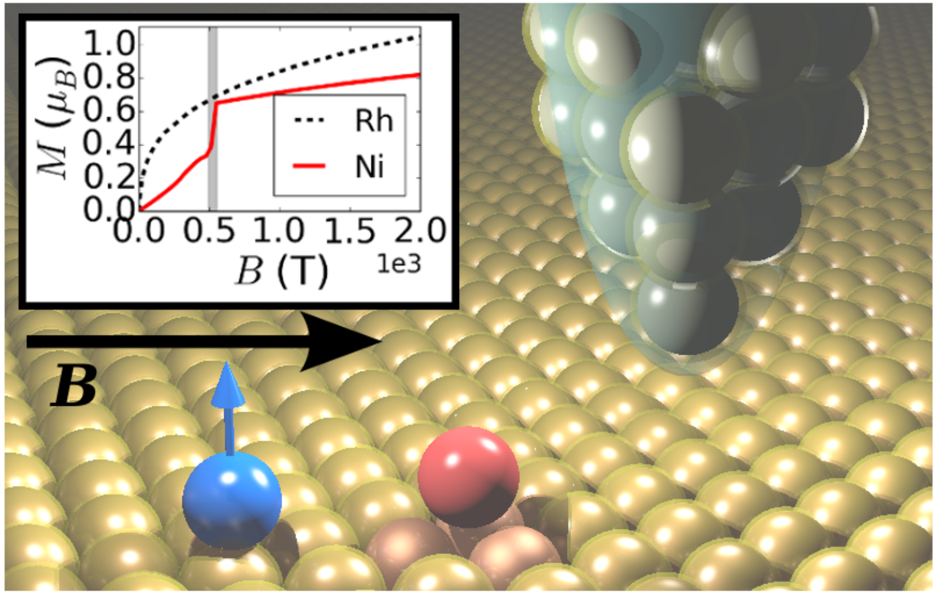
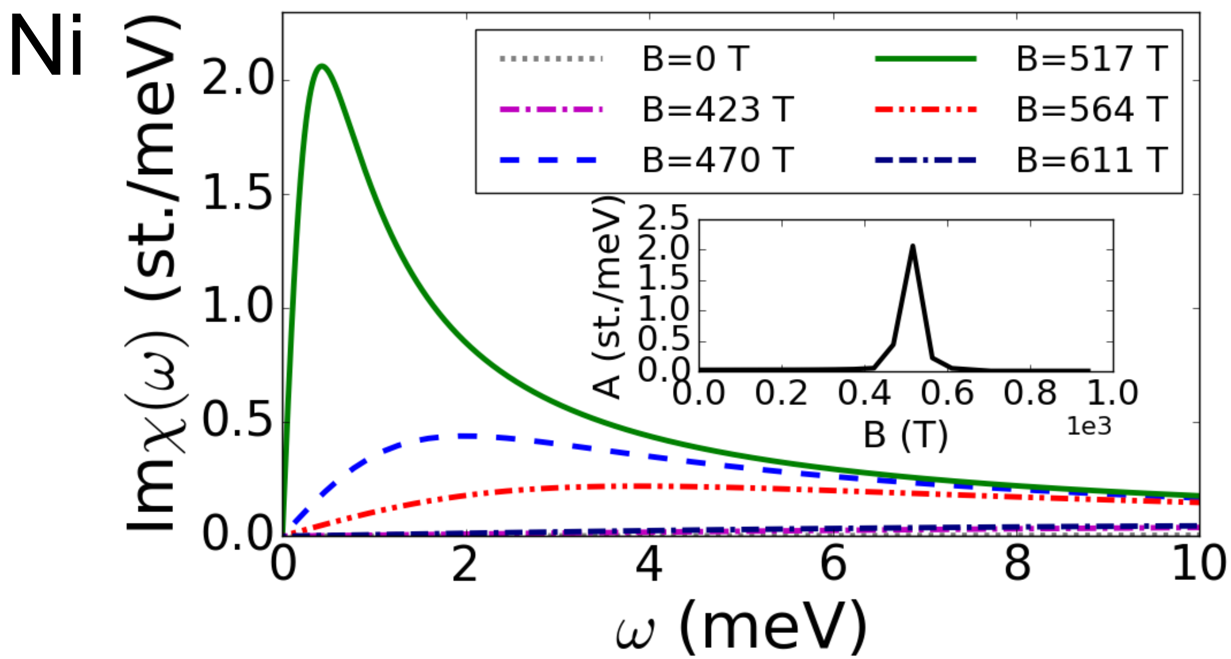
Magnetic transition from a proximity-effect





Azpiroz, dos Santos Dias, Schweflinghaus, Blügel, Lounis, PRL (2017); Editor's suggestion