Electron transport simulations from first principles

Krisztián Palotás
Budapest University of Technology and Economics
Department of Theoretical Physics
Budapest, Hungary

Methods

- Tunneling & ballistic transport:
  - Tight-binding (hopping)
  - Kubo-Greenwood linear response
  Implemented into the fully relativistic SKKR code
  Suitable to study magnetotransport, reletivistic effects (SOC, AMR)
  - Nonequilibrium Green's functions

- Tunneling transport only:
  STM simulations, different levels of theories:
  - 1D WKB (QM)
  - 3D WKB (atom superposition)
  - Tersoff-Hamann (LDOS)
  - Bardeen (perturbation theory, transfer Hamiltonian)
  - multiple scattering theory (Green's function methods)

- All above based on first principles electronic structure data
  first principles = ab initio = parameter-free, no fitting
  (Schrödinger equation or relativistic Dirac equation)

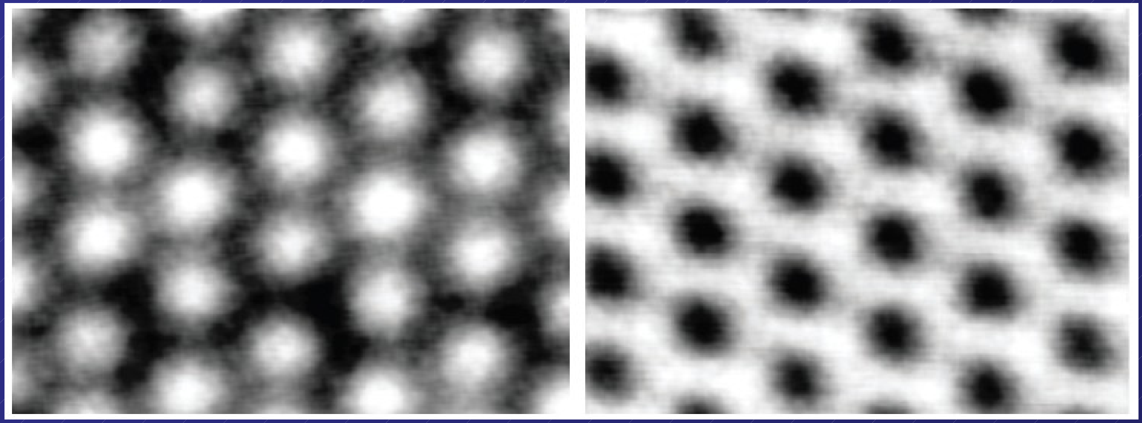
STM simulations

- **New SP-STM/STS simulation package** developed based on electronic structure data (from first principles), extending the work of Heinze, Appl. Phys. A 85, 407 (2006).
- Main features:
  1. Imaging noncollinear surface magnetic structures
  2. **Tip electronic structure** considered
  3. Bias voltage included
  4. Energy dependence of local spin quantization axes included
  5. **Easy combination with any electronic structure code**
- Studied examples:
  1. Tip-sensitivity of SP-STS: Fe(001)
  2. SP-STS: Cr ML on Ag(111)
  3. Bias-dependent magnetic contrast of SP-STM: Cr ML on Ag(111)
  4. Orbital dependent tunneling: contrast inversion on W(110)
- Conclusions

Motivation

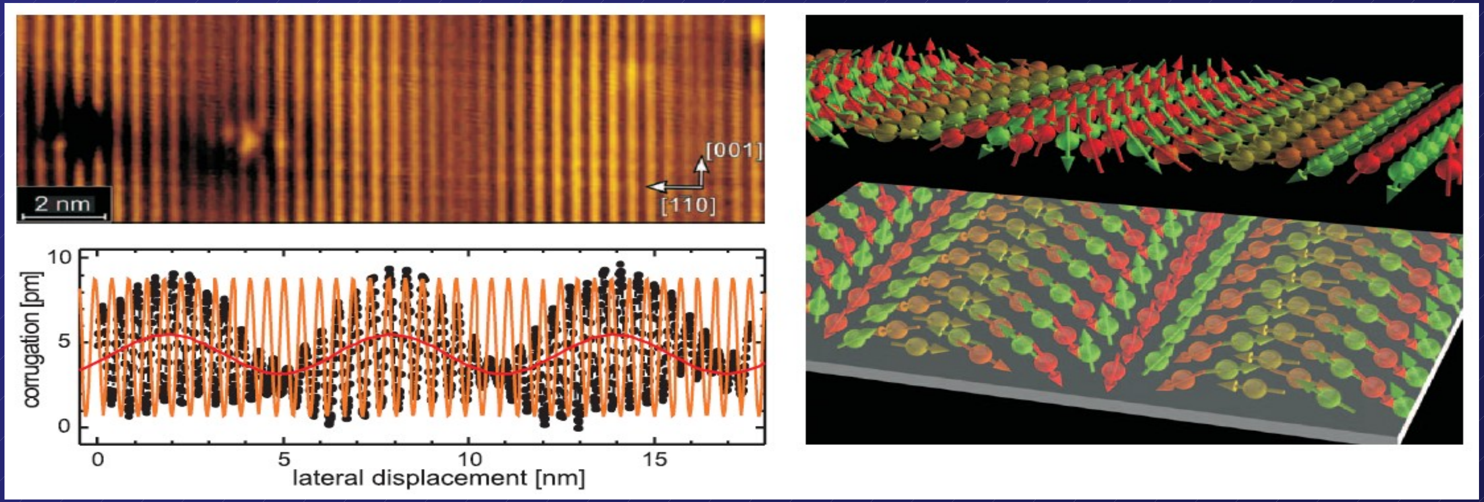
Recent experimental advances in spin-polarized STM:

Frustrated antiferromagnets: Mn/Ag(111), Gao and Wulfhekel, J.Phys.Cond.Matt. 22, 084021 (2010)



Another Review: Wiesendanger, Rev. Mod. Phys. 81, 1495 (2009)

Spin spirals: Mn/W(110), Bode et al., Nature 447, 190 (2007)



Recipe

Determine the **ground state magnetic structure** of the studied system (from first principles: Density Functional Theory; For larger systems: considering model Hamiltonians describing magnetic interactions or micromagnetic simulations)
Magnetic interactions from first principles: e.g.
Antal et al., Phys. Rev. B 77, 174429 (2008)
Multiscale approach: e.g.
Udvardi et al., Physica B 403, 402 (2008)
Self-consistent method based on band energy derivatives:
Balogh et al., Phys. Rev. B 86, 024406 (2012)

Calculate electronic structure and **simulate STM/STS** (**New SP-STM/STS simulation package**)

Compare the simulation results to experiments

Theoretical description

Heinze model [Appl. Phys. A 85, 407 (2006)]:

$$LDOS(\underline{R}_{TIP}(x,y,z),E_F) = \sum_{\alpha} e^{-2\kappa|\underline{R}_{TIP}-\underline{R}_{\alpha}|}\left(1 + P_T(E_F)P_S^{\alpha}(E_F)\cos\varphi_{\alpha}\right)$$

Assumption made:

Contribution to vacuum LDOS from spherical tail of atomic wave functions (**Independent orbital approximation**)

LDOS considered in our model at arbitrary energies:

$$LDOS(x,y,z,E,V) = \Delta E \sum_{\alpha} e^{-2\kappa(E,V)|\underline{R}_{TIP}(x,y,z)-\underline{R}_{\alpha}|} n_T(E) n_S^{\alpha}(E)[1+P_T(E)P_S^{\alpha}(E)cos\varphi_{\alpha}(E)]$$

Energy dependent vacuum decay: $\kappa(E,V) = \frac{1}{\hbar}\sqrt{2m\left(\frac{\phi_S+\phi_T+eV}{2}+E_F^S-E\right)}$

Virtual diff. conductance: $\frac{dI}{dU}(U,V) = \frac{e^2}{h}\Delta E \cdot LDOS(E_F^S+eU,V)$

Total current: $I(V) = \int_0^V dU \frac{dI}{dU}(U,V)$ Palotás et al., PRB 84, 174428

Diff. conductance: $\frac{dI}{dV}(V') = \frac{dI}{dU}(V',V') + \int_0^{V'} dU \left.\frac{\partial}{\partial V}\frac{dI}{dU}(U,V)\right|_{V=V'}$

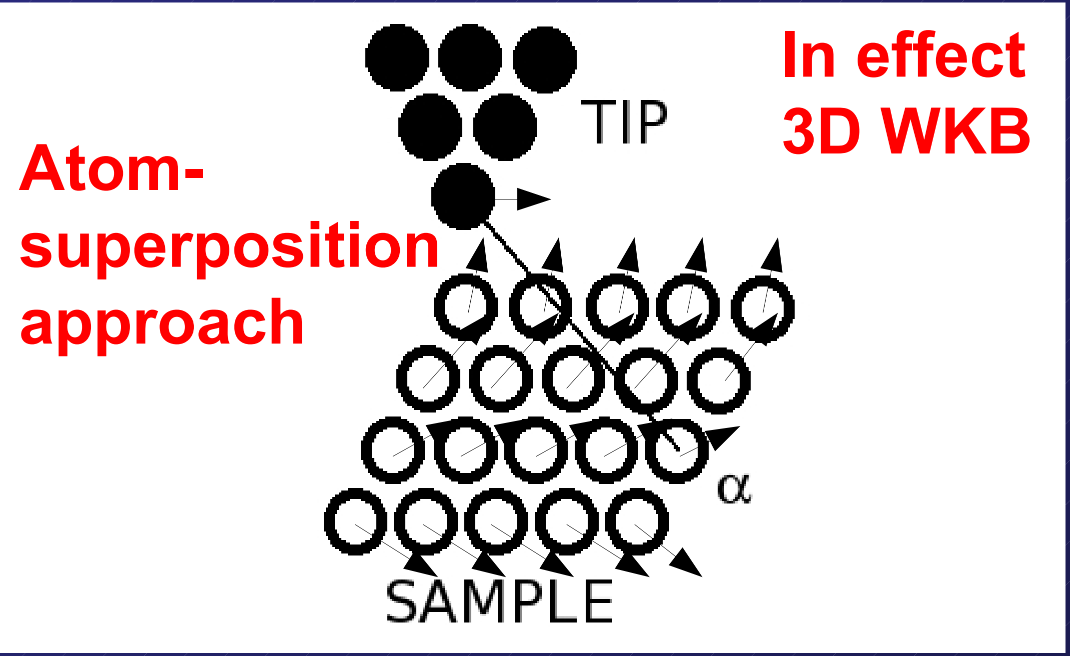
Theoretical description

Modified electron local density of states at tip apex position $\underline{R}_{TIP}$ at energy E in flavour of the **spin-pol. Tersoff-Hamann model**:

$$LDOS(x,y,z,E,V) = \Delta E \sum_{\alpha} e^{-2\kappa(E,V)|\underline{R}_{TIP}(x,y,z)-\underline{R}_{\alpha}|} n_T(E) n_S^{\alpha}(E)[1+P_T(E)P_S^{\alpha}(E)cos\varphi_{\alpha}(E)]$$

Topographic **TOPO**: $n_T n_S$ and magnetic **MAGN**: $m_T m_S \cos\varphi$ contributions

Sum over α has to be carried out over all atoms on the surface:



Palotás et al., Phys. Rev. B 83, 214410 (2011)

Theoretical description

$$LDOS(x,y,z,E,V)=\Delta E\sum_{\alpha} e^{-2\kappa(E,V)|\underline{R}_{TIP}(x,y,z)-\underline{R}_{\alpha}|}n_T(E)n_S^{\alpha}(E)[1+P_T(E)P_S^{\alpha}(E)cos\varphi_{\alpha}(E)]$$

φ_α: angle between local spin quant. axes of tip apex and the αth atom.

P_T and P_S is the spin polarization of tip apex and sample atoms, respectively.

The atom-projected charge and magnetization DOS (PDOS):

$$n(E)=n_{\uparrow}(E)+n_{\downarrow}(E)$$
$$m(E)=n_{\uparrow}(E)-n_{\downarrow}(E)$$

Spin polarization (**COLLINEAR calc.**):

$$P_{T,S}(E)=\left(n_{T,S}^{\uparrow}(E)-n_{T,S}^{\downarrow}(E)\right)/\left(n_{T,S}^{\uparrow}(E)+n_{T,S}^{\downarrow}(E)\right)$$

NONCOLLINEAR calc. [Palotás et al., PRB 84, 174428 (2011)]:

$$n_{T,S}(E)=\sum_{\underline{k}}\sum_{j}\frac{1}{G\sqrt{\pi}}e^{-\left(E-\varepsilon^{j}_{T,S}(\underline{k})\right)^2/G^2}\int_{atomic\ volume} d^3r\,\Psi^{j\underline{k}\dagger}_{T,S}(\underline{r})\Psi^{j\underline{k}}_{T,S}(\underline{r})$$

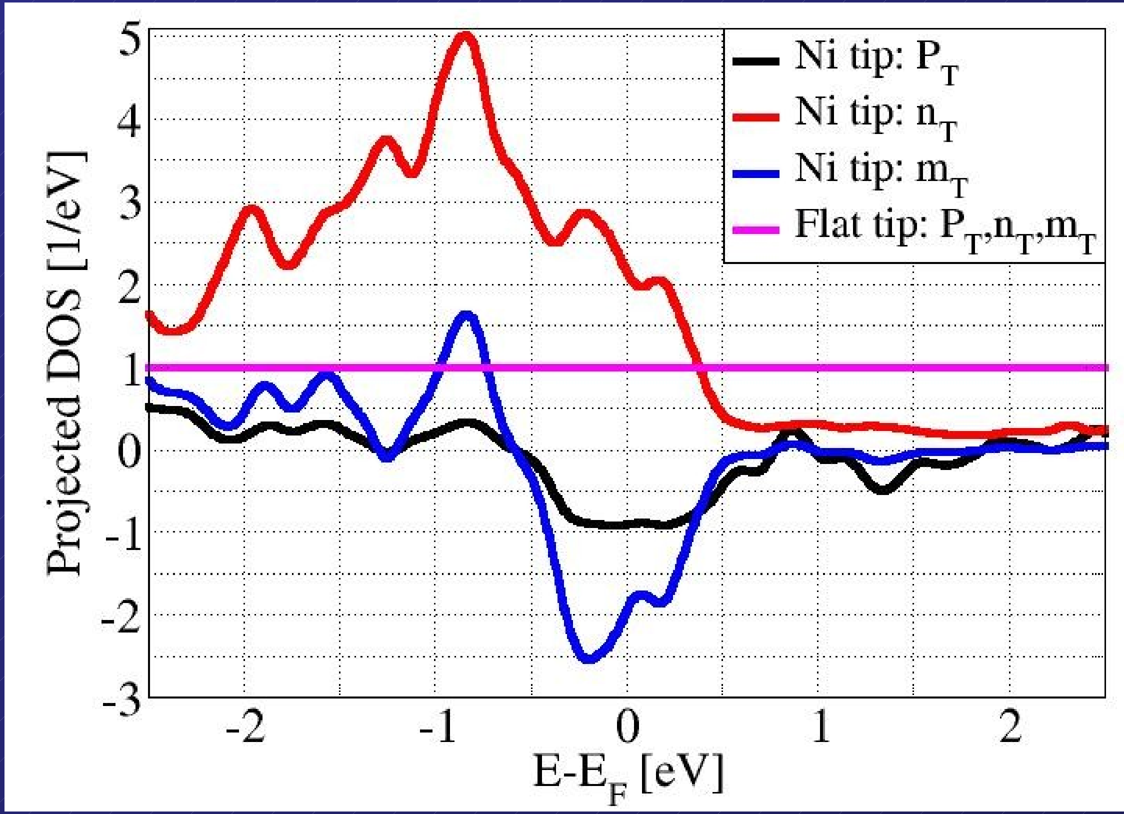
$$\underline{m}_{T,S}(E)=\sum_{\underline{k}}\sum_{j}\frac{1}{G\sqrt{\pi}}e^{-\left(E-\varepsilon^{j}_{T,S}(\underline{k})\right)^2/G^2}\int_{atomic\ volume} d^3r\,\Psi^{j\underline{k}\dagger}_{T,S}(\underline{r})\underline{\sigma}\Psi^{j\underline{k}}_{T,S}(\underline{r})$$

Spin polarization vector: $\underline{P}_{T,S}(E)=\frac{\underline{m}_{T,S}(E)}{n_{T,S}(E)}$

Model tips

Three tip models considered:

1. **Ideal** maximally spin-polarized electronically **flat tip**
2. **Ni(110) tip** with single Ni atom apex, VASP+PAW, GGA-PW91
   Symm. 7 lay. Ni(110) slab+apex atom, 3x3 cell, 36 IBZ k-points
   P_T close to -1 in the energy range [-0.3eV,+0.3eV], ϕ_T= 4.52 eV
3. **Fe(001) tip with Cr apex**, data from Ferriani et al. PRB 82, 054411 (2010)



Projected DOS onto the tip apex atom: Charge (*n*) and magnetization (*m*) DOS:

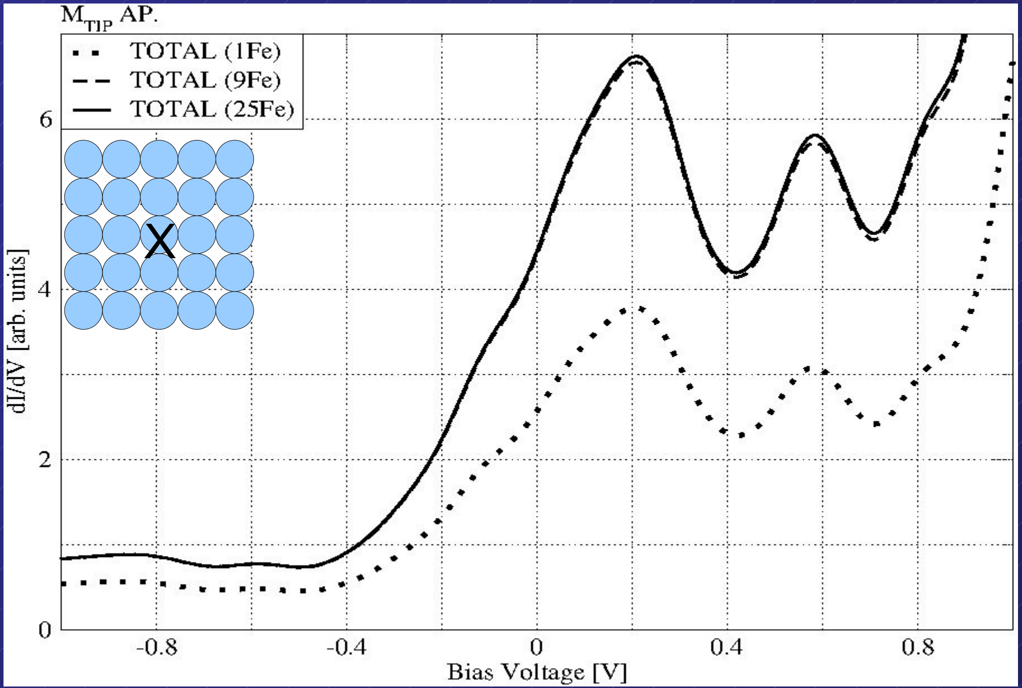
$$n(E) = n_\uparrow(E) + n_\downarrow(E)$$
$$m(E) = n_\uparrow(E) - n_\downarrow(E)$$

Spin-polarization:
$P(E)=m(E)/n(E)$

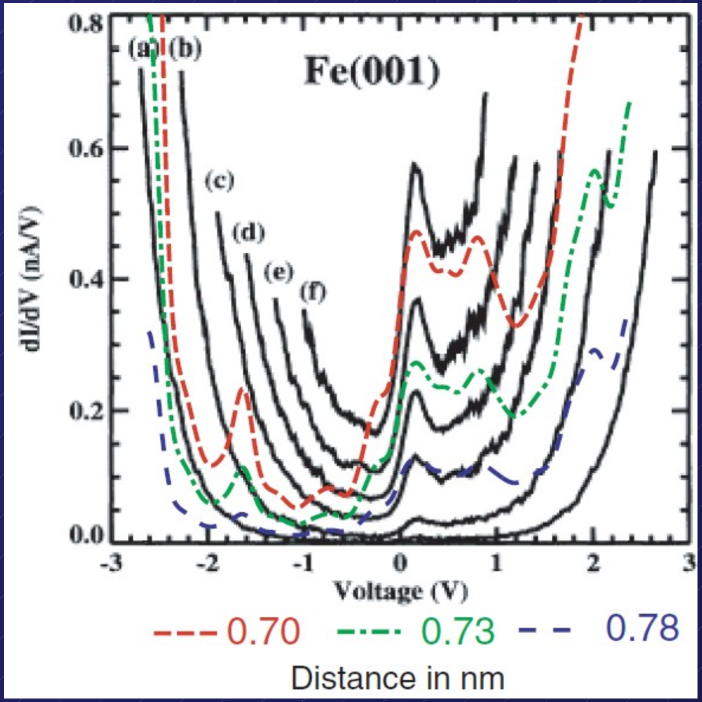
Differential tunnelling spectrum of Fe(001)

Simulation details: VASP+PAW, GGA-PW91,
Symmetric 13 layers Fe(001) slab, 1x1 cell, 72 k-points in IBZ

Ideal tip



Experiment and BSKAN:



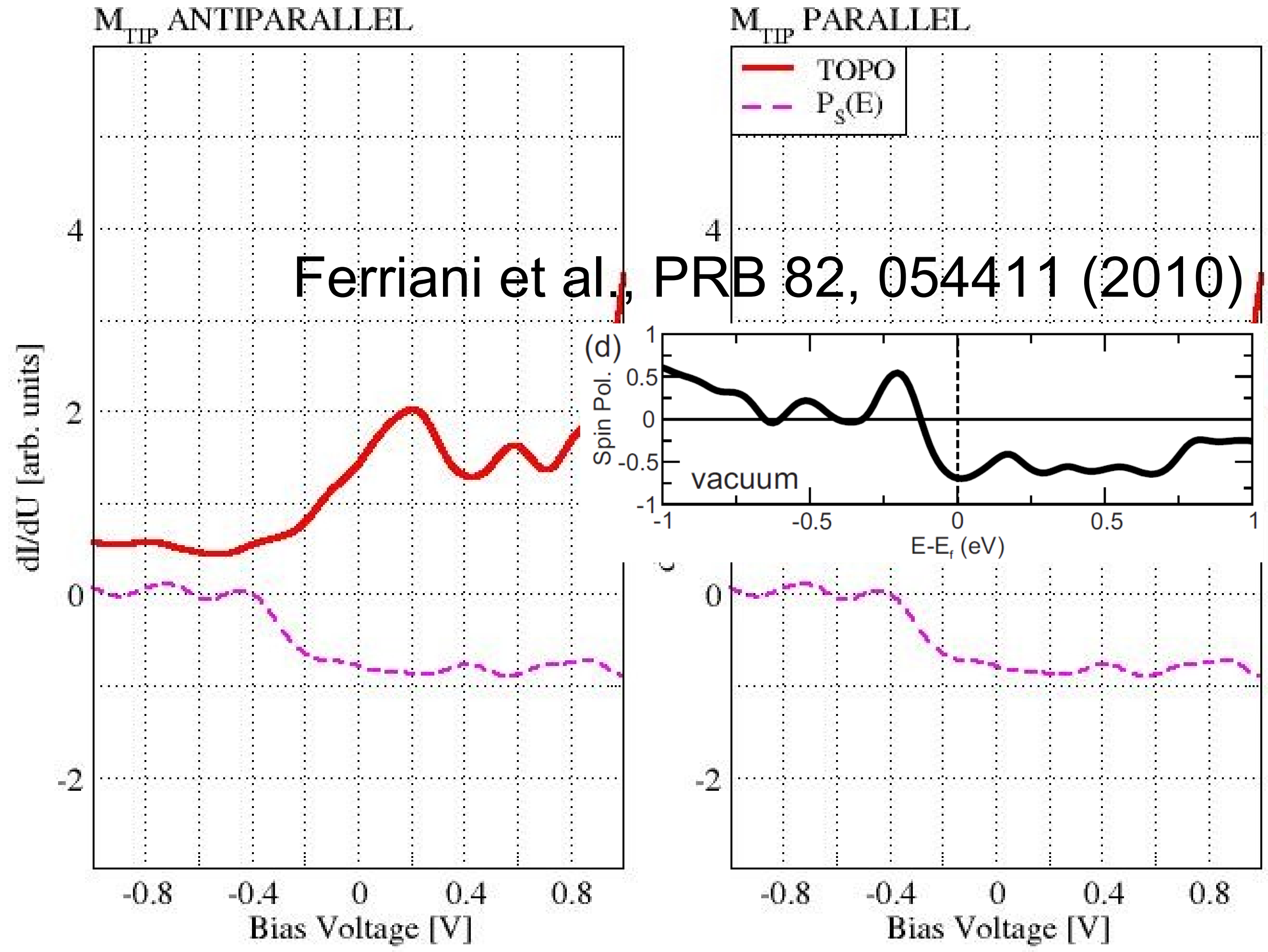
Peak position at +0.20V agrees with exp. and more sophisticated calc.
Experiment: Stroscio et al. PRL 75, 2960 (1995).
Theor. results from multiple scattering theory of tunnelling (BSKAN code):
Palotás and Hofer: J. Phys. Cond. Matt. 17, 2705 (2005).

Differential tunnelling spectrum of Fe(001)

Ideal tip: ***dI/dU(U)***

Palotás et al., PRB 83, 214410 (2011)

Ferriani et al., PRB 82, 054411 (2010)



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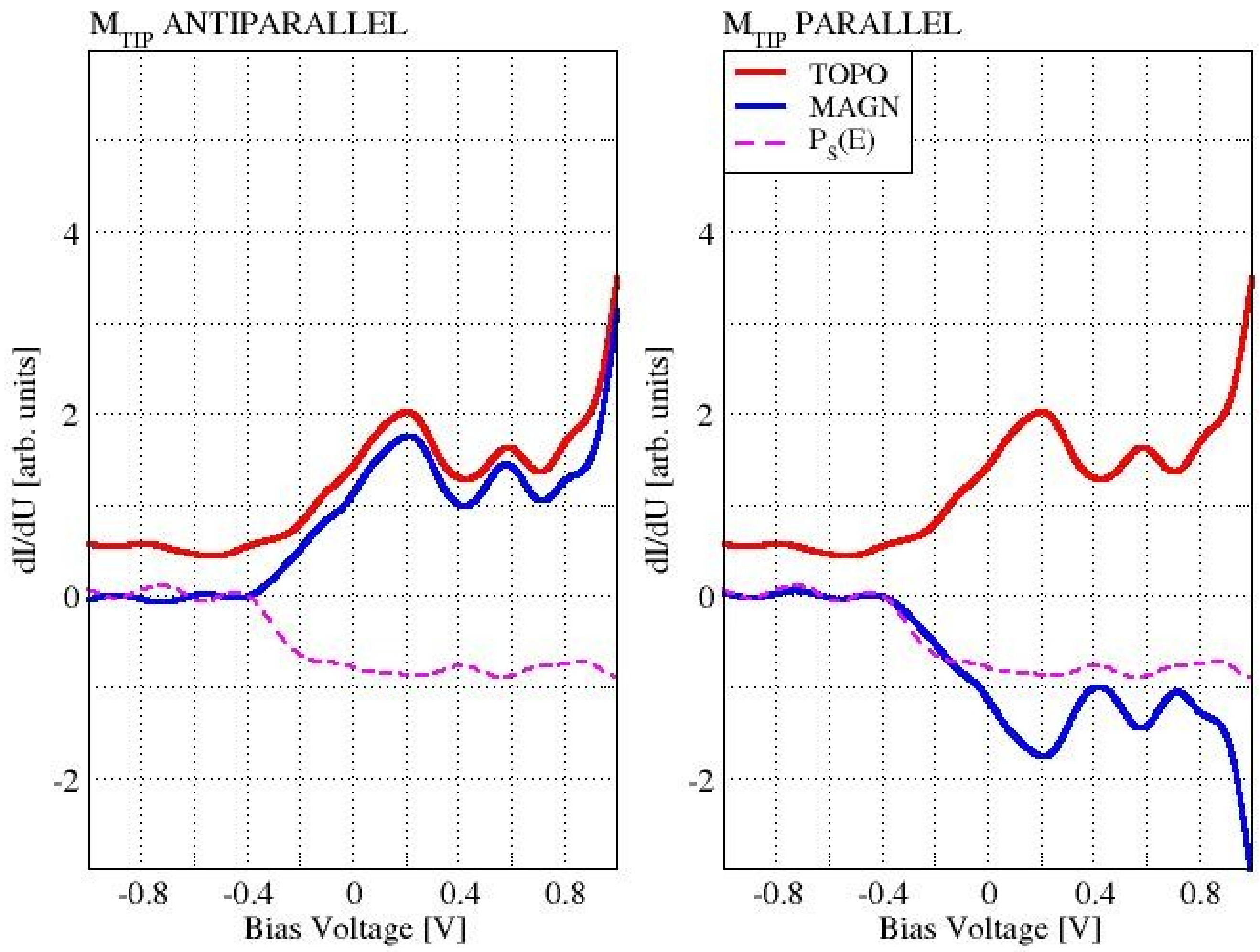

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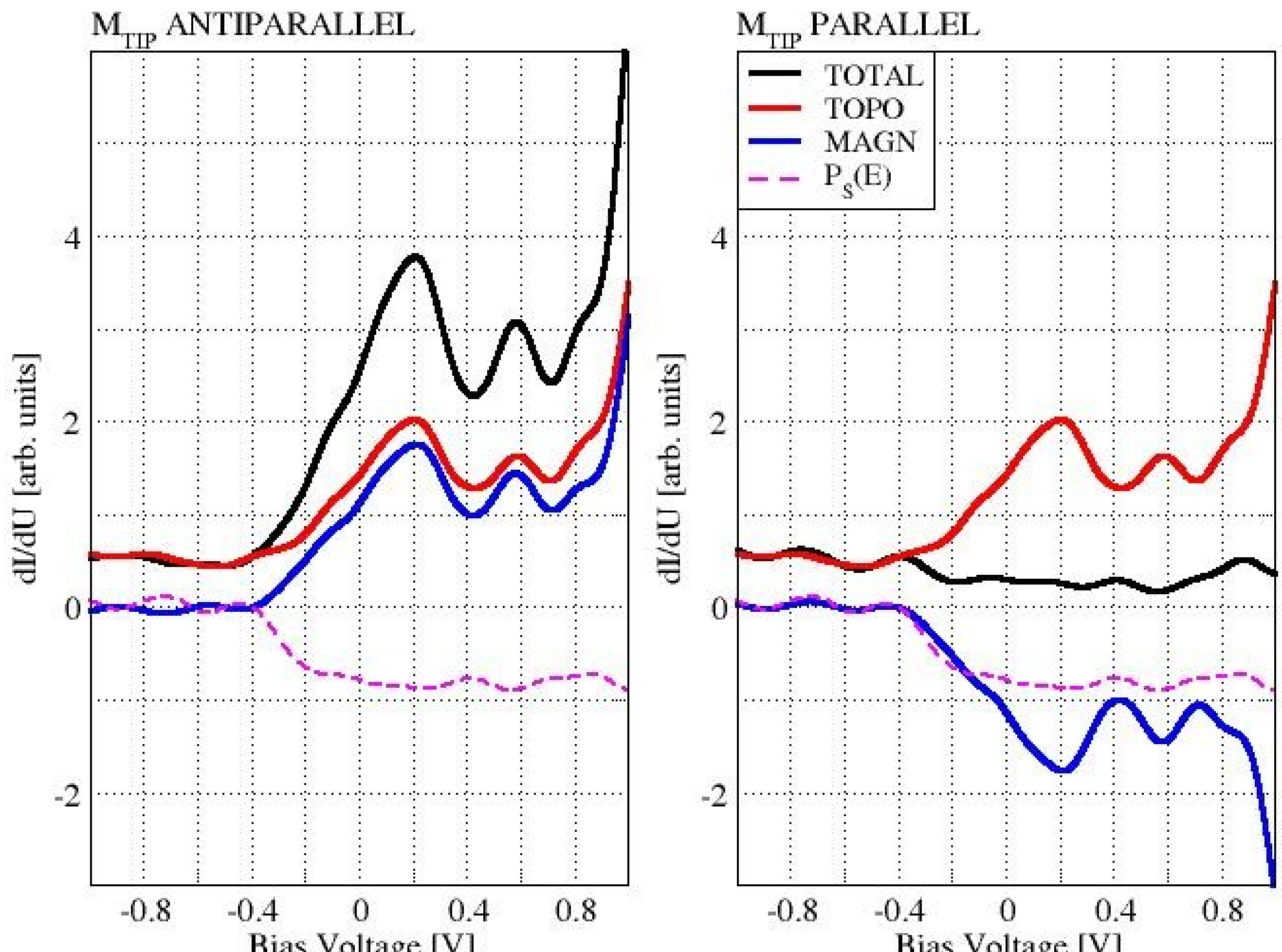
Ideal tip: ***dI/dU(U)***

Palotás et al., PRB 83, 214410 (2011)



Sensitivity of STS can be tuned by changing tip magnetization direction!

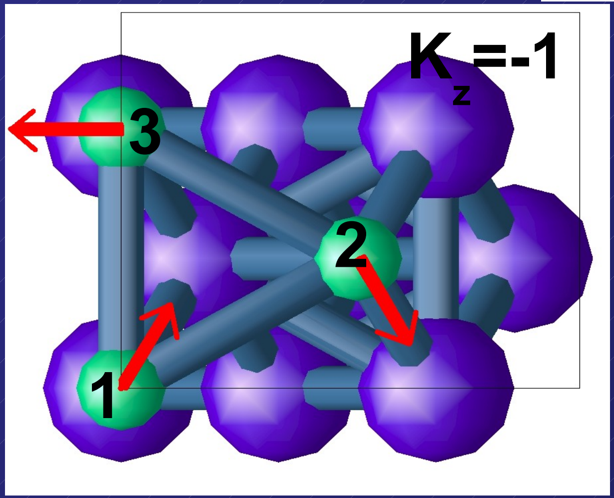
Enhanced sensitivity is possible!

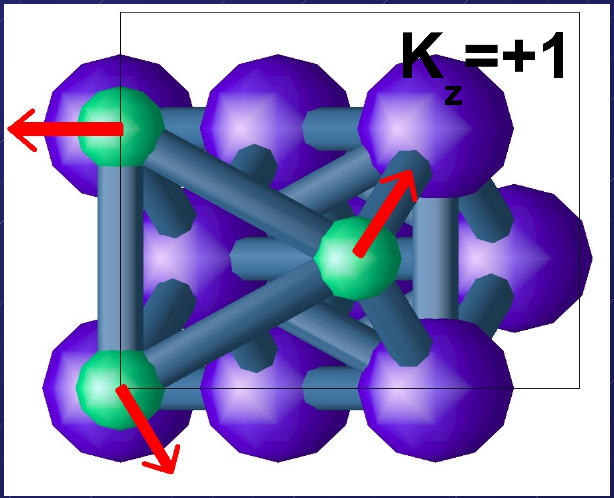
Imaging noncollinear surface magnetic structures
Cr monolayer on Ag(111) surface

Simulation details: VASP+PAW+SOC, GGA-PW91
Symmetric 5 layers Ag slab+Cr layers, 121 BZ k-points
Two different magnetic chiralities characterized by

$$\underline{K} = \frac{2}{3\sqrt{3}}\left(\underline{e}_S^1 \times \underline{e}_S^2 + \underline{e}_S^2 \times \underline{e}_S^3 + \underline{e}_S^3 \times \underline{e}_S^1\right)$$ chirality vector

Magnetic unit cell: $\left(\sqrt{3} \times \sqrt{3}\right) R30°$ Palotás et al., PRB 84, 174428

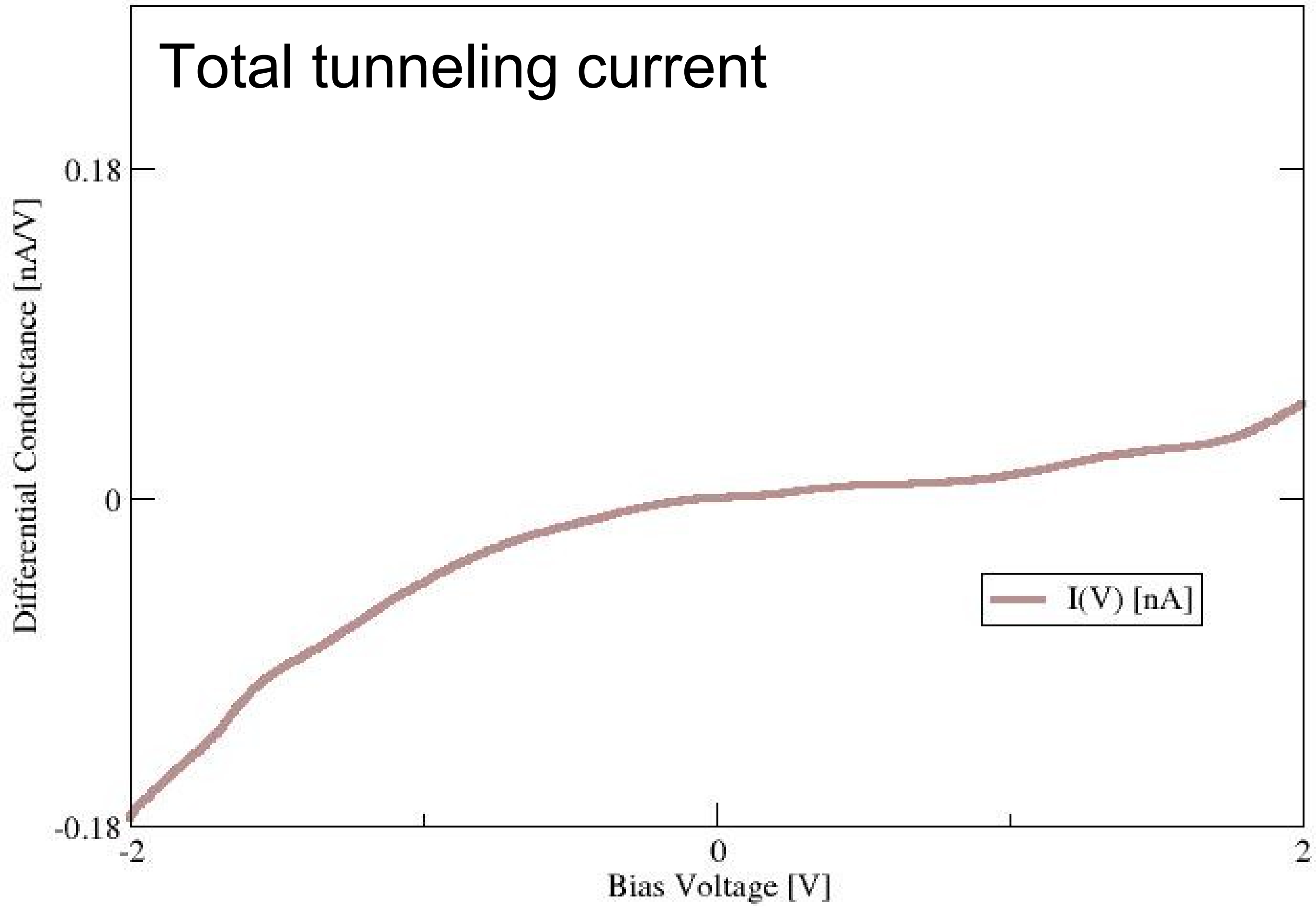




K_z=-1 energetically favored by 1.1 meV (FM state 1.04 eV higher)
Cr: AFM coupling → noncollinear 120˚ Néel state, $|M_{Cr}|$=3.73 μ_B

Cr monolayer on Ag(111) surface

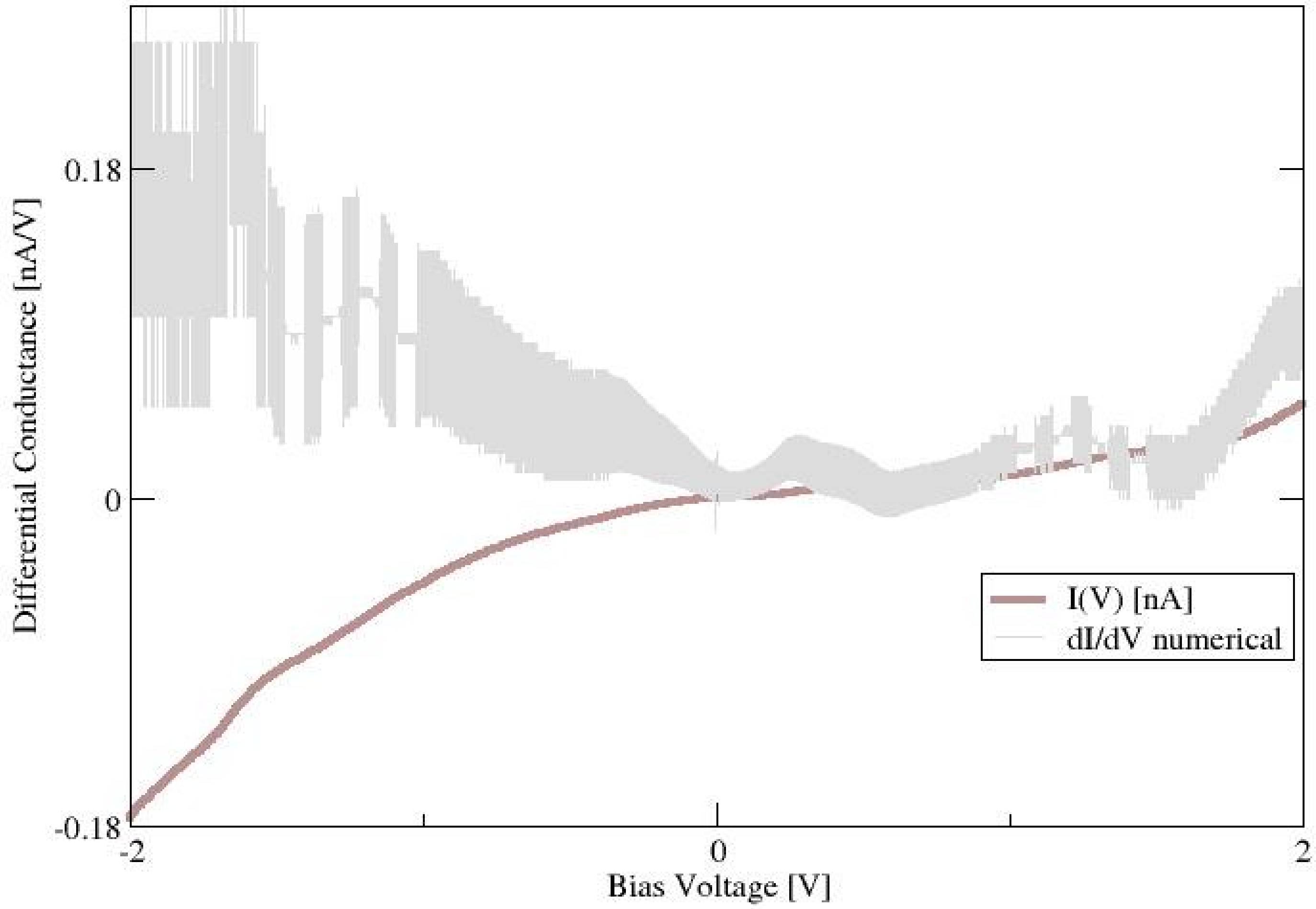
Tip: Cr adatom on Fe(001) [Ferriani et al. PRB 82, 054411 (2010)]
@ z=3.5 Angstoms above surface Cr atom



Palotás et al., Phys. Rev. B 85, 205427 (2012)

Cr monolayer on Ag(111) surface

Differential conductance dI/dV



Palotás et al., Phys. Rev. B 85, 205427 (2012)

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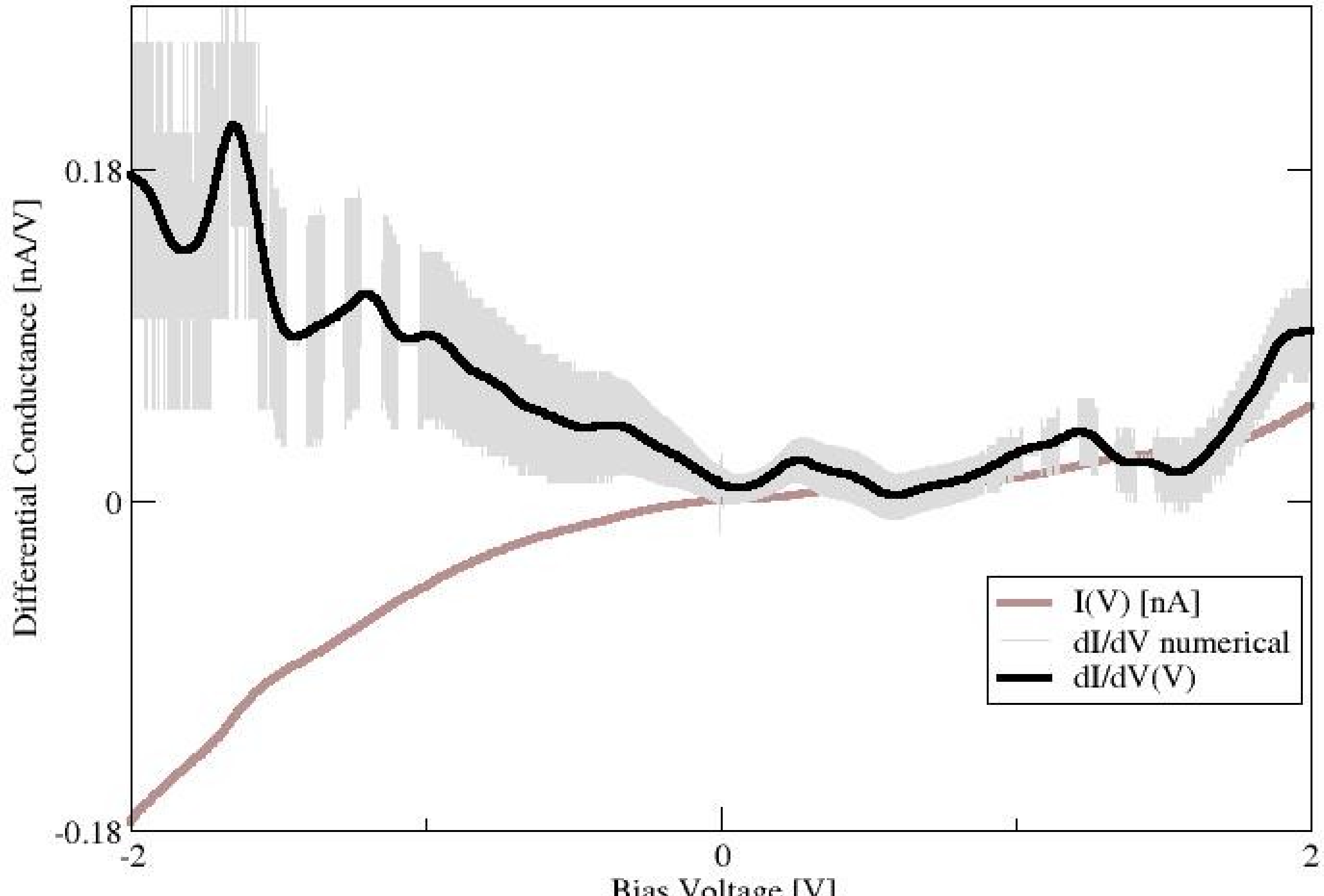
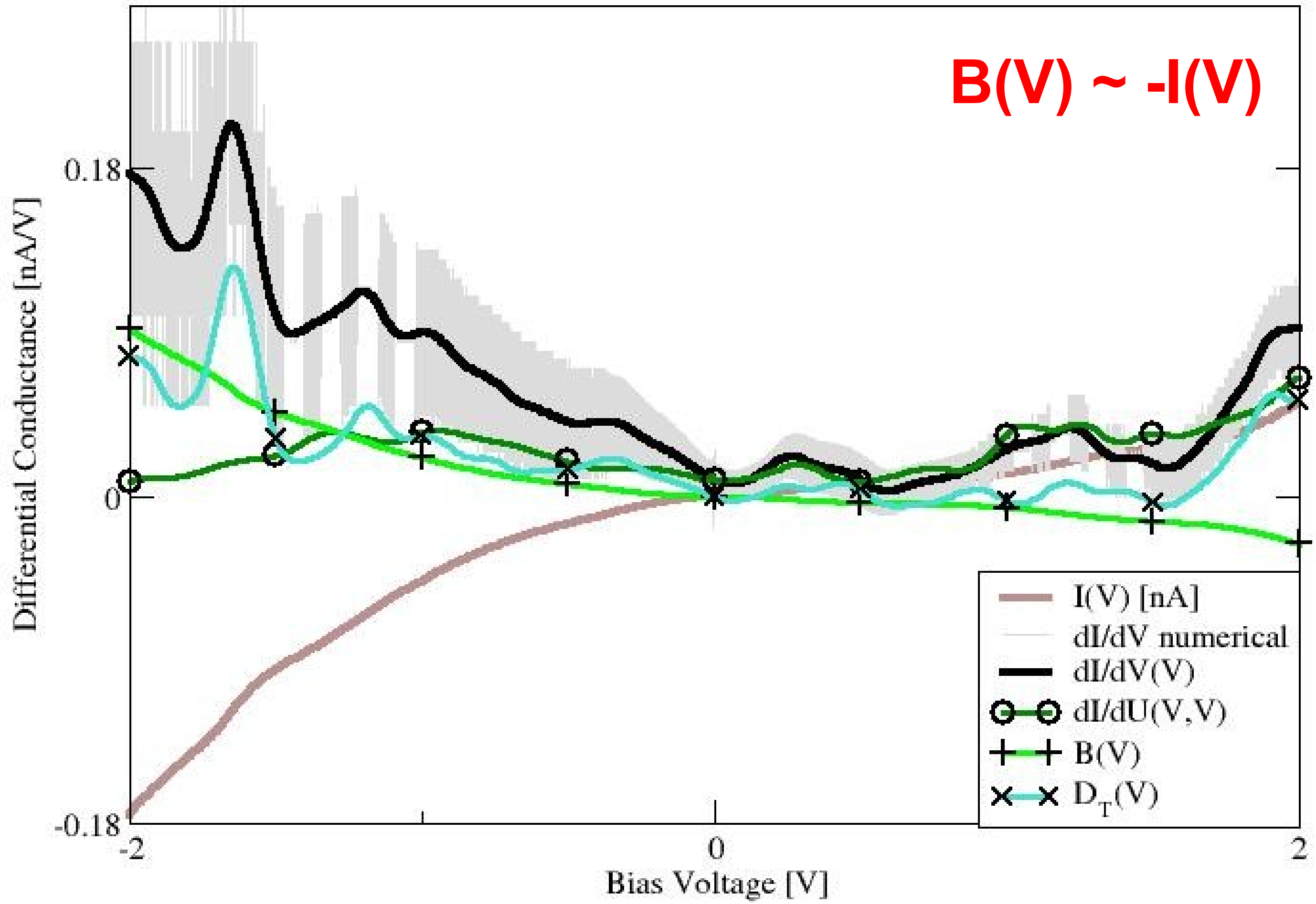


Palotás et al., Phys. Rev. B 85, 205427 (2012)

Cr monolayer on Ag(111) surface

$$\frac{dI_{TOTAL}}{dV}(x,y,z,V) = \frac{dI}{dU}(x,y,z,V,V) + B(x,y,z,V) + D_T(x,y,z,V)$$



Palotás et al., Phys. Rev. B 85, 205427 (2012)

Magnetic asymmetry: $A_{MAGN}(x,y,z,V) = \frac{dI^P/dV(x,y,z,V) - dI^{AP}/dV(x,y,z,V)}{dI^P/dV(x,y,z,V) + dI^{AP}/dV(x,y,z,V)}$.
Relation to the effective spin polarization

Differential conductance:

$$\frac{dI_{TOTAL}}{dV}(x,y,z,V) = \frac{dI}{dU}(x,y,z,V,V) + B(x,y,z,V) + D_T(x,y,z,V)$$

~LDOS

background ($\partial T/\partial V$)

tip-derivative ($\partial n_T/\partial V$)

Magnetic asymmetry:

$$A^{dI/dV}(x,y,z,V) = \frac{dI^P_{\mathrm{MAGN}}/dV(x,y,z,V)}{dI_{\mathrm{TOPO}}/dV(x,y,z,V)}$$

≠ESP

$$= \frac{dI^P_{\mathrm{MAGN}}/dU(x,y,z,V,V) + B^P_{\mathrm{MAGN}}(x,y,z,V) + D_T^{\mathrm{MAGN},P}(x,y,z,V)}{dI_{\mathrm{TOPO}}/dU(x,y,z,V,V) + B_{\mathrm{TOPO}}(x,y,z,V) + D_T^{\mathrm{TOPO}}(x,y,z,V)}$$

Effective spin polarization:

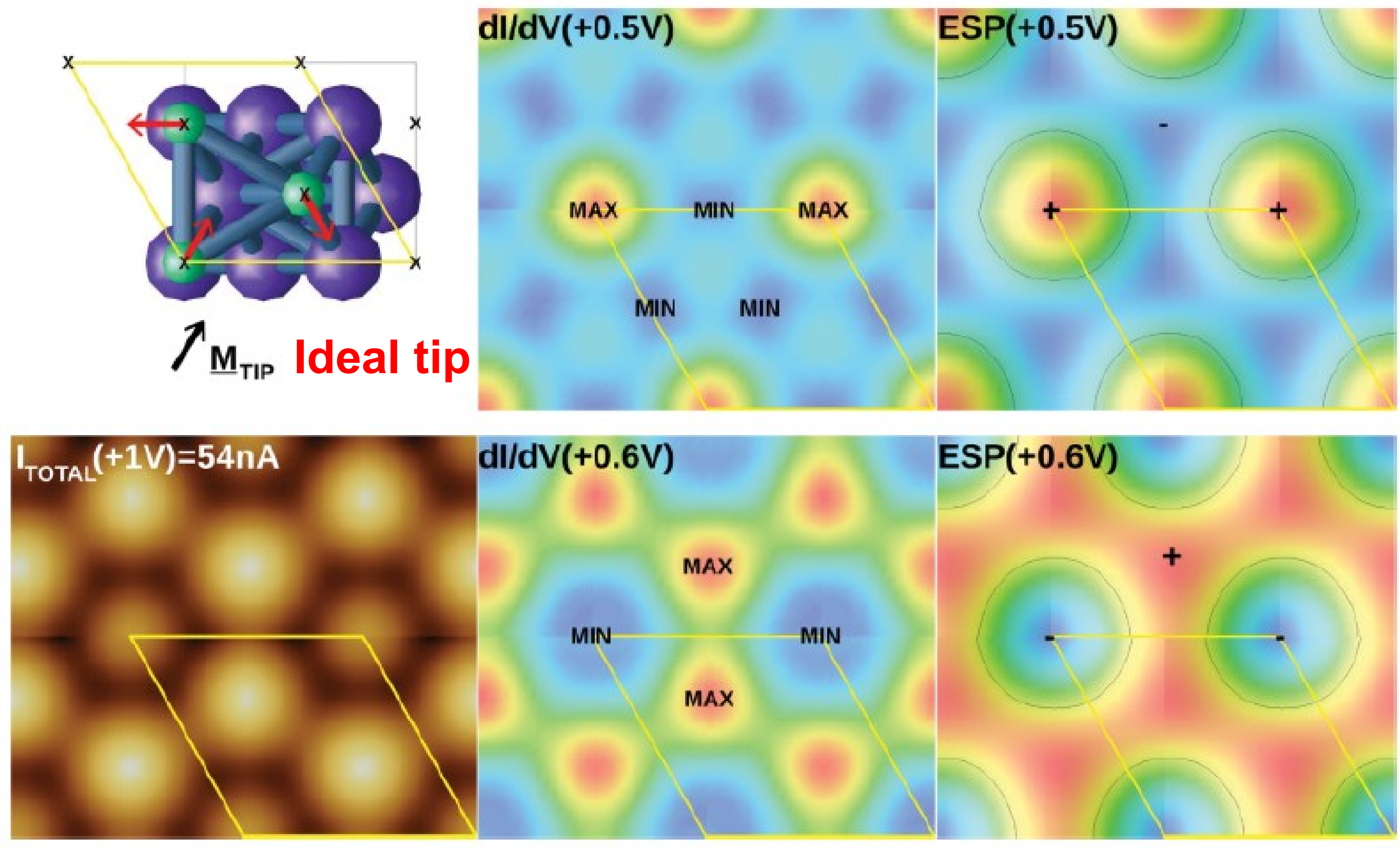
$$A^{dI/dU}(x,y,z,V) = \frac{dI^P_{\mathrm{MAGN}}/dU(x,y,z,V,V)}{dI_{\mathrm{TOPO}}/dU(x,y,z,V,V)}$$

$$= \underline{P}_T(E_F^T)\underline{P}_S(x,y,z,E_F^S + eV)$$

Palotás et al.,
PRB 85, 205427 (2012)

Cr monolayer on Ag(111) surface

2D dI/dV & ESP maps on constant current contour



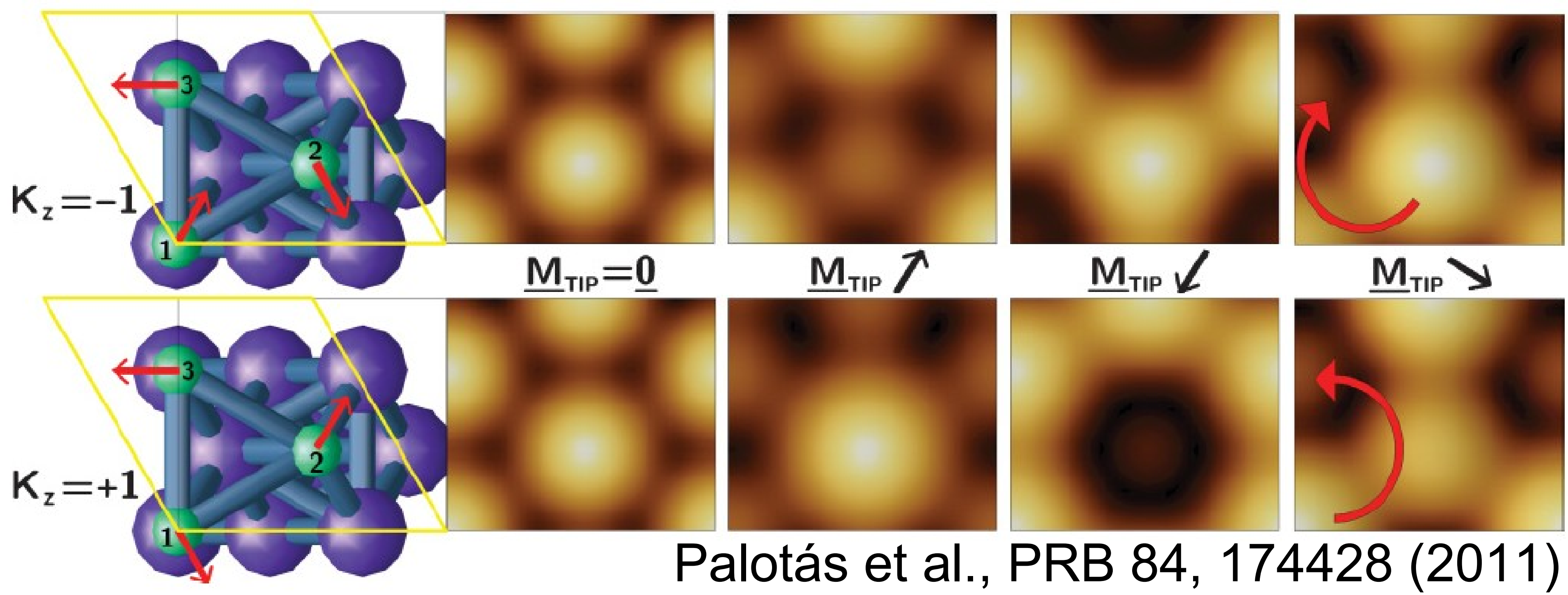
Palotás et al., Phys. Rev. B 85, 205427 (2012)

Cr monolayer on Ag(111) surface

Dependence of magnetic contrast on tip magnetization orientation

Ideal magnetic tip, 0 V bias, ϕ_S= 4.47 eV

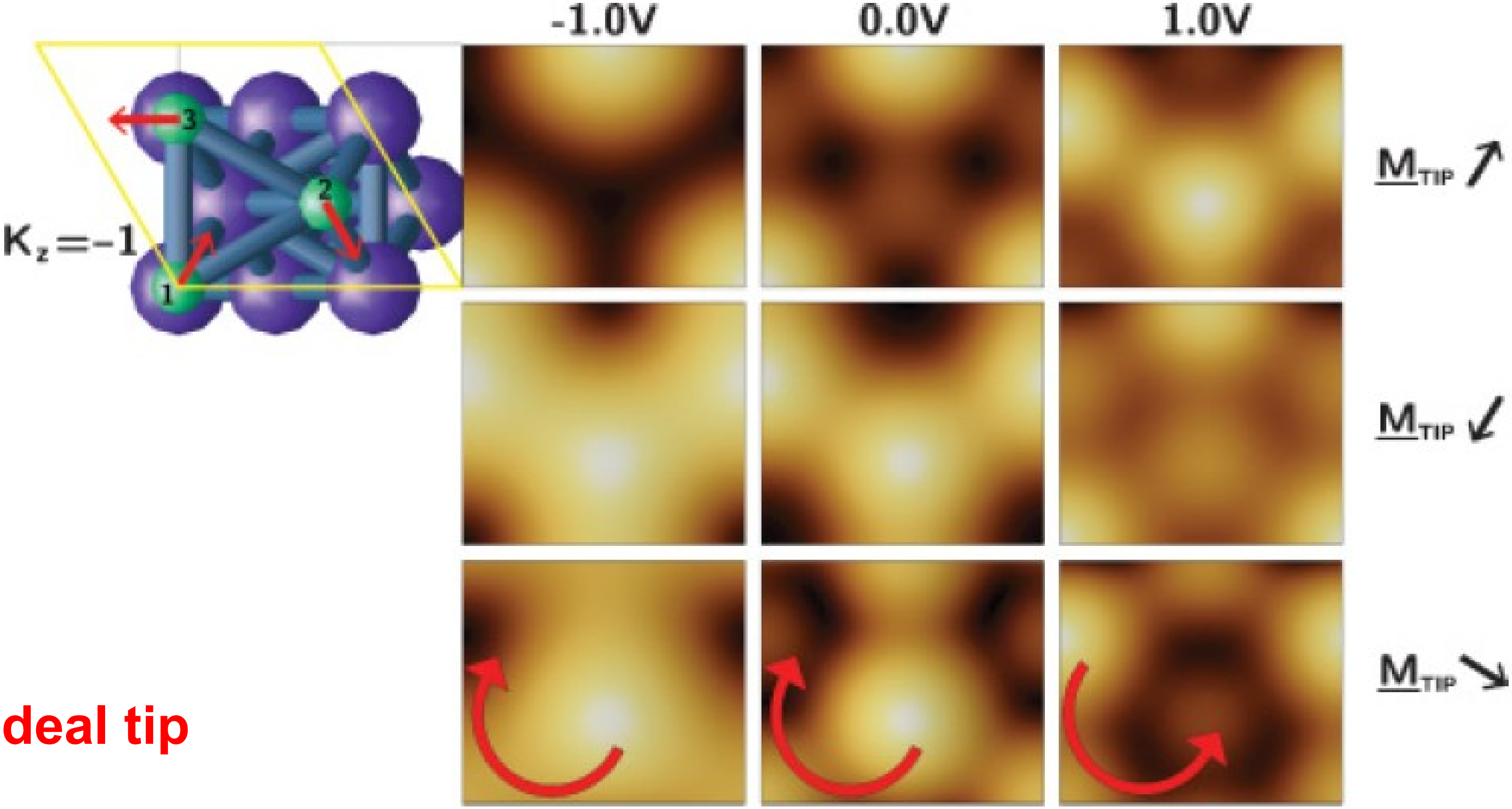
Qualitatively similar images obtained in SP-STM exp./sim. for Néel states:
Cr/Ag(111) Heinze, Appl. Phys. A 85, 407 (2006) (sim.),
Mn/Ag(111) Gao and Wulfhekel, Phys. Rev. Lett. 101, 267205 (2008) (exp.),
Cr/Pd(111) Waśniowska et al., Phys. Rev. B 82, 012402 (2010) (exp.+sim.)



Palotás et al., PRB 84, 174428 (2011)

Cr monolayer on Ag(111) surface

Bias dependent magnetic contrast

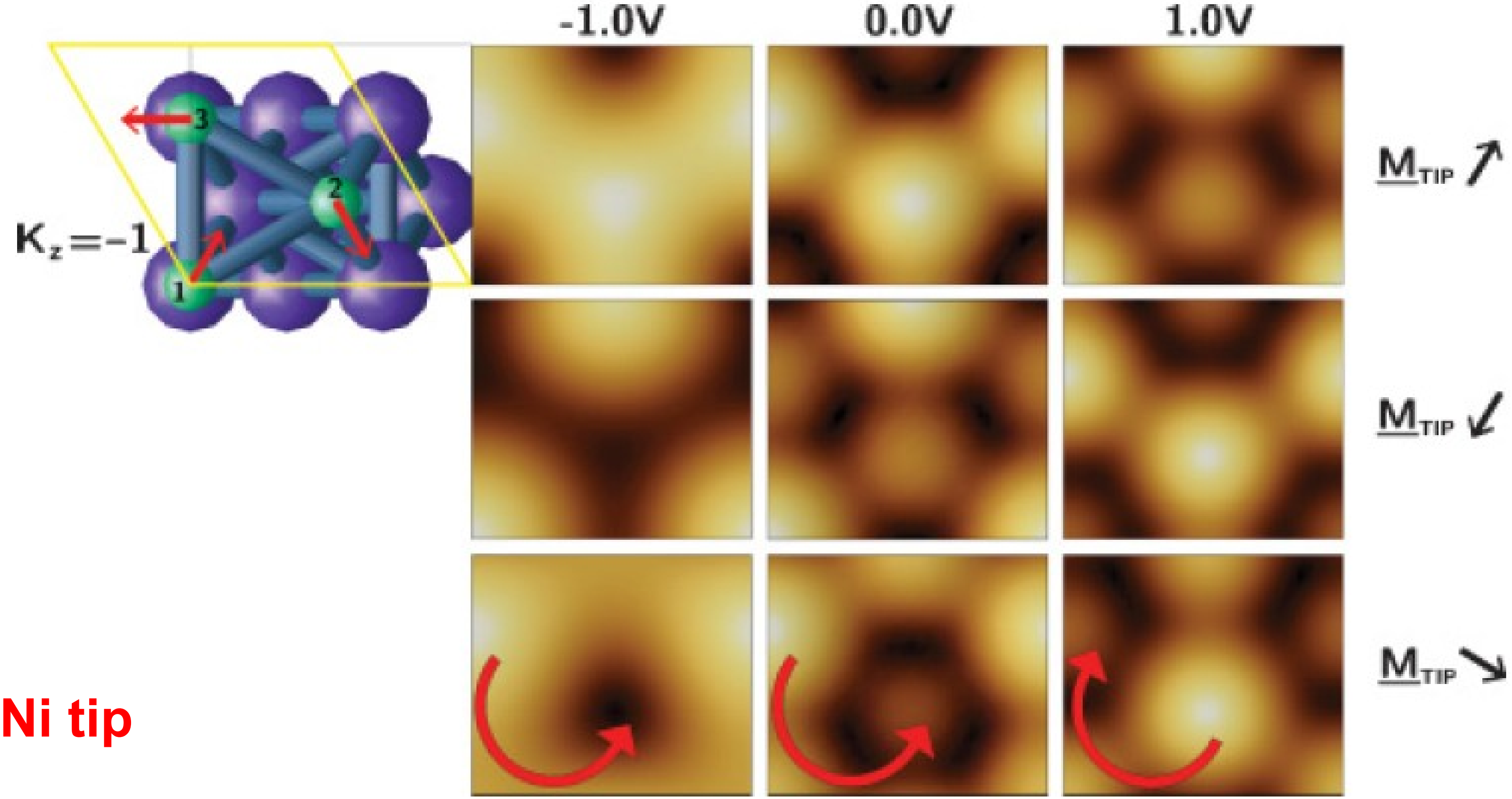


Ideal tip

Palotás et al., PRB 84, 174428 (2011)

Cr monolayer on Ag(111) surface

Bias dependent magnetic contrast



Ni tip

Be careful when interpreting SP-STM images!

Palotás et al., PRB 84, 174428 (2011)

Relation between constant current and constant height STM images

Height contrast between A and B lateral surface points in nonmagnetic STM: (Chen: Introduction to STM, 1993)

$$\Delta z^{AB}_{\text{nonmagn}}(z_1,V) = -\frac{\Delta I^{AB}(z_1,V)}{\partial I^{\text{av}}/\partial z(z_1,V)}$$

Total contrast in spin-polarized STM:

$$\begin{aligned}\Delta z^{AB}(z_1,V) &= \Delta z^{AB}_{\text{TOPO}}(z_1,V) + \Delta z^{AB}_{\text{MAGN}}(z_1,V)\\ &= -\frac{\Delta I^{AB}_{\text{TOPO}}(z_1,V)}{\partial I^{\text{av}}_{\text{TOT}}/\partial z(z_1,V)} - \frac{\Delta I^{AB}_{\text{MAGN}}(z_1,V)}{\partial I^{\text{av}}_{\text{TOT}}/\partial z(z_1,V)}\end{aligned}$$

Averaged current over the scan area:

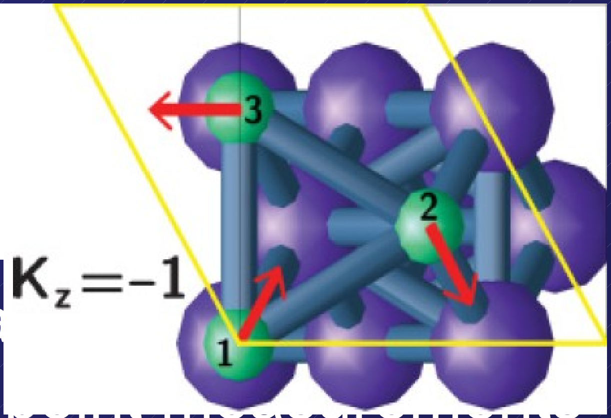
$$I^{\text{av}}_{\text{TOT}}(z,V) = \frac{1}{N_x N_y}\sum_{i=1}^{N_x}\sum_{j=1}^{N_y} I_{\text{TOT}}(x_i,y_j,z,V)$$

Palotás, Phys. Rev. B 87, 024417 (2013)

Magnetic contrast estimation

Assumptions: Atomically flat surface consisting of chemically equivalent & magnetically inequivalent atoms

$$\Delta z^{AB}(z_1,V) = \Delta z^{AB}_{TOPO}(z_1,V) + \Delta z^{AB}_{MAGN}(z_1,V)$$
$$= -\frac{\Delta I^{AB}_{TOPO}(z_1,V)}{\partial I^{av}_{TOT}/\partial z(z_1,V)} - \frac{\Delta I^{AB}_{MAGN}(z_1,V)}{\partial I^{av}_{TOT}/\partial z(z_1,V)}$$



We want to avoid scanning the full scan a
predict the magnetic contrast from single

→ 2 propositions: (measurements over points A and B needed)

$$\Delta z^{AB}_{I}(z_1,V) = -\frac{\Delta I^{AB}_{MAGN}(z_1,V)}{\partial I^{A}_{TOPO}/\partial z(z_1,V)} = \frac{I^{A}_{MAGN}(z_1,V) - I^{B}_{MAGN}(z_1,V)}{2\kappa^{A}_{TOPO}(V) I^{A}_{TOPO}(z_1,V)}$$

$$\Delta z^{AB}_{II}(z_1,V) = -\frac{\Delta I^{AB}_{MAGN}(z_1,V)}{\partial I^{av.AB}_{TOT}/\partial z(z_1,V)} = \frac{I^{A}_{MAGN}(z_1,V) - I^{B}_{MAGN}(z_1,V)}{2\kappa^{av.AB}_{TOT}(V) I^{av.AB}_{TOT}(z_1,V)}$$

Palotás, Phys. Rev. B 87, 024417 (2013)

Magnetic contrast estimation

$$\Delta z_I^{AB}(z_1,V) = -\frac{\Delta I_{\mathrm{MAGN}}^{AB}(z_1,V)}{\partial I_{\mathrm{TOPO}}^{A}/\partial z(z_1,V)} = \frac{I_{\mathrm{MAGN}}^{A}(z_1,V) - I_{\mathrm{MAGN}}^{B}(z_1,V)}{2\kappa_{\mathrm{TOPO}}^{A}(V) I_{\mathrm{TOPO}}^{A}(z_1,V)}$$

$$\Delta z_{II}^{AB}(z_1,V) = -\frac{\Delta I_{\mathrm{MAGN}}^{AB}(z_1,V)}{\partial I_{\mathrm{TOT}}^{\mathrm{av}.AB}/\partial z(z_1,V)} = \frac{I_{\mathrm{MAGN}}^{A}(z_1,V) - I_{\mathrm{MAGN}}^{B}(z_1,V)}{2\kappa_{\mathrm{TOT}}^{\mathrm{av}.AB}(V) I_{\mathrm{TOT}}^{\mathrm{av}.AB}(z_1,V)}$$

Motivation:
Magnetic modulation superimposed on topographic image

$$\Delta z_{\mathrm{nonmagn}}^{AB}(z_1,V) = -\frac{\Delta I^{AB}(z_1,V)}{\partial I^{\mathrm{av}}/\partial z(z_1,V)}$$

$$\Delta I^{AB} \to \Delta I_{\mathrm{MAGN}}^{AB}$$

$$I^{\mathrm{av}} \to I_{\mathrm{TOPO}}$$

$$I_{\mathrm{TOPO}}^{A}(z,V) = I_{\mathrm{TOPO}}^{A0}(V) e^{-2\kappa_{\mathrm{TOPO}}^{A}(V) z}$$

$$I_{\mathrm{TOT}}^{\mathrm{av}}(z,V) = \frac{1}{N_x N_y}\sum_{i=1}^{N_x}\sum_{j=1}^{N_y} I_{\mathrm{TOT}}(x_i,y_j,z,V)$$

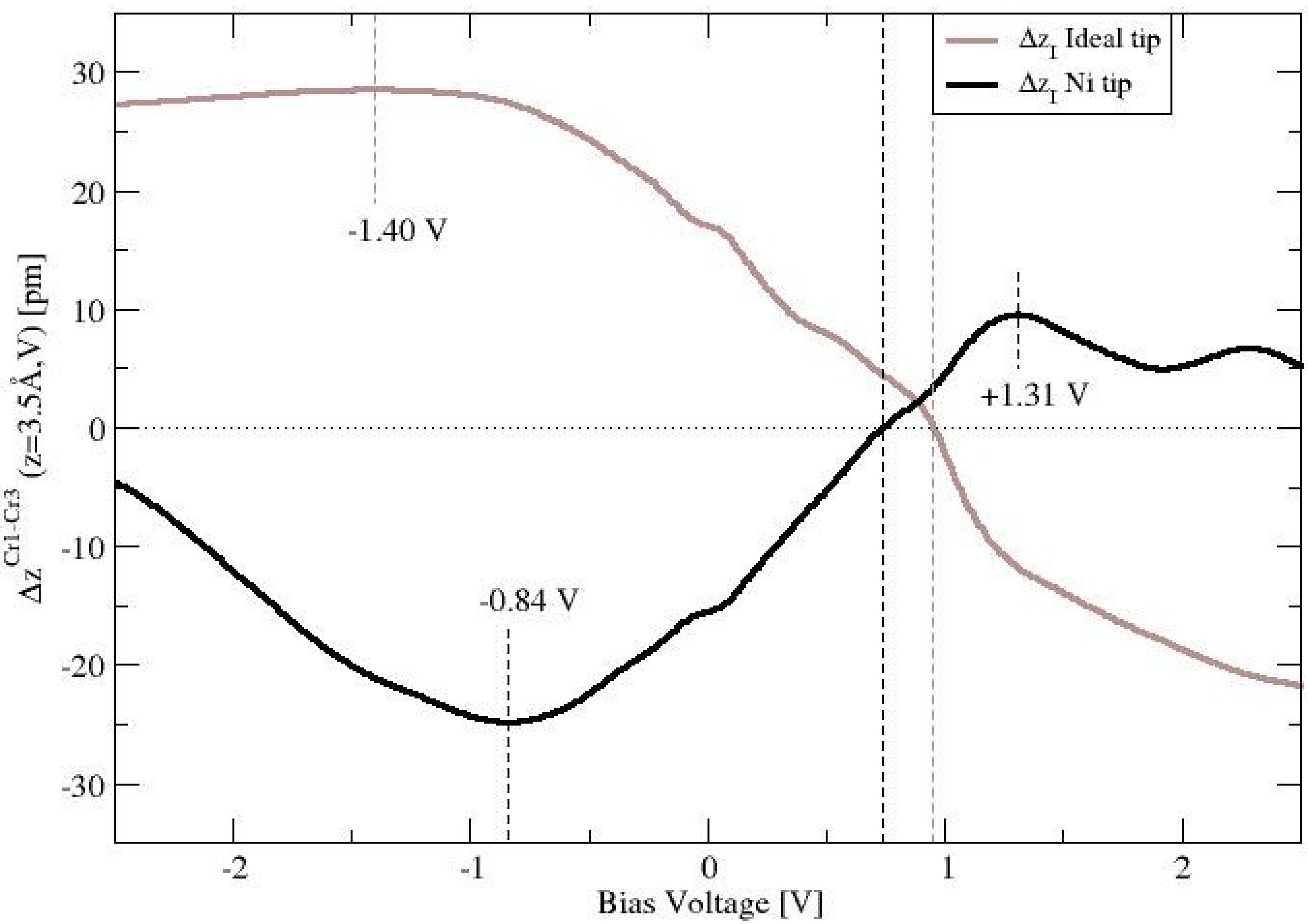
Average over scan area
→ average over A & B

$$I_{\mathrm{TOT}}^{\mathrm{av}.AB}(z,V) = \frac{I_{\mathrm{TOT}}^{A}(z,V) + I_{\mathrm{TOT}}^{B}(z,V)}{2} = I_{\mathrm{TOT}}^{\mathrm{av}.AB0}(V) e^{-2\kappa_{\mathrm{TOT}}^{\mathrm{av}.AB}(V) z}.$$

Palotás, Phys. Rev. B 87, 024417 (2013)

Prediction of bias dependent magnetic contrast

$$\Delta z_I^{AB}(z_1, V) = -\frac{\Delta I_{\mathrm{MAGN}}^{AB}(z_1, V)}{\partial I_{\mathrm{TOPO}}^{A} / \partial z(z_1, V)}$$



Palotás, Phys. Rev. B 87, 024417 (2013)

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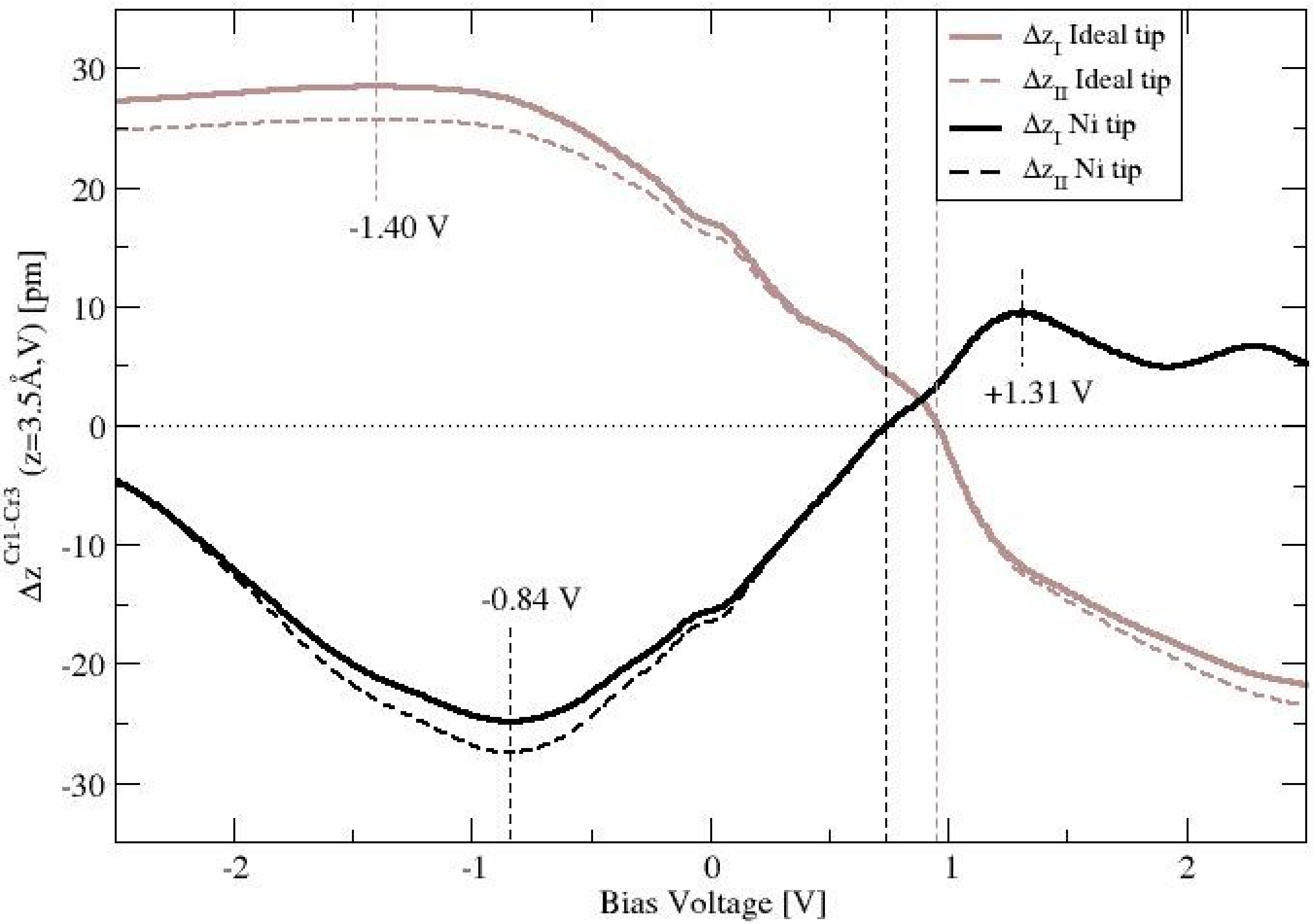

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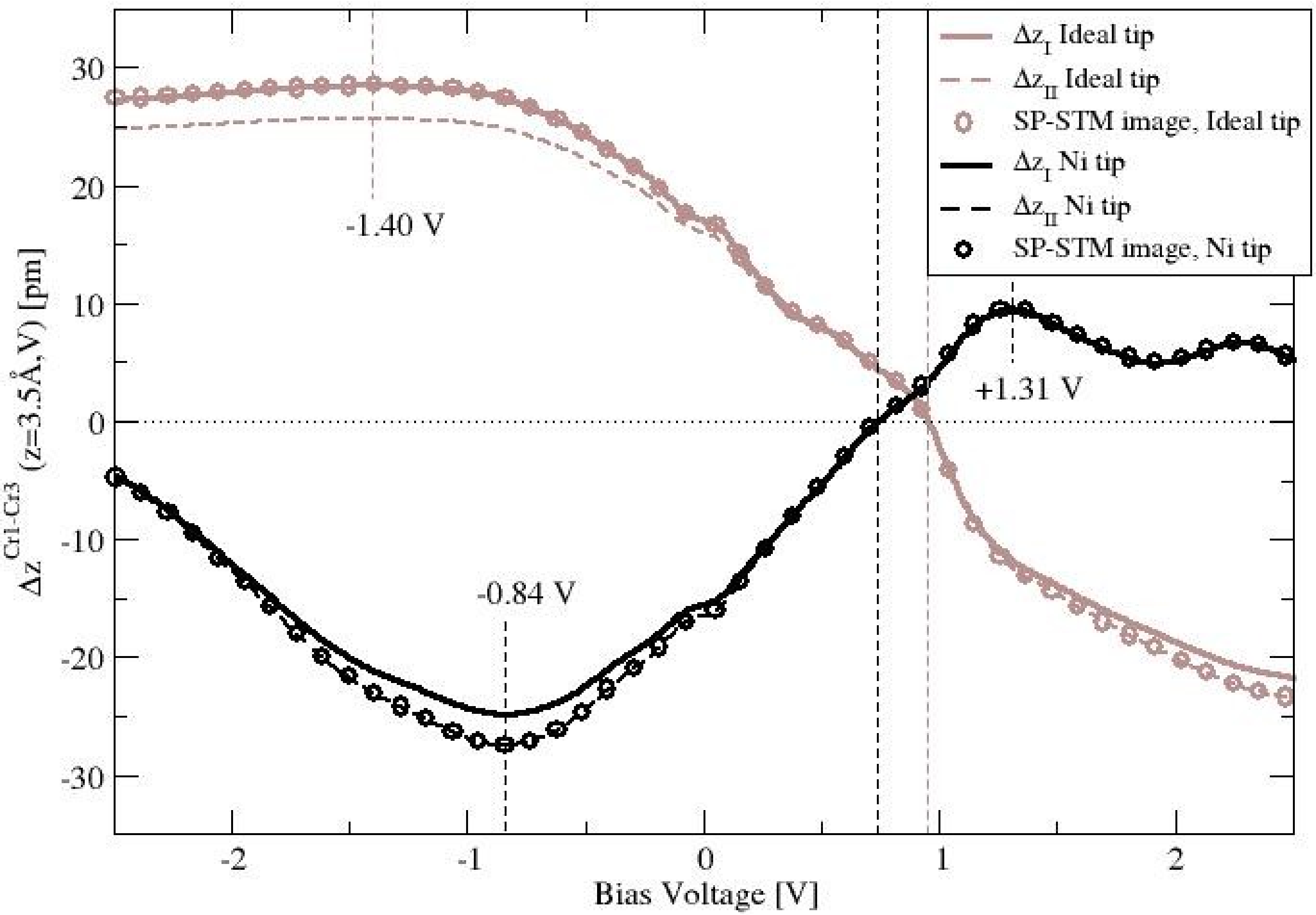
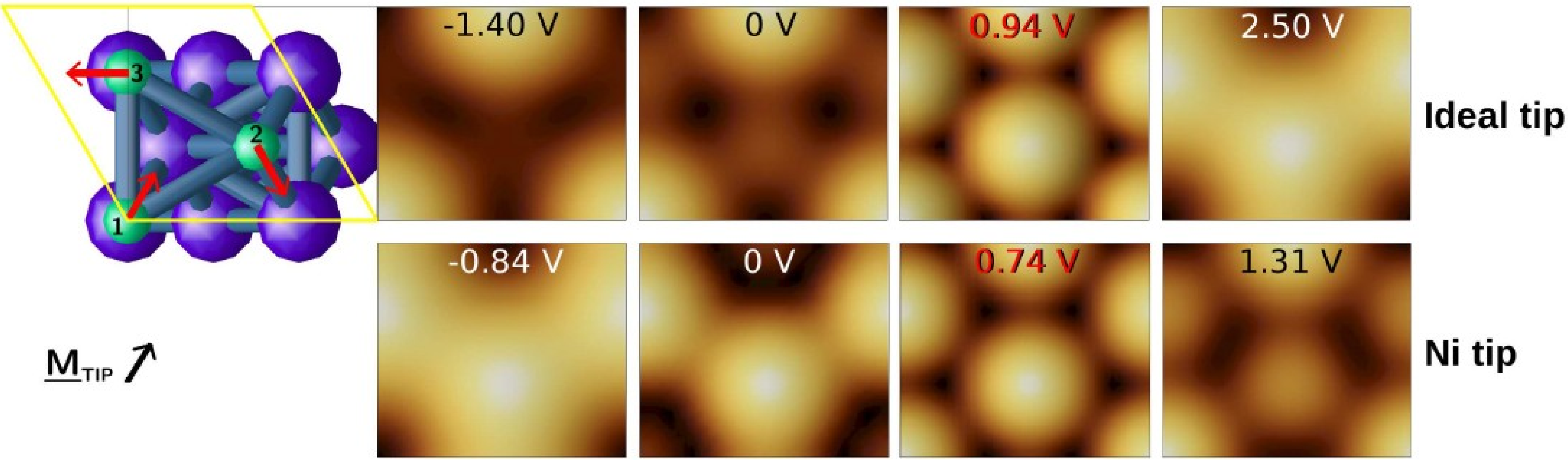


Palotás, Phys. Rev. B 87, 024417 (2013)

Cr monolayer on Ag(111) surface
Bias dependent magnetic contrast



Contrast reversal observed using ideal tip
→ effect of surface electronic structure
Tip electronic structure plays a role as well!
Experimental verification is needed!

Palotás, Phys. Rev. B 87, 024417 (2013)
Palotás et al., Phys. Rev. B 84, 174428 (2011)

PRB 86, 235415 (2012)

Orbital independent tunneling
Theoretical description

$$I(x,y,z,V) = \int_0^V \frac{dI}{dU}(x,y,z,U,V)dU$$

$$\frac{dI}{dU}(x,y,z,U,V) = \varepsilon^2 \frac{e^2}{h} \times \sum_\alpha T(E_F^S + eU, V, d_\alpha(x,y,z)) n_T(E_F^T + eU - eV) n_S^\alpha(E_F^S + eU)$$

$$T(E_F^S + eU, V, d_\alpha) = e^{-2\kappa(U,V)d_\alpha}$$

Independent orbital approximation

$$\kappa(U,V) = \frac{1}{\hbar}\sqrt{2m\left(\frac{\phi_S + \phi_T + eV}{2} - eU\right)}$$

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Orbital dependent tunneling
Theoretical description

$$n_S^\alpha(E) = \sum_\beta n_{S\beta}^\alpha(E)$$

$$n_T(E) = \sum_\gamma n_{T\gamma}(E)$$

Orbital decomposition of PDOS

$$\beta, \gamma \in \{s, p_y, p_z, p_x, d_{xy}, d_{yz}, d_{3z^2-r^2}, d_{xz}, d_{x^2-y^2}\}$$

Generalization

$$\frac{dI}{dU}(x,y,z,U,V) = \varepsilon^2 \frac{e^2}{h} \quad (10)$$

$$\times \sum_\alpha \sum_{\beta,\gamma} T_{\beta\gamma}(E_F^S + eU, V, d_\alpha(x,y,z)) n_{T\gamma}(E_F^T + eU - eV) n_{S\beta}^\alpha(E_F^S + eU),$$

$$I(x,y,z,V) = \sum_{\beta,\gamma} I_{\beta\gamma}(x,y,z,V)$$

$$I_{\beta\gamma}(x,y,z,V) = \varepsilon^2 \frac{e^2}{h}$$

$$\times \sum_\alpha \int_0^V T_{\beta\gamma}(E_F^S + eU, V, d_\alpha(x,y,z)) n_{T\gamma}(E_F^T + eU - eV) n_{S\beta}^\alpha(E_F^S + eU) dU$$

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Orbital dependent tunneling
Theoretical description

Generalized transmission function:

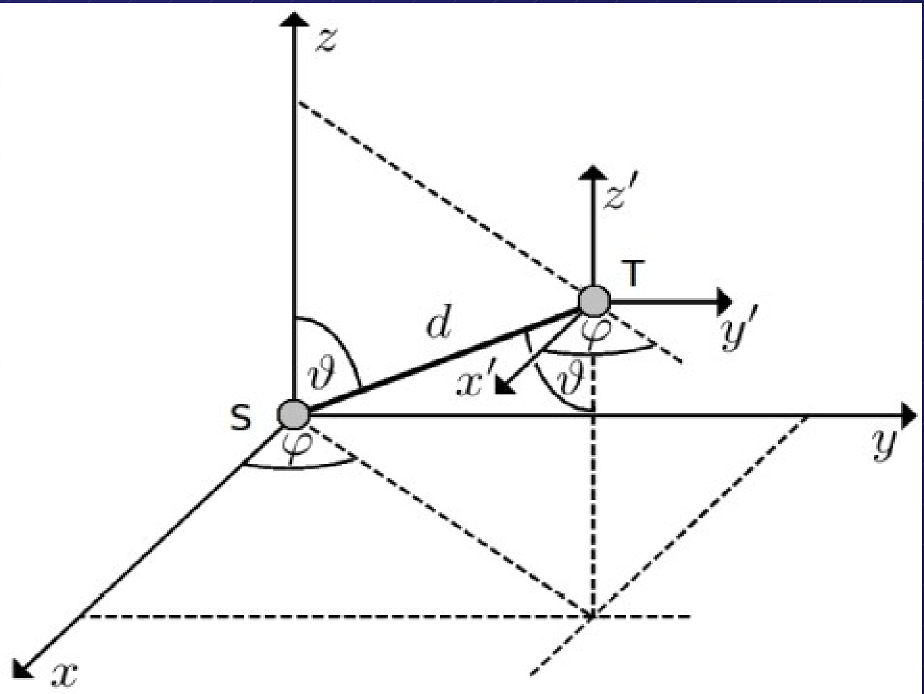
orbital-independent

$$T_{\beta\gamma}(E_F^S + eU, V, d_\alpha) = e^{-2\kappa(U,V)d_\alpha} t_{\beta\gamma}(\vartheta_\alpha, \varphi_\alpha)$$

orbital dependent

$$t_{\beta\gamma}(\vartheta_\alpha, \varphi_\alpha) = [\chi_\beta(\vartheta_\alpha, \varphi_\alpha)]^2 \times [\chi_\gamma(\vartheta_\alpha + \pi, \varphi_\alpha + \pi)]^2$$

orbital	index	definition	$\chi(\vartheta,\varphi)$
s	1	Y_0^0	1
p_y	2	$Y_1^1 - Y_1^{-1}$	$sin(\vartheta)sin(\varphi)$
p_z	3	Y_1^0	$cos(\vartheta)$
p_x	4	$Y_1^1 + Y_1^{-1}$	$sin(\vartheta)cos(\varphi)$
d_{xy}	5	$Y_2^2 - Y_2^{-2}$	$sin^2(\vartheta)sin(2\varphi)$
d_{yz}	6	$Y_2^1 - Y_2^{-1}$	$sin(2\vartheta)sin(\varphi)$
$d_{3z^2-r^2}$	7	Y_2^0	$\frac{1}{2}(3cos^2(\vartheta) - 1)$
d_{xz}	8	$Y_2^1 + Y_2^{-1}$	$sin(2\vartheta)cos(\varphi)$
$d_{x^2-y^2}$	9	$Y_2^2 + Y_2^{-2}$	$sin^2(\vartheta)cos(2\varphi)$



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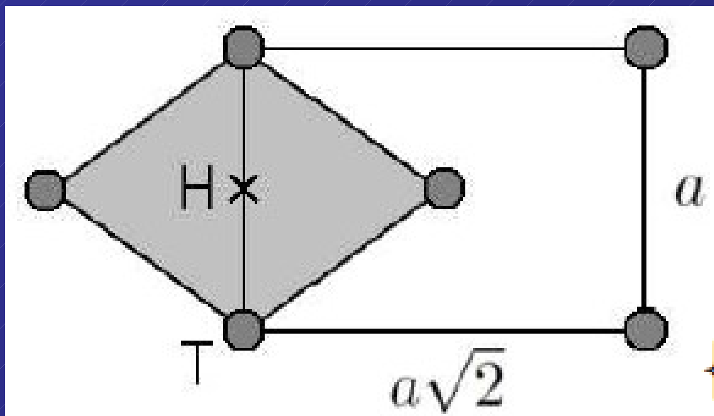
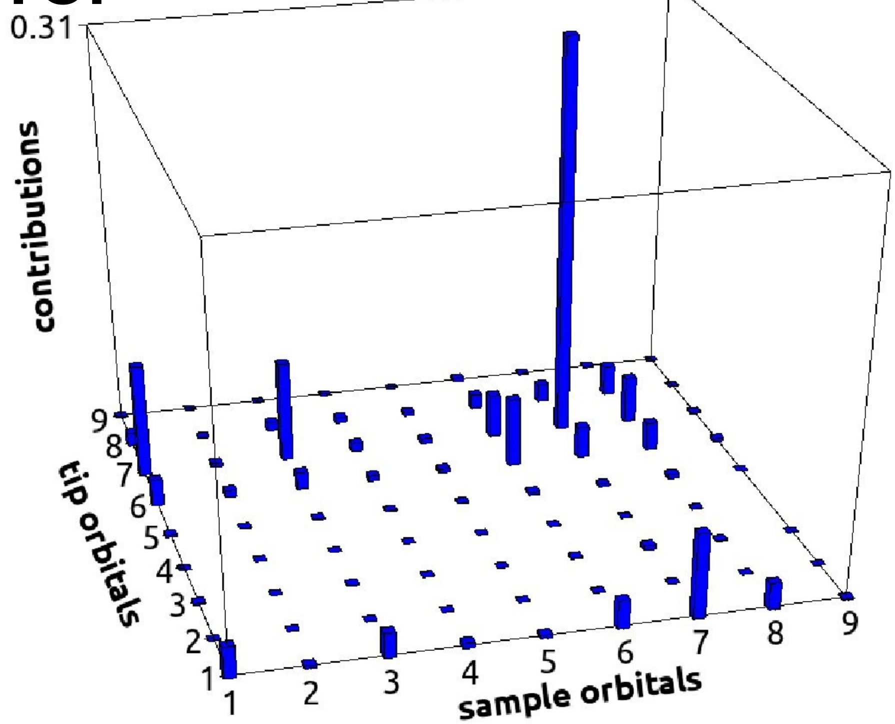
Orbital contributions to the current on W(110)



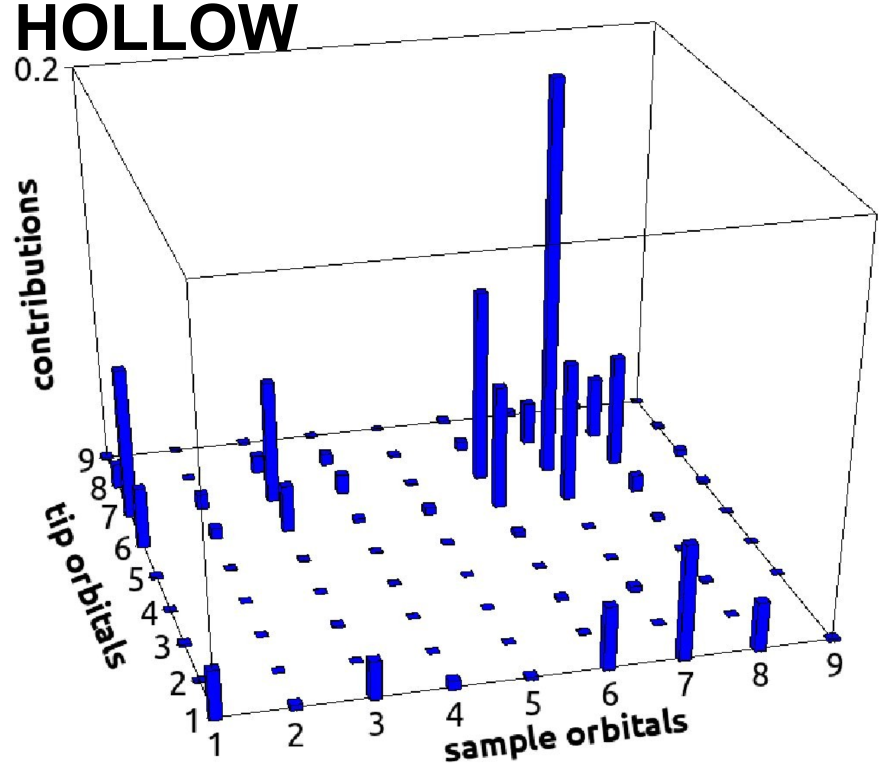
V = -0.1 V, z = 4.5 Angströms

$$\{s, p_y, p_z, p_x, d_{xy}, d_{yz}, d_{3z^2-r^2}, d_{xz}, d_{x^2-y^2}\}$$

TOP



HOLLOW



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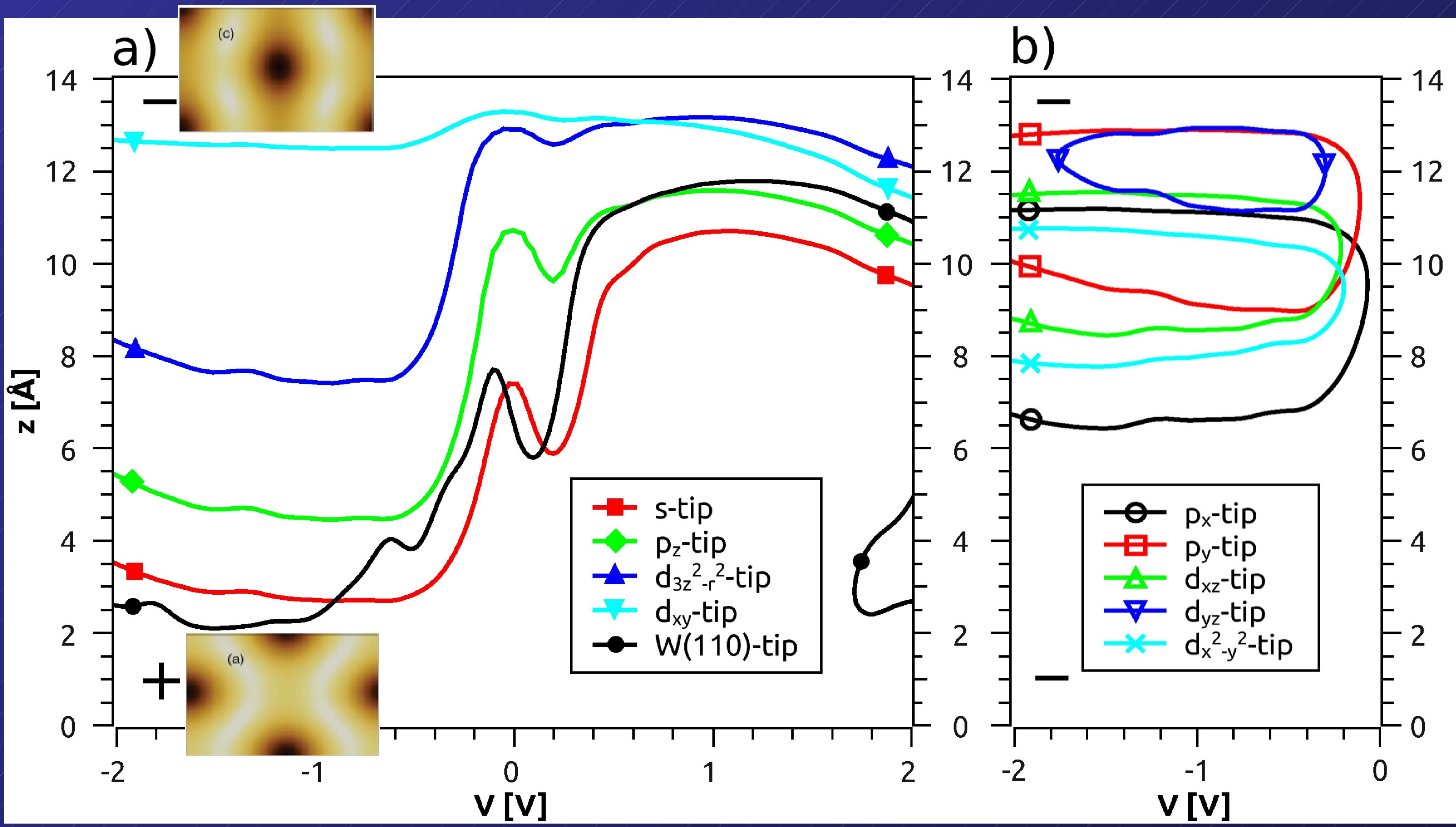
Corrugation inversion on W(110)

Dependence on tip-symmetry, bias, and tip-sample distance



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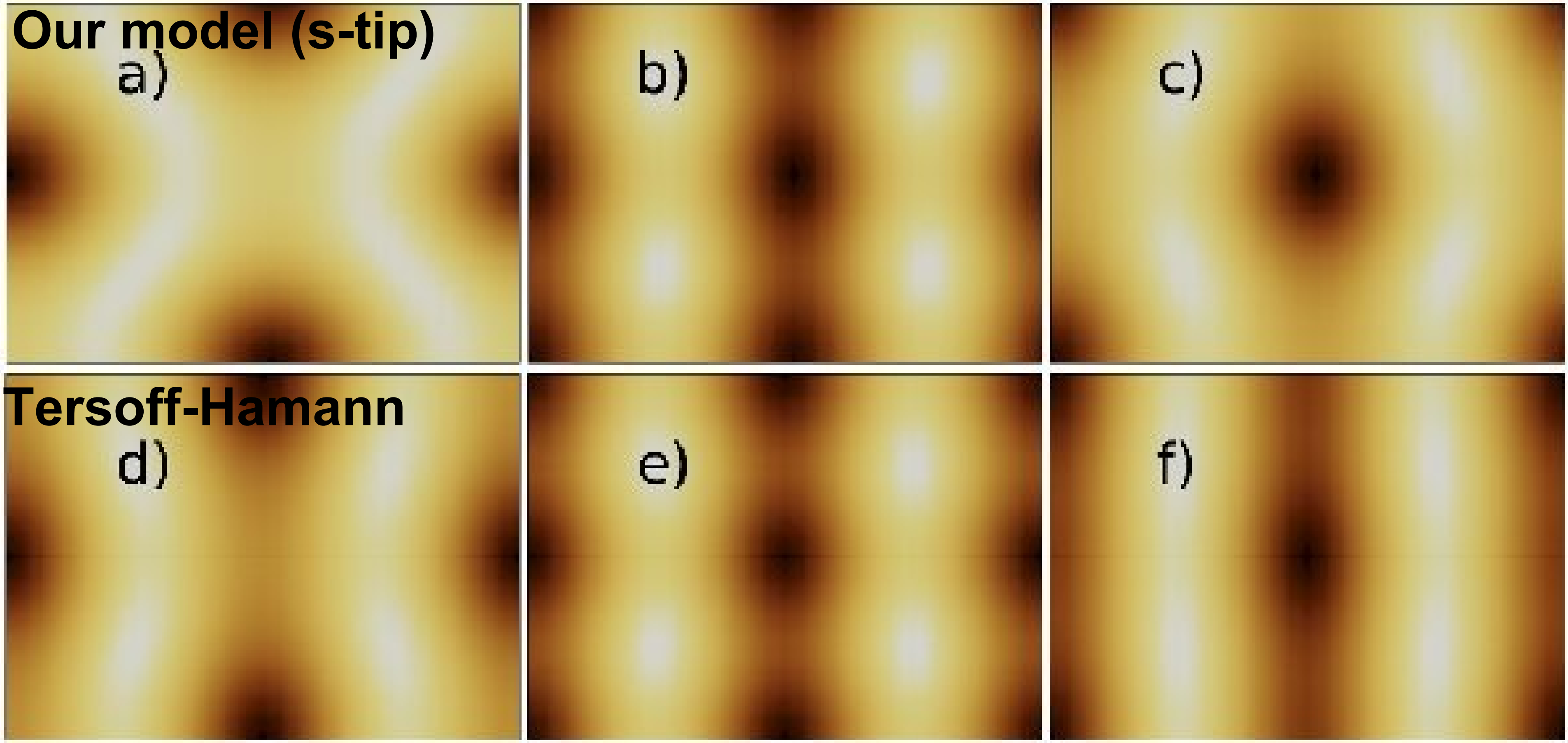
Corrugation inversion on W(110)

Simulated STM images, V=-0.25 V



Good agreement of contrast reversal height: 4.15 vs 4.21 Å

Good agreement with Heinze et al., PRB 58, 16432 (1998)

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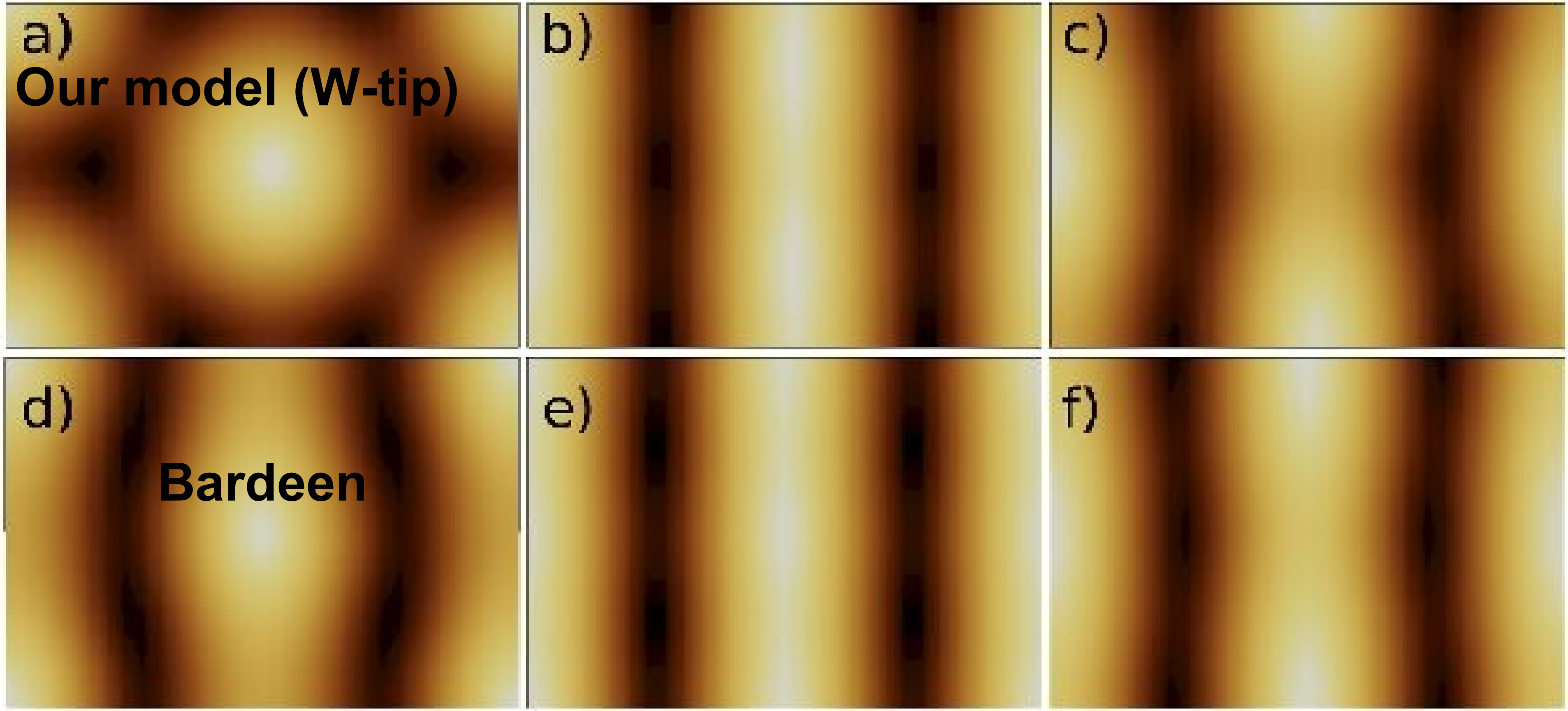
Corrugation inversion on W(110)

Simulated STM images, V=-0.25 V



Good agreement of contrast reversal height: 5.80 vs 5.55 Å

Computational time of our model does not depend on k-point sampling of BZ!

Example: Sample 41x41x5, Tip 11x15x5 k-set: Our model **8500** times **faster**!

Summary

- **New SP-STM/STS simulation package** developed based on first principles electronic structure data and the work of Heinze, Appl. Phys. A 85, 407 (2006).
- Main features:
  1. Imaging noncollinear surface magnetic structures
  2. Tip electronic structure considered
  3. Bias voltage included
  4. Energy dependence of local spin quantization axes included
  5. Orbital dependent tunneling transmission
- Main advantages:
  1. **Easy combination with any electronic structure code**
  2. **Possible combination of different levels of electronic structure methods for tip and surface**
  3. **Computationally cheap**
  4. **Easy to parallelize → fast**

Work in progress - Outlook

- Going beyond the independent orbital approximation considering tunneling between **directional orbitals**
  - arbitrary tip orientations (comparison to experiments, at the moment graphite(0001) surface)
  - extension to study magnetic systems reveal contrast mechanisms

  PhD work in Budapest: Gábor Mándi
- Local electronic properties of surfaces with Moiré structure
  TDK work in Budapest: Mátyás Seress
- Improve tunneling theory for complex magnetic surfaces (**BSKAN code - Werner Hofer, Liverpool interface to noncollinear VASP code**)
- Study of magnetic atomic contacts (at the moment Ir contacts, domain walls in Co contacts)

Conclusions

- Reproduced Fe(001) surface state peak at +0.20V in the SP-STS spectrum
- Sensitivity of SP-STS on magnetic samples can be enhanced by using proper magnetic tips. Role of effective spin polarization! PRB 83, 214410 (2011)
- dI/dV: background and tip-derivative terms considered
- 2D dI/dV map, Magn. Asymm. map → 2D Eff. Spin-Pol. map PRB 85, 205427 (2012)
- Cr/Ag(111): Evidence for tip and bias dependent magnetic contrast PRB 84, 174428 (2011); PRB 87, 024417 (2013)
- Orbital dependent tunneling: W(110), PRB 86, 235415 (2012)

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Thank YOU for your attention!

palotas@phy.bme.hu