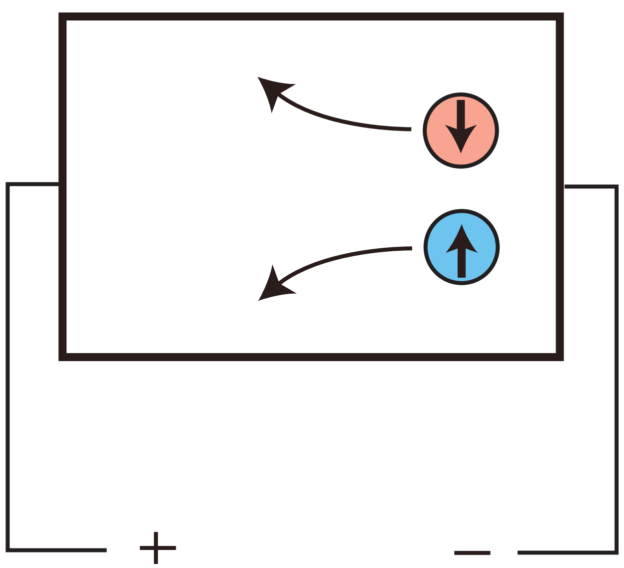
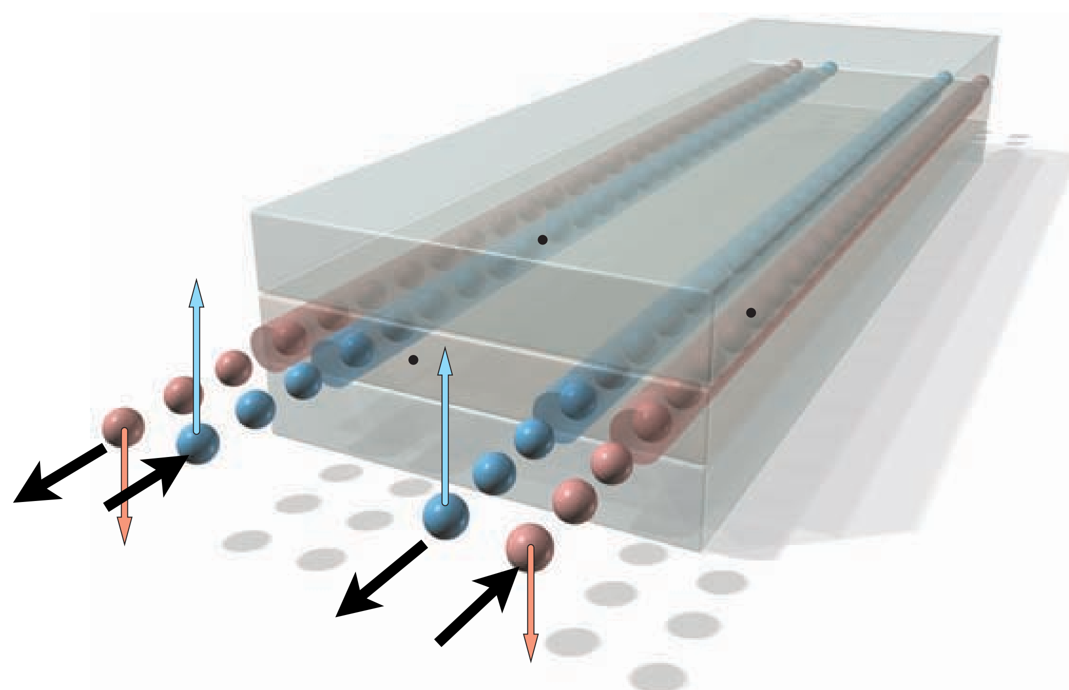
Electron Dynamics in Systems with Strong Spin-Orbit Coupling

pure spin
Hall effect



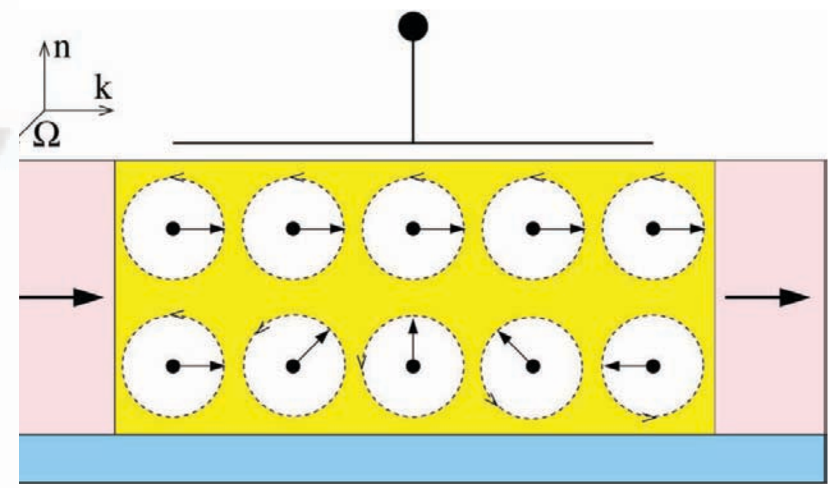
J. Sinova et al., Physical Review Letters **92**, 126603 (2004)
Y. K. Kato et al. Science **306**, 1910 (2004).

quantum spin
Hall effect



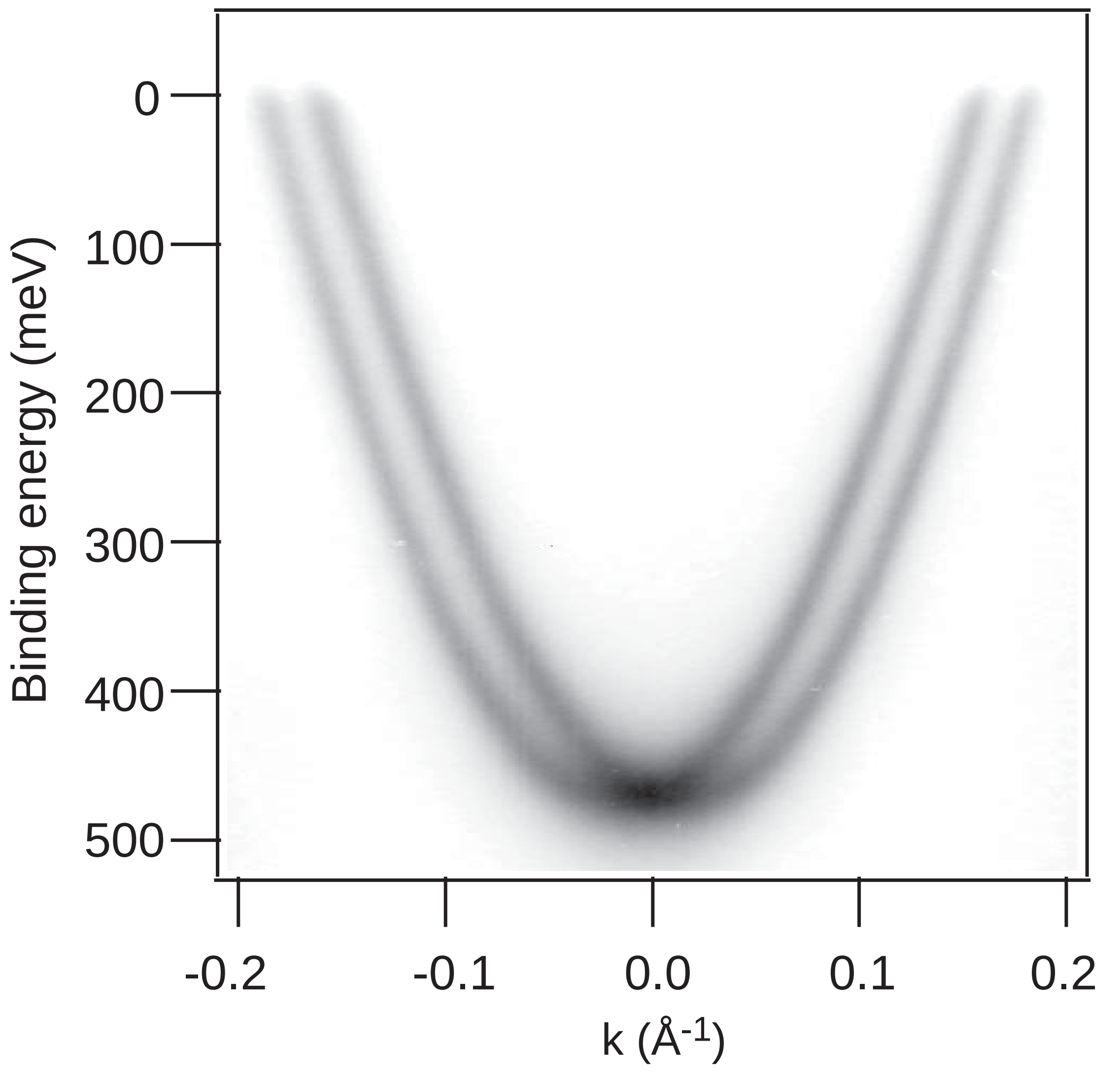
M. Konig et al., Science **318**, 766 (2007).

Datta-Das
spin FET



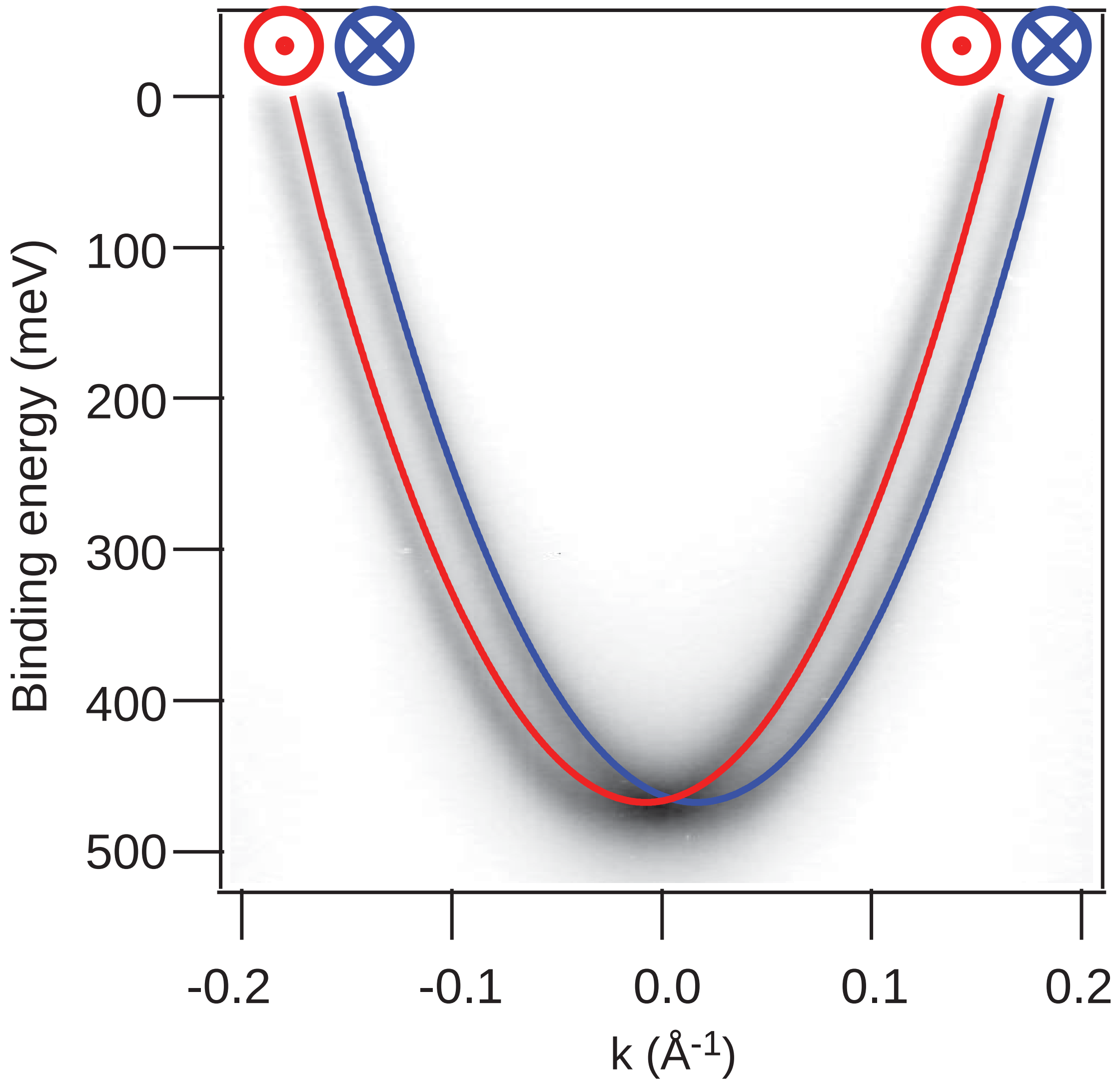
atta and B. Das, Appl. Phys. Lett. **56**, 665 (1990)
Fig. from I. Zutic et al. Rev. Mod. Phys. **76**, 323 (2004)
experiment: H. C. Koo et al., Science **325**, 1515 (2009)

Au(111)



S. LaShell, B.A. McDougall and E. Jensen, PRL **77**, 3419 (1996)
I. A. Nechaev et al. PRB **80**, 113402 (2009)

Au(111)



dispersion $$E = \frac{\hbar^2 k^2}{2m} \pm \alpha \hbar k$$

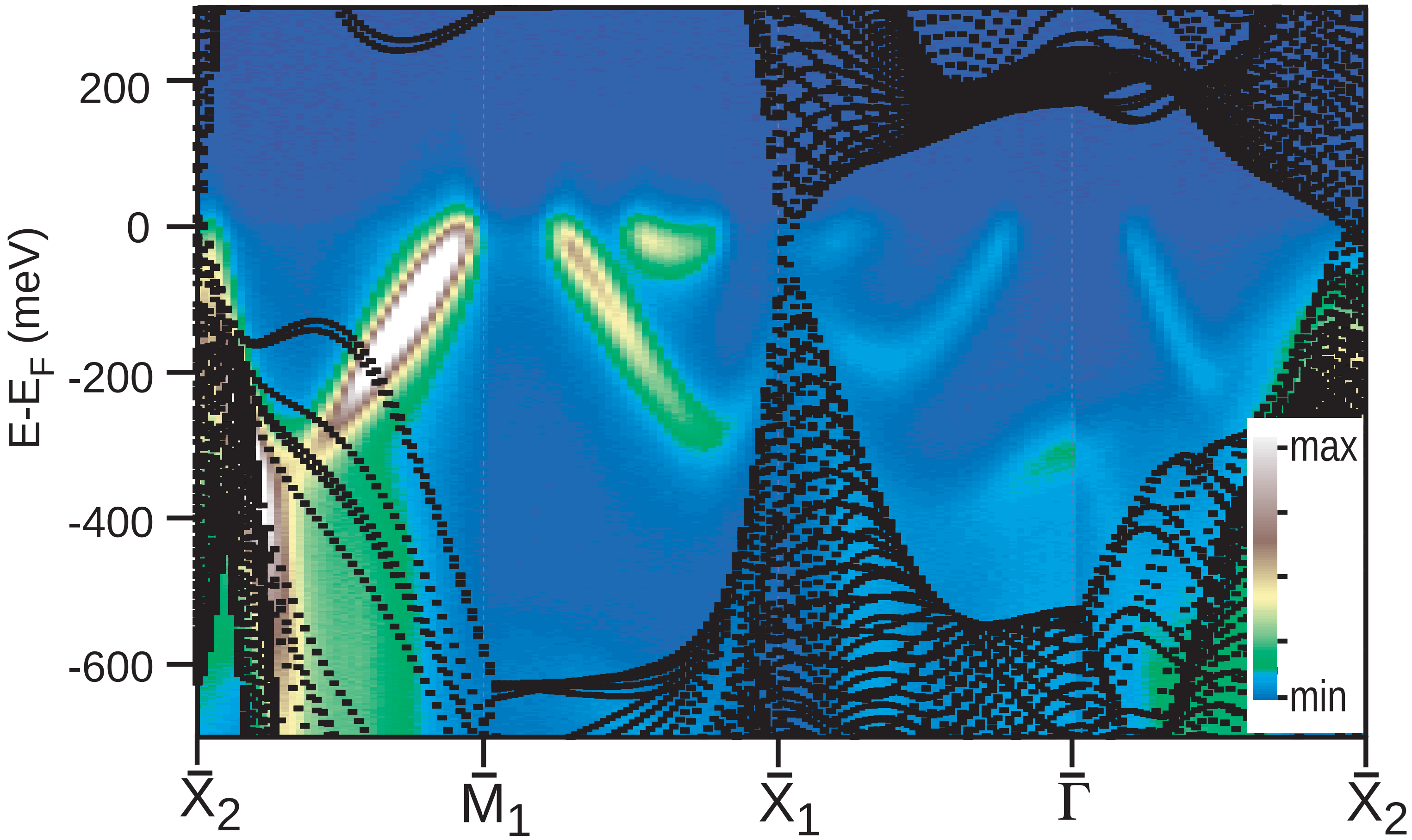
symmetry

$$\epsilon(\vec{k}, \uparrow) = \epsilon(-\vec{k}, \downarrow)$$

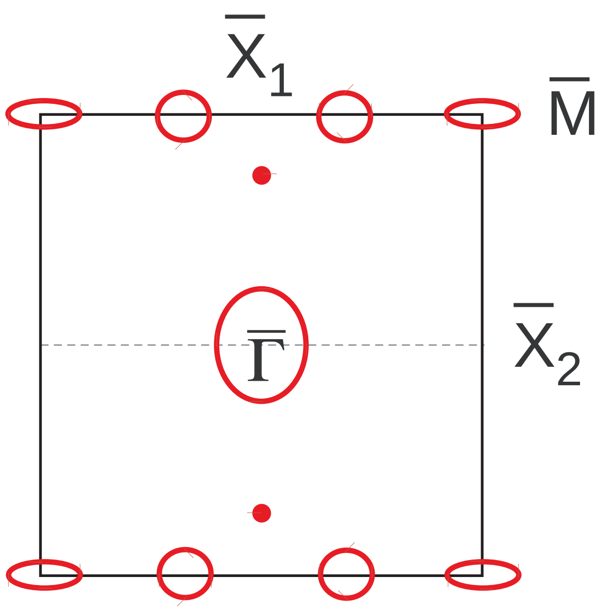
$$\epsilon(\vec{k}_{\parallel} = 0, \uparrow) = \epsilon(-\vec{k}_{\parallel} = 0, \downarrow)$$

S. LaShell, B.A. McDougall and E. Jensen, PRL **77**, 3419 (1996)
I. A. Nechaev et al. PRB **80**, 113402 (2009)

Bi(110)



S. Agergaard et al. NJP **3**, 15 (2001)

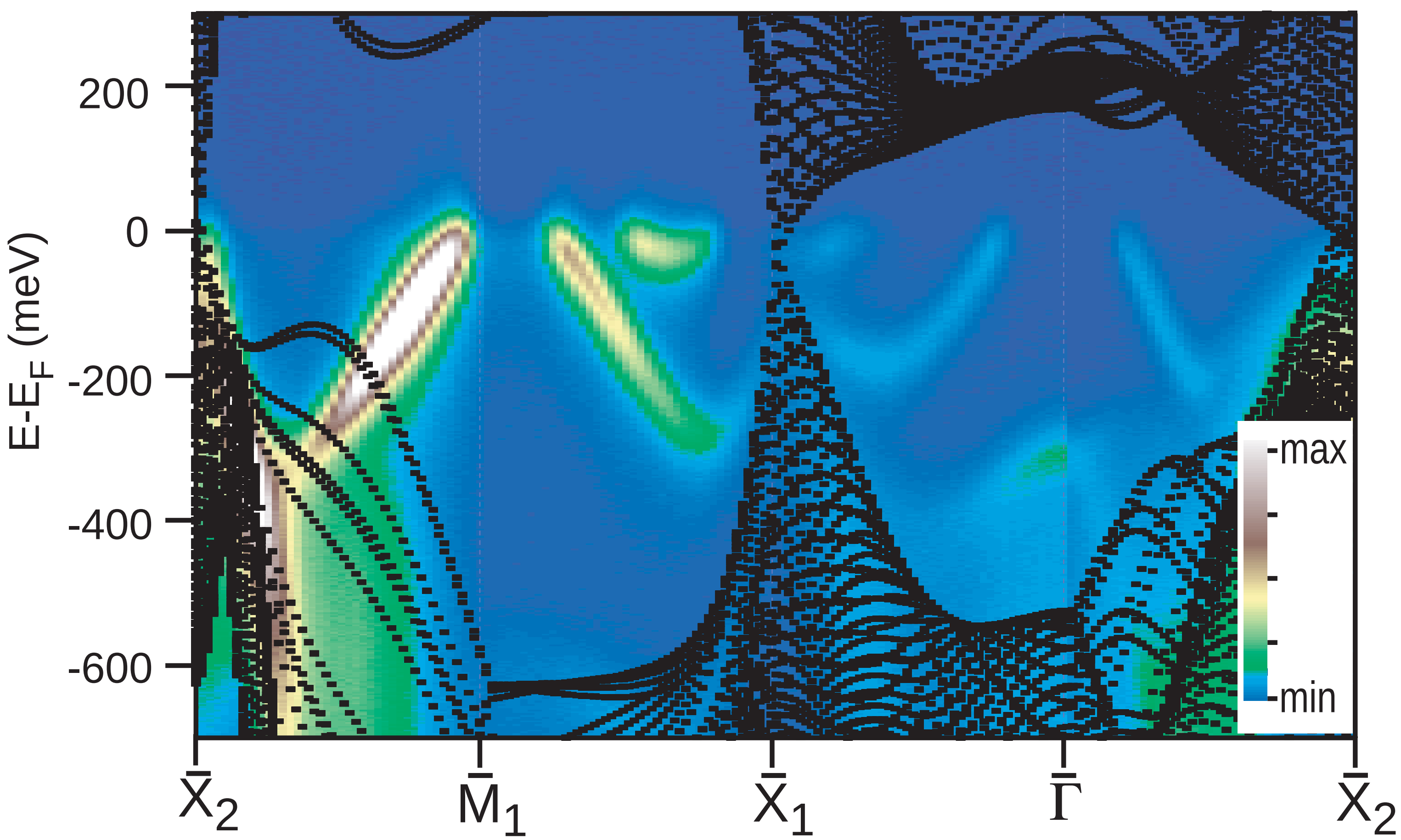


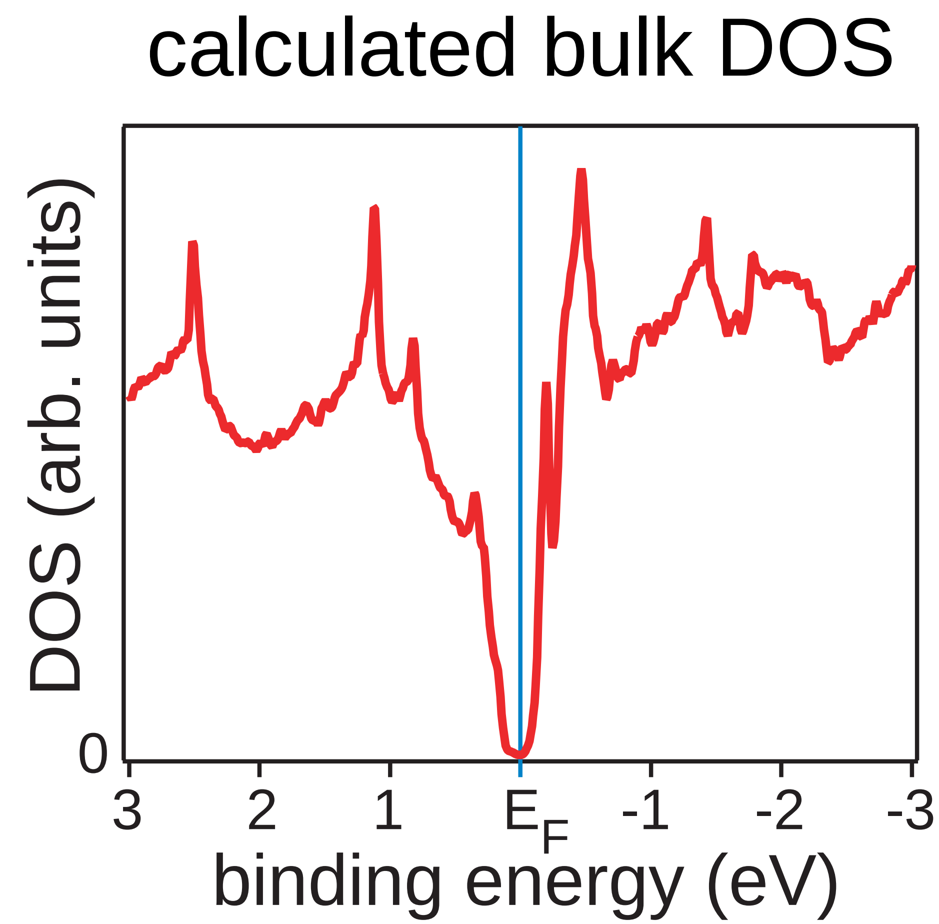
$$\epsilon(0, \uparrow) = \epsilon(0, \downarrow)$$

$$\epsilon(\bar{M}, \uparrow) = \epsilon(\bar{M}, \downarrow)$$

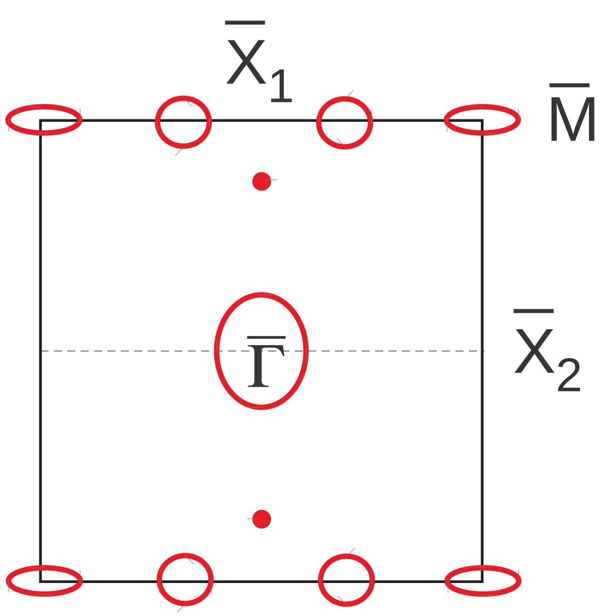
$$\epsilon(\bar{X}_i, \uparrow) = \epsilon(\bar{X}_i, \downarrow)$$

Bi(110)





S. Agergaard et al. NJP **3**, 15 (2001)

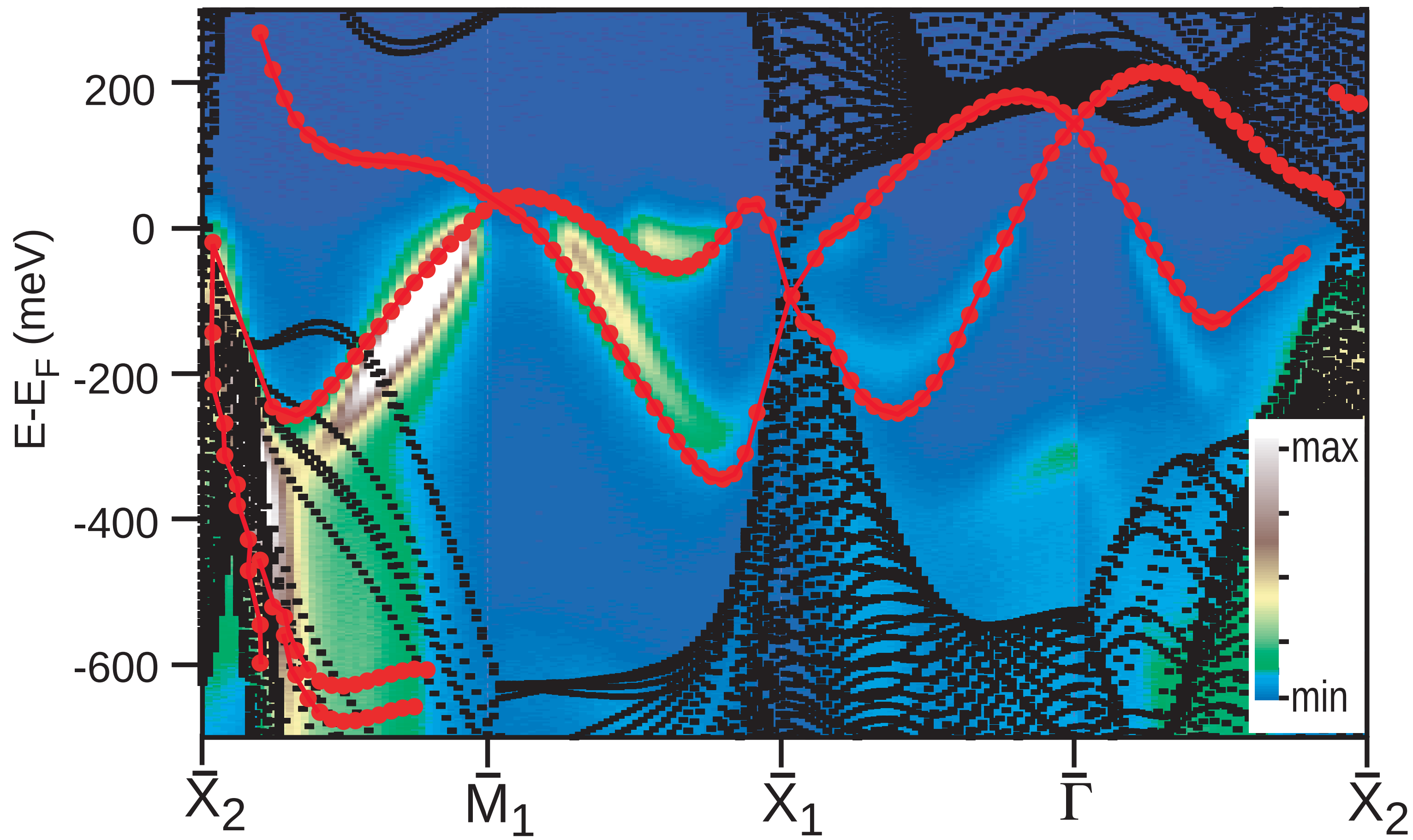


$$\epsilon(0,\uparrow) = \epsilon(0,\downarrow)$$

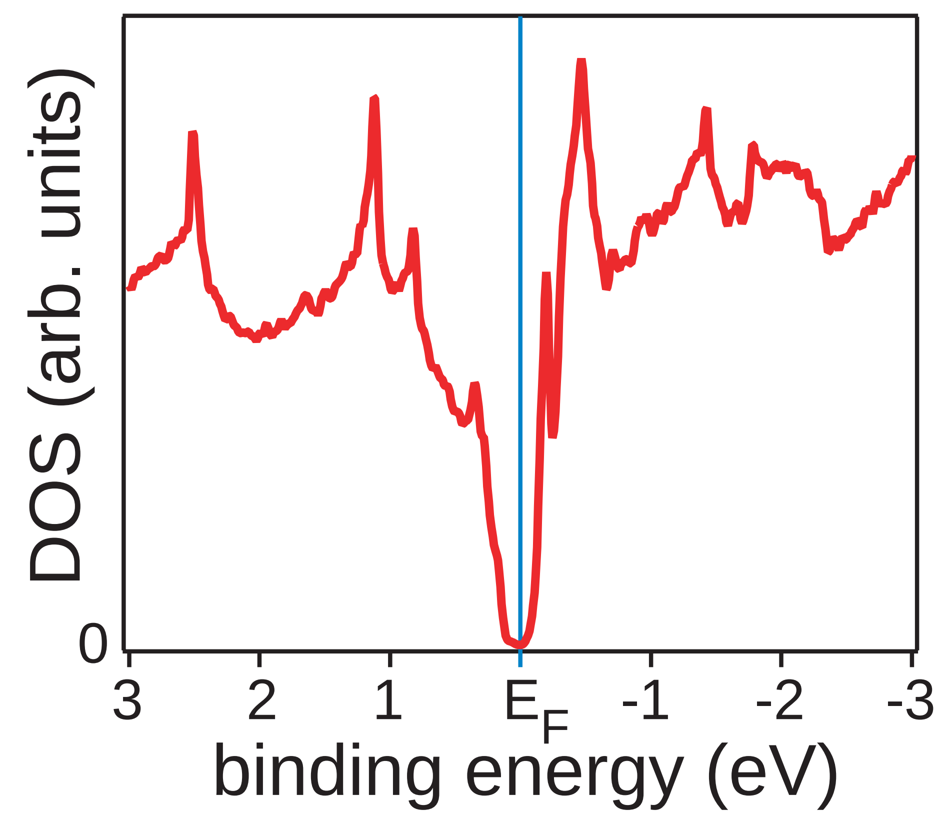
$$\epsilon(\bar{M},\uparrow) = \epsilon(\bar{M},\downarrow)$$

$$\epsilon(\bar{X}_i,\uparrow) = \epsilon(\bar{X}_i,\downarrow)$$

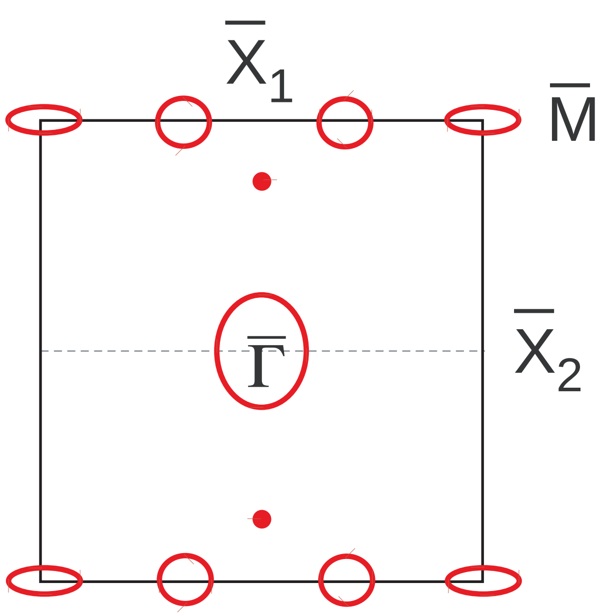
Bi(110)



calculated bulk DOS



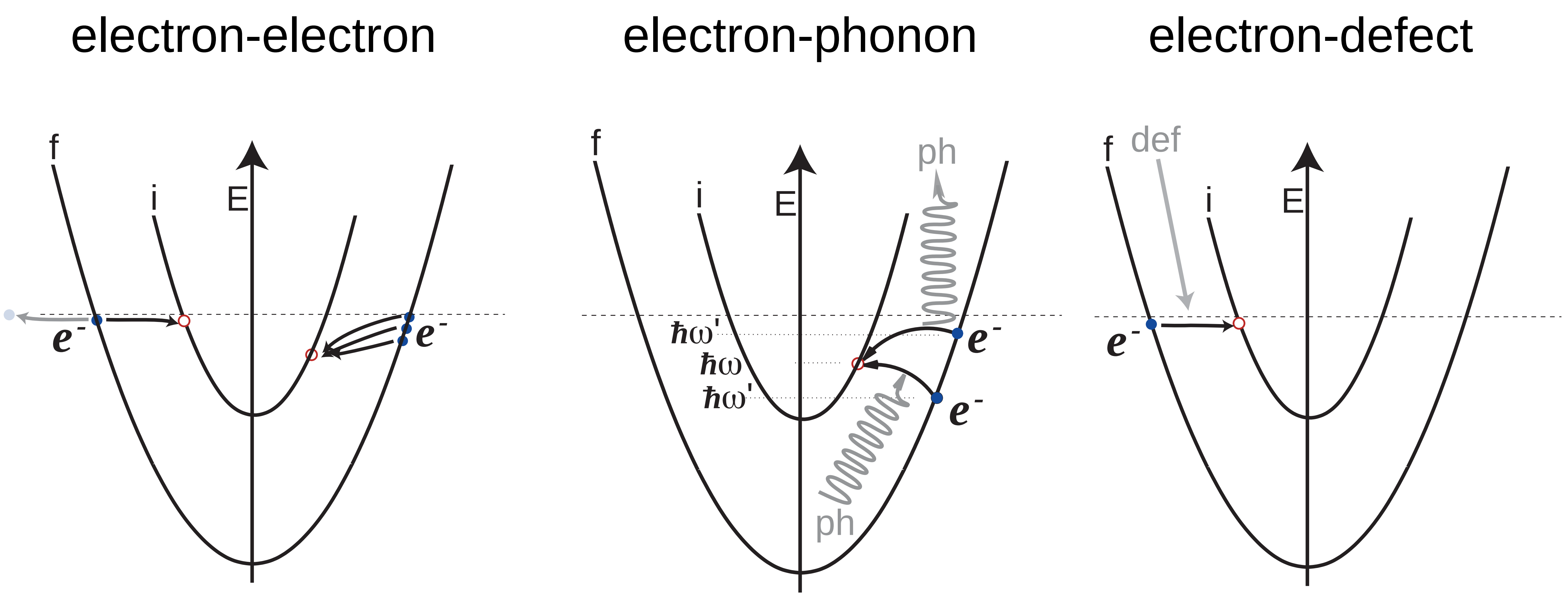
S. Agergaard et al. NJP **3**, 15 (2001)



$$\epsilon(0,\uparrow) = \epsilon(0,\downarrow)$$
$$\epsilon(\bar{M},\uparrow) = \epsilon(\bar{M},\downarrow)$$
$$\epsilon(\bar{X}_i,\uparrow) = \epsilon(\bar{X}_i,\downarrow)$$

Yu. M. Koroteev et al. PRL **93**, 046403 (2004)

electron / hole lifetimes

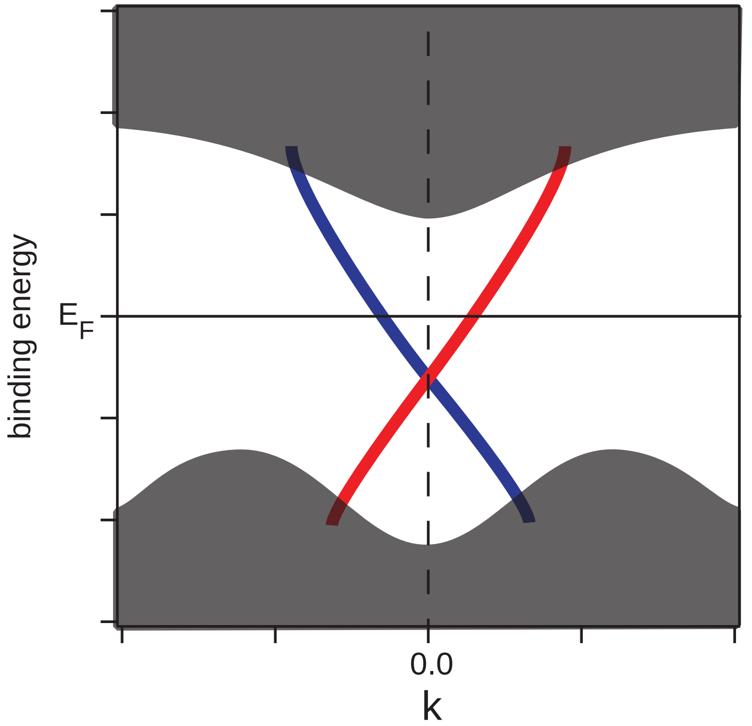


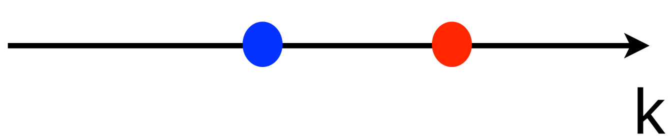
$$\alpha^2 F_{\vec{k}_i}(\omega) = \sum_{\vec{q},\nu,f} |g_{i,f}^{\vec{q},\nu}|^2 \delta(\omega - \omega_{\vec{q},\nu}) \delta(\epsilon_{\vec{k}_i} - \epsilon_{\vec{k}_f})$$

- matrix elements
- density of states
- spin (?)

electron / hole lifetimes

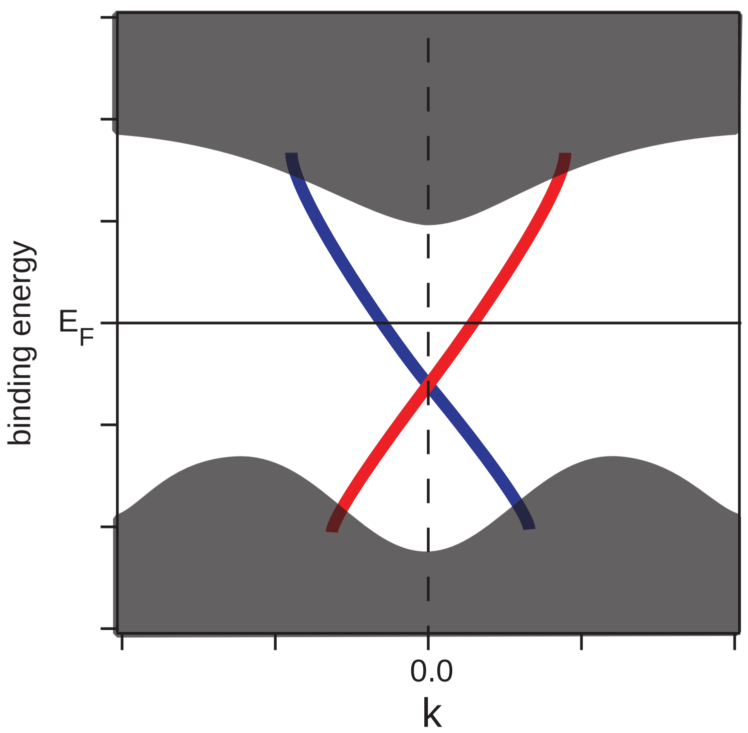
1D

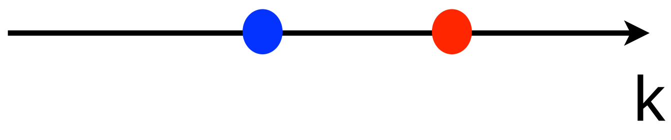




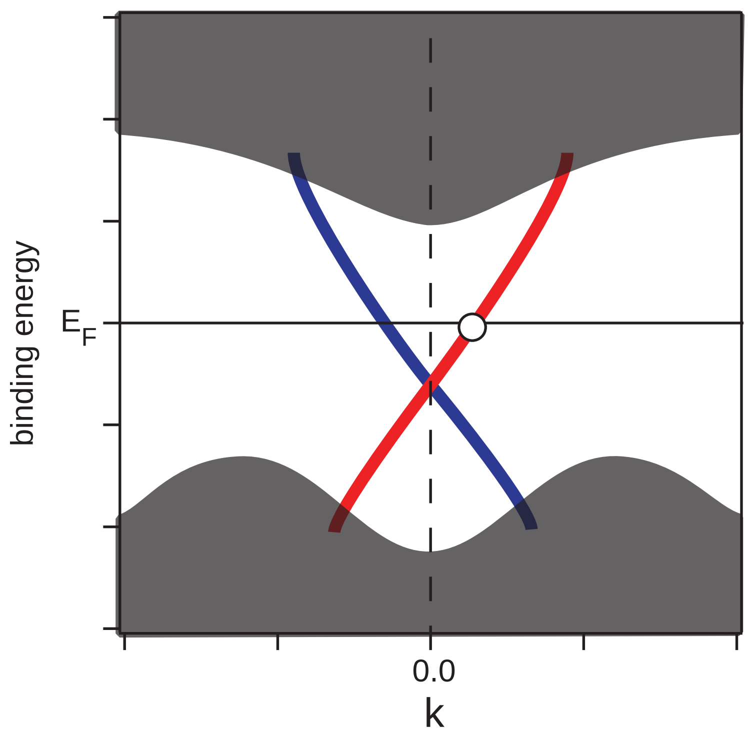
electron / hole lifetimes

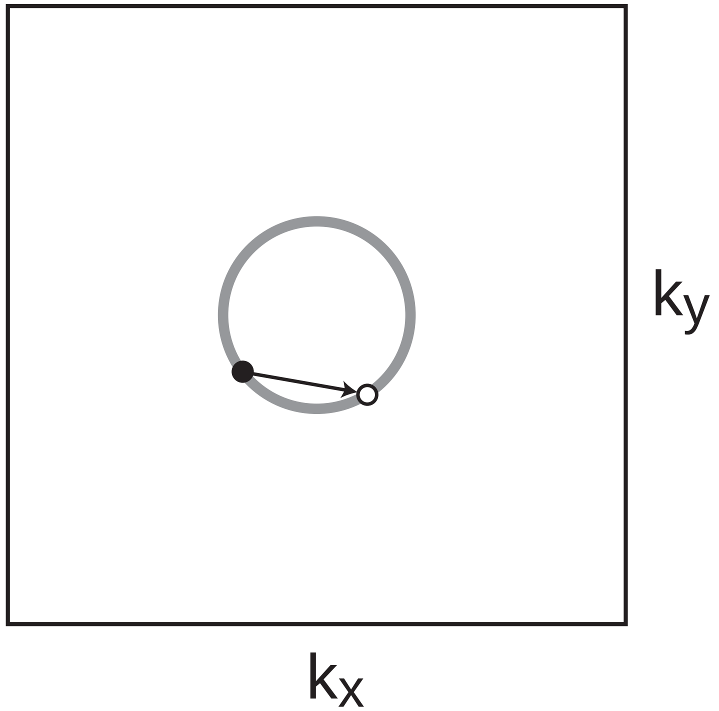
1D



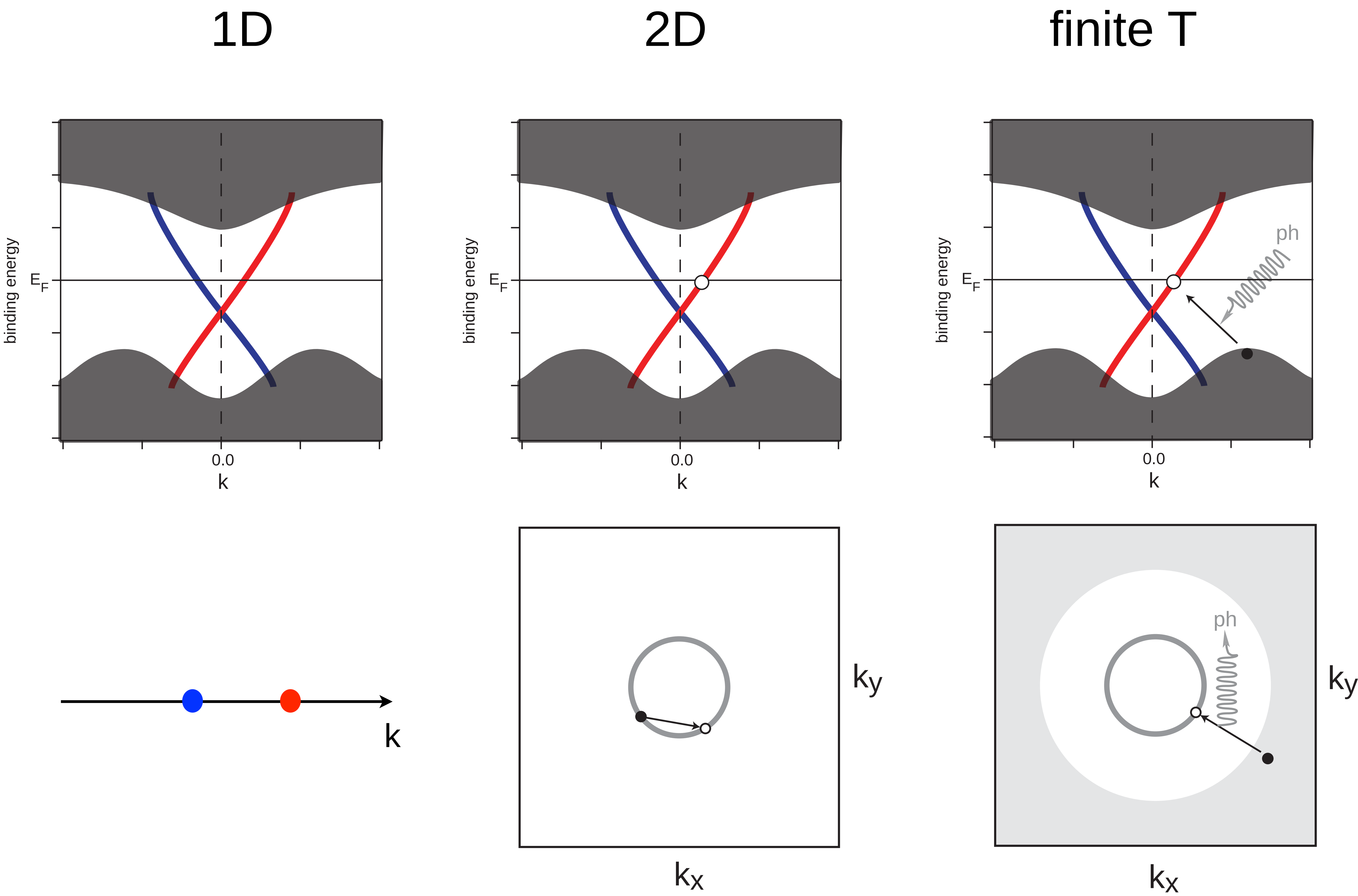


2D





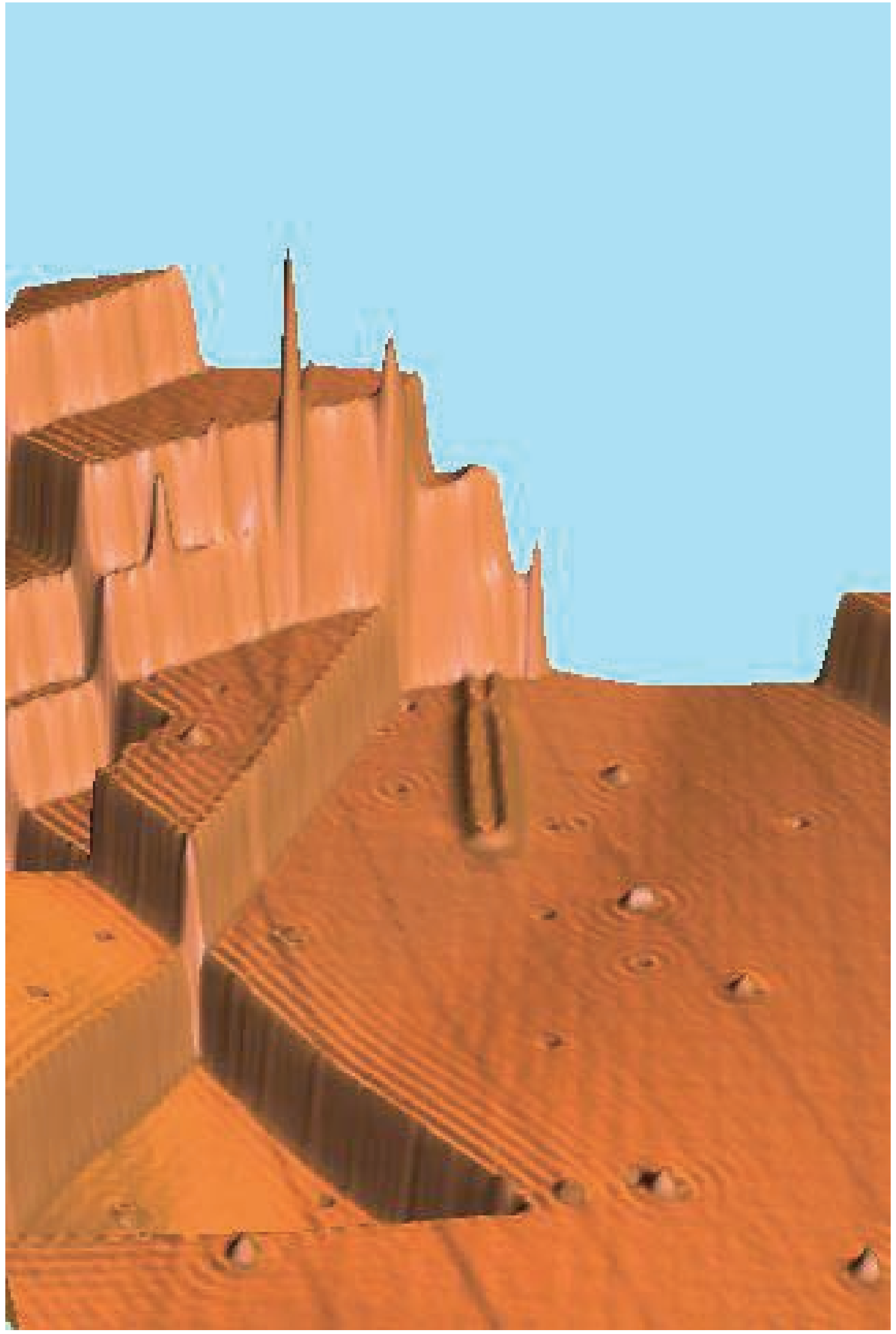
electron / hole lifetimes



cases

- quasiparticle interference
- lifetime in Rashba systems
- detailed calculations of spin polarization

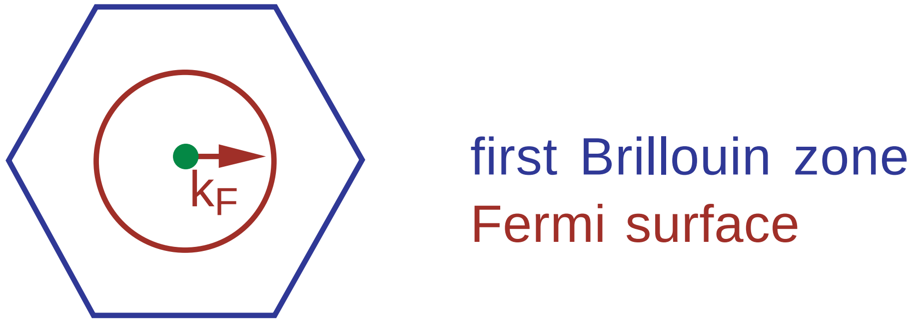
quasiparticle interference



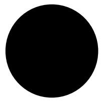
standing electron waves on Cu(111) at 4K
Crommie, Lutz, Eigler, Nature **363**, 524 (1993)

Origin of the waves at E_F (very small V_{bias})

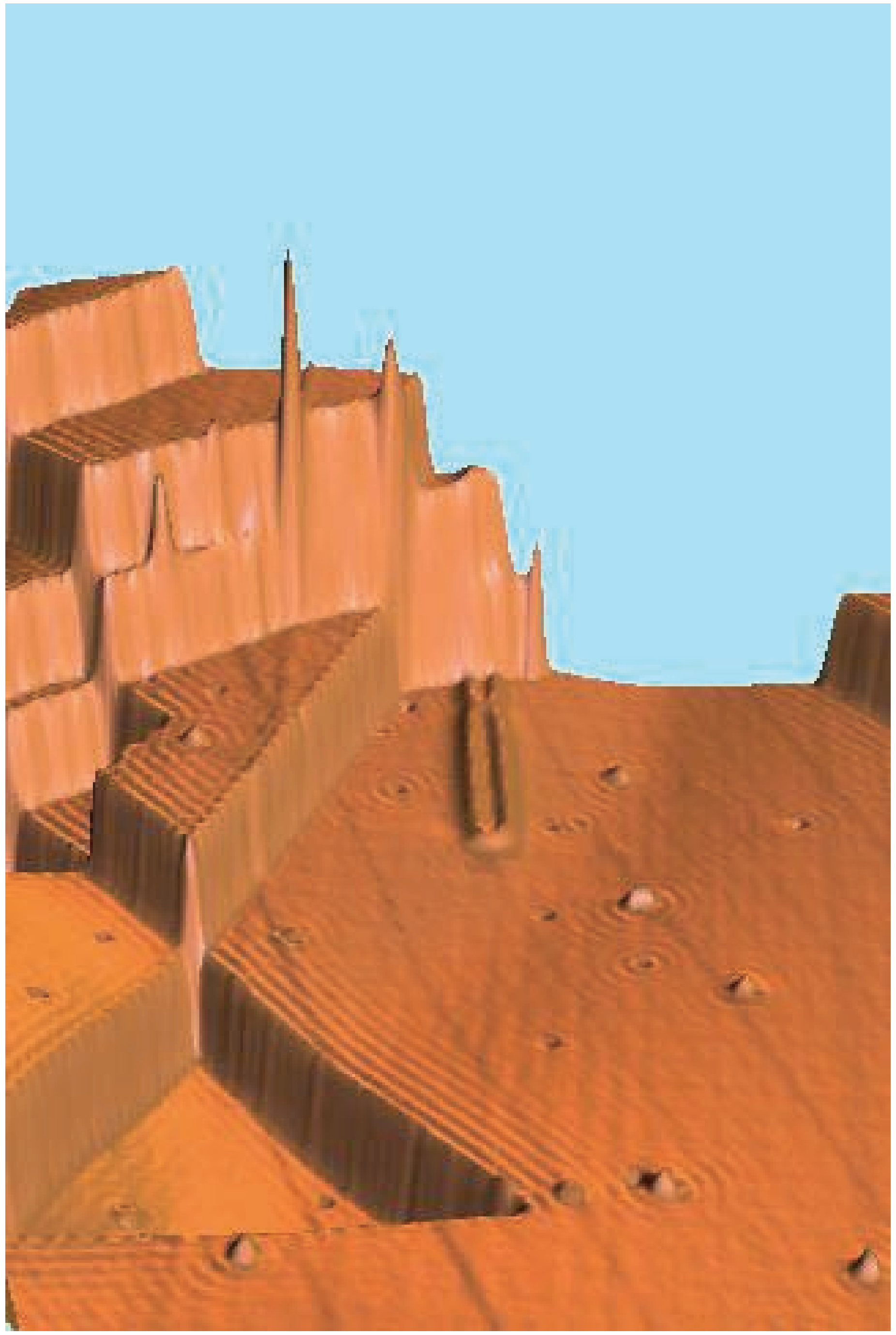
reciprocal space



point defect in real space

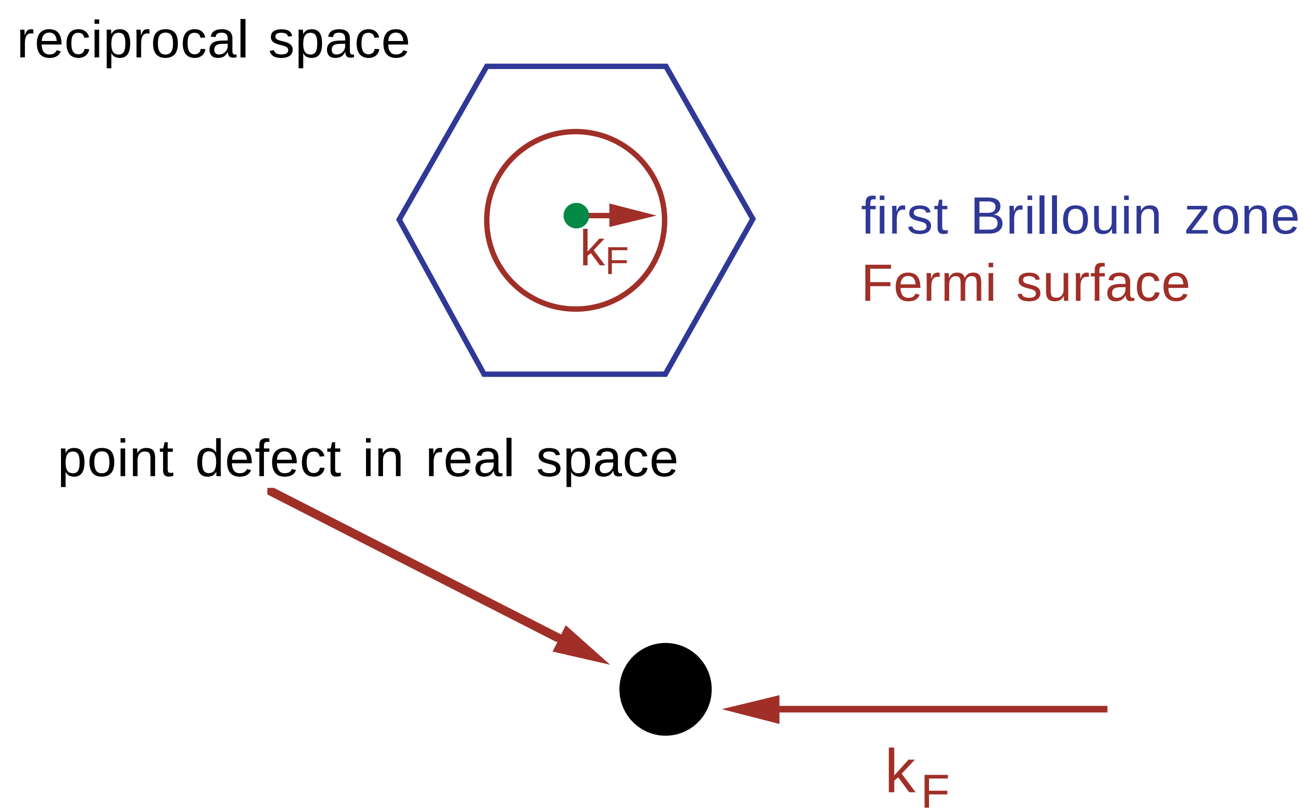


quasiparticle interference

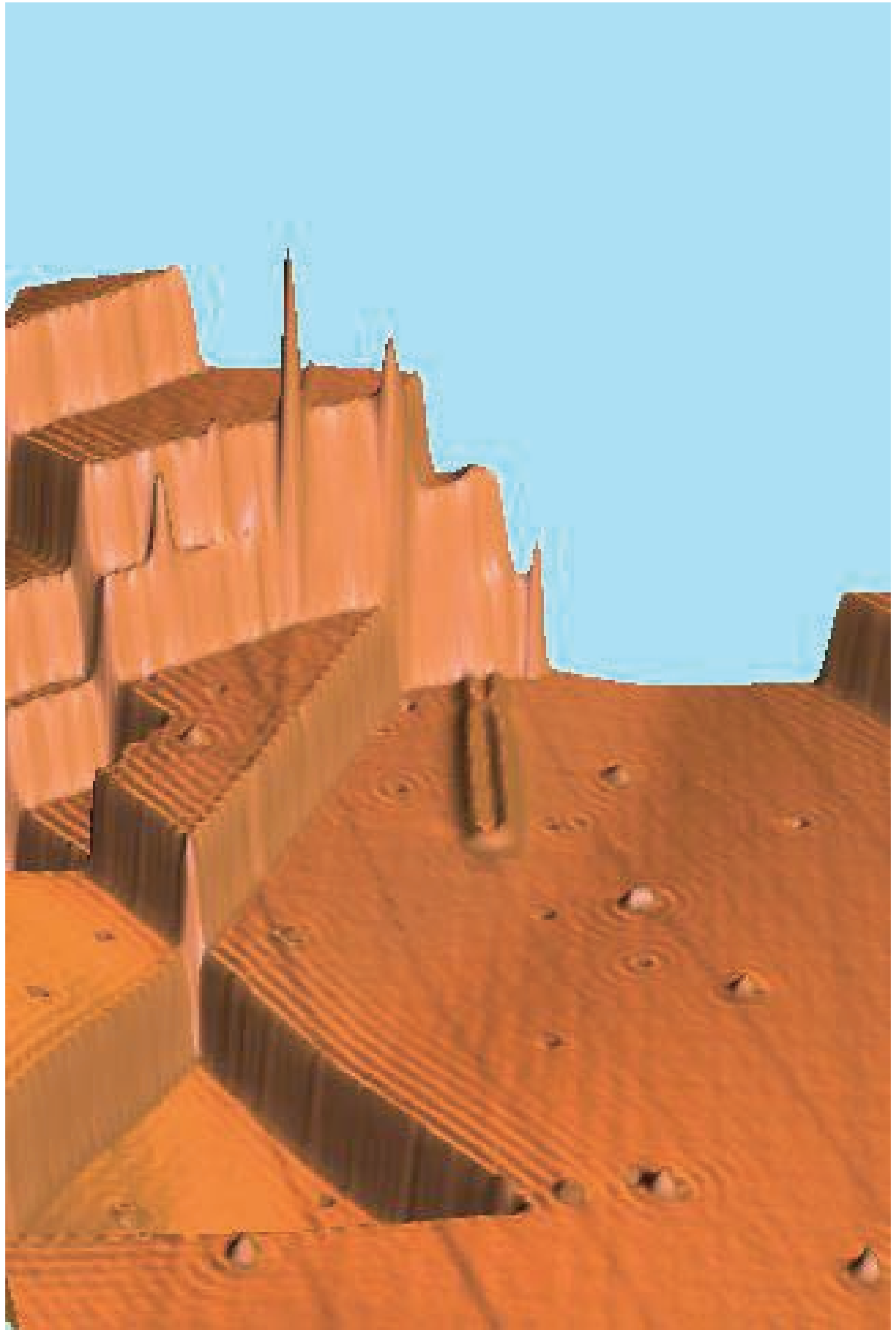


standing electron waves on Cu(111) at 4K
Crommie, Lutz, Eigler, Nature **363**, 524 (1993)

Origin of the waves at E_F (very small V_{bias})

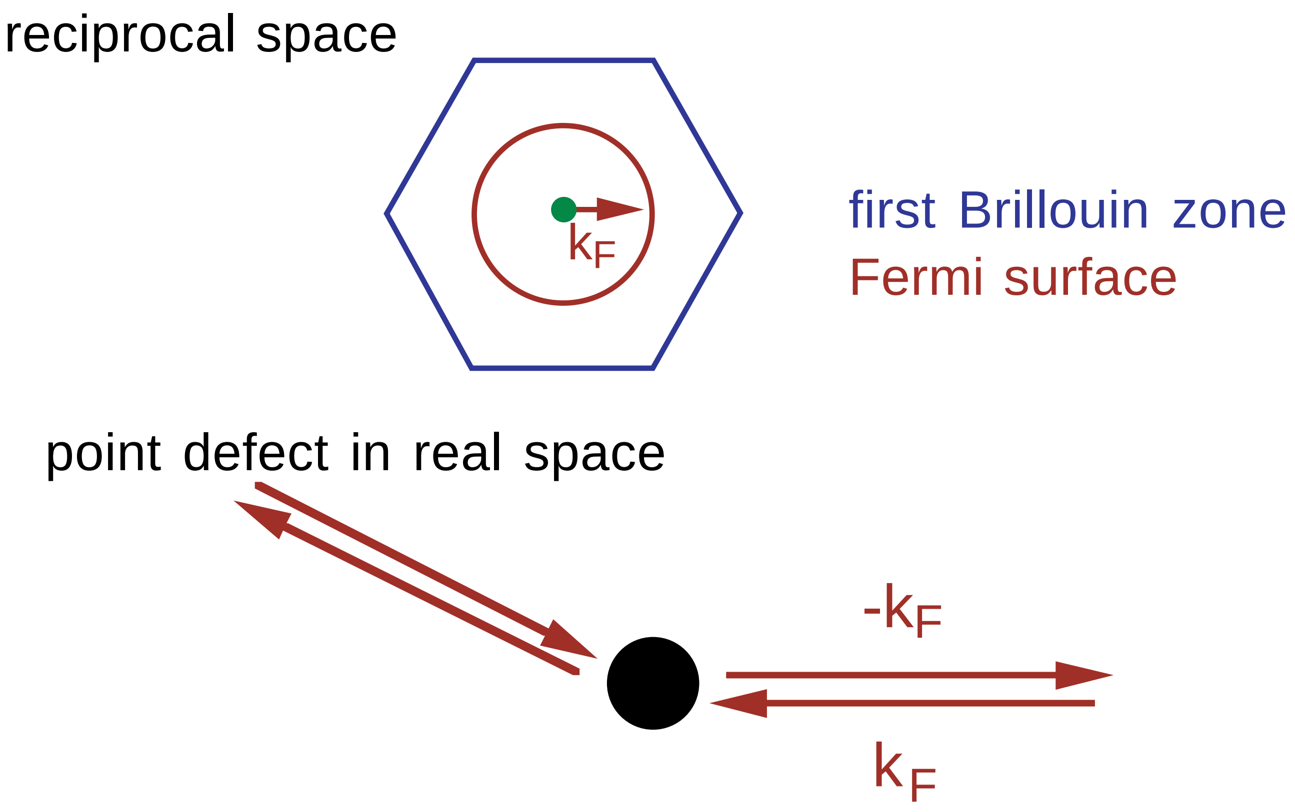


quasiparticle interference

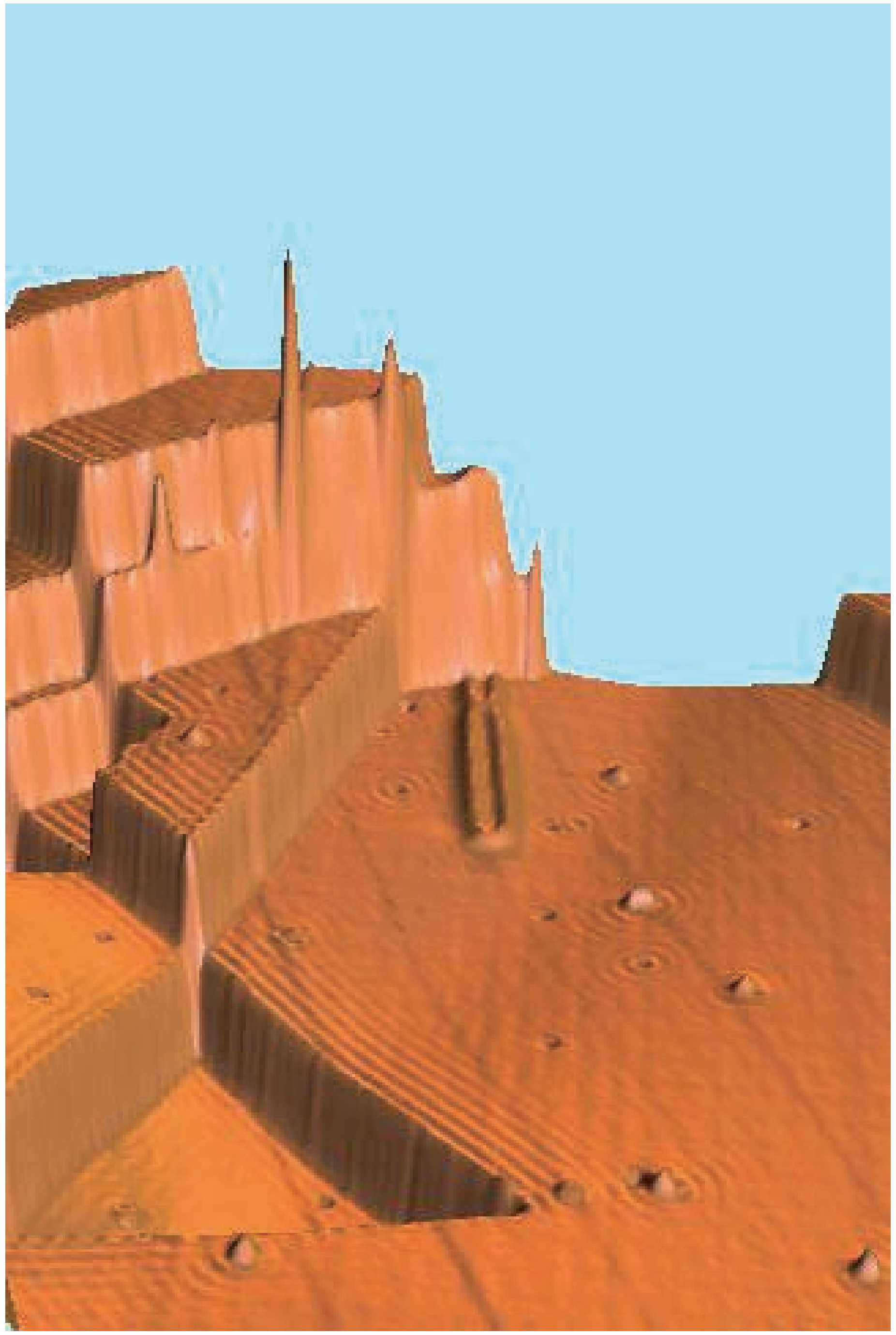


standing electron waves on Cu(111) at 4K
Crommie, Lutz, Eigler, Nature **363**, 524 (1993)

Origin of the waves at E_F (very small V_{bias})



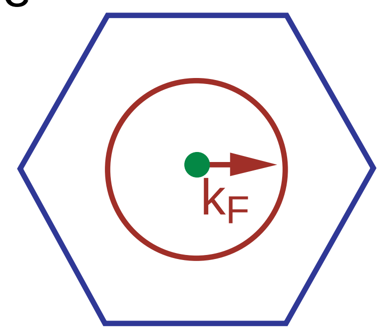
quasiparticle interference



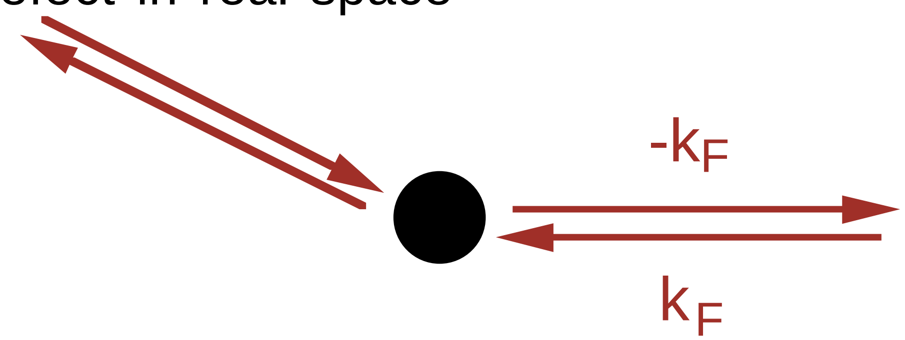
standing electron waves on Cu(111) at 4K
Crommie, Lutz, Eigler, Nature **363**, 524 (1993)

Origin of the waves at E_F (very small V_{bias})

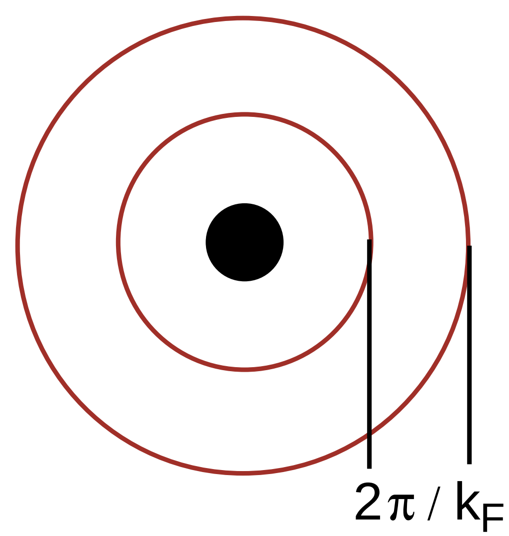
reciprocal space



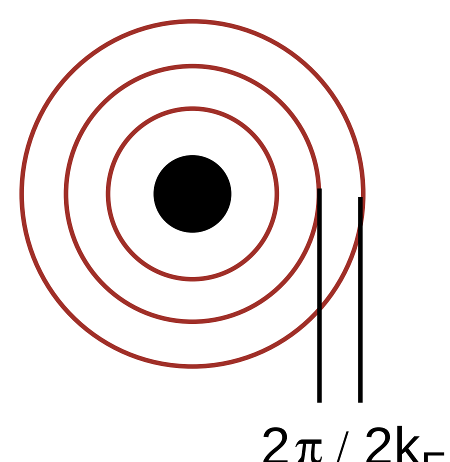
point defect in real space



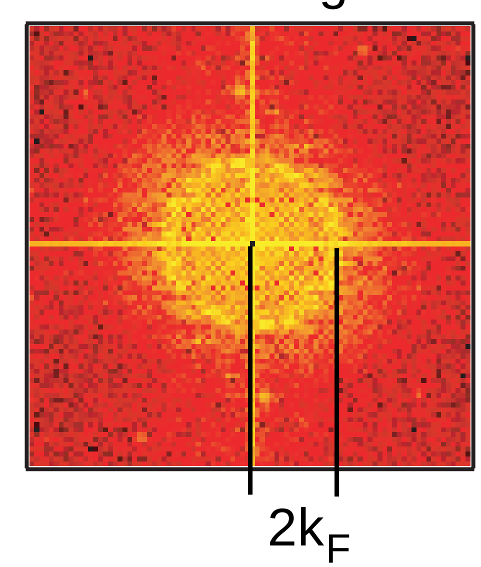
wave functions



LDOS

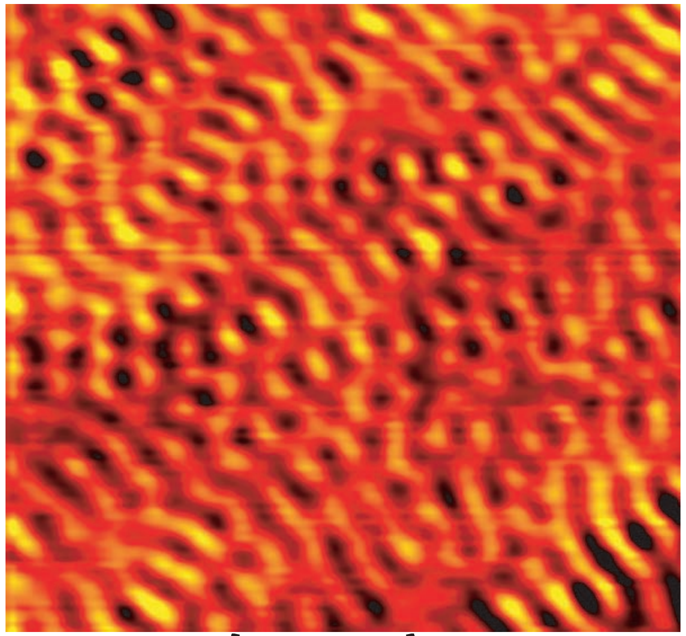


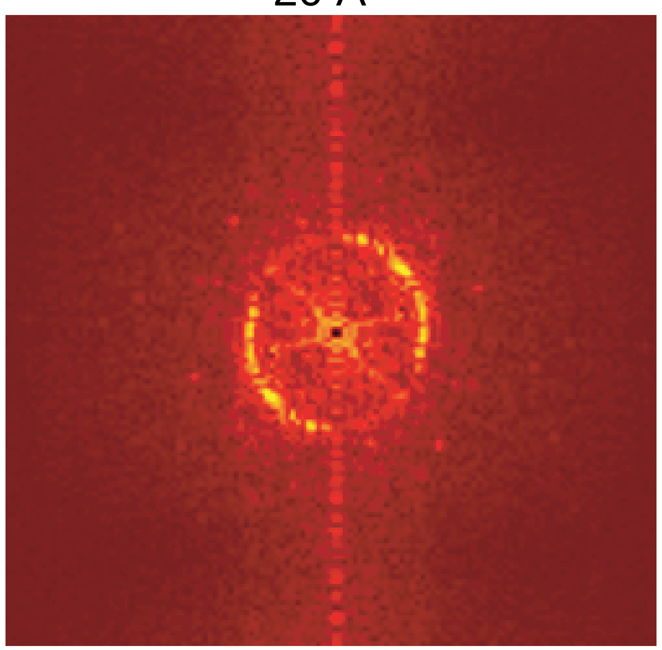
Fourier transform of STM image



fermi surfaces by Fourier-transform STM

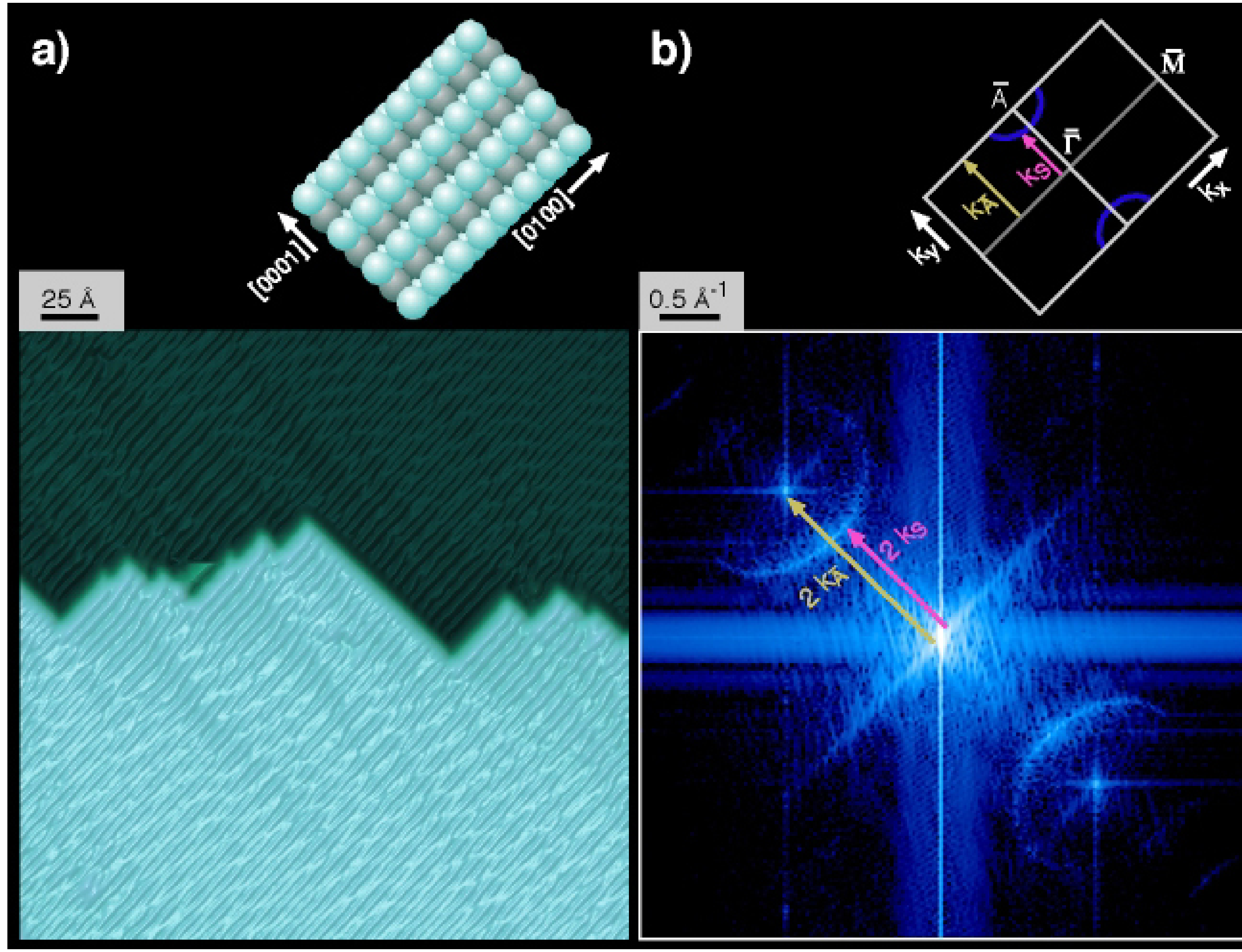
Be(0001)





Ph. Sprunger et al., Science **275**, 1764 (1997).

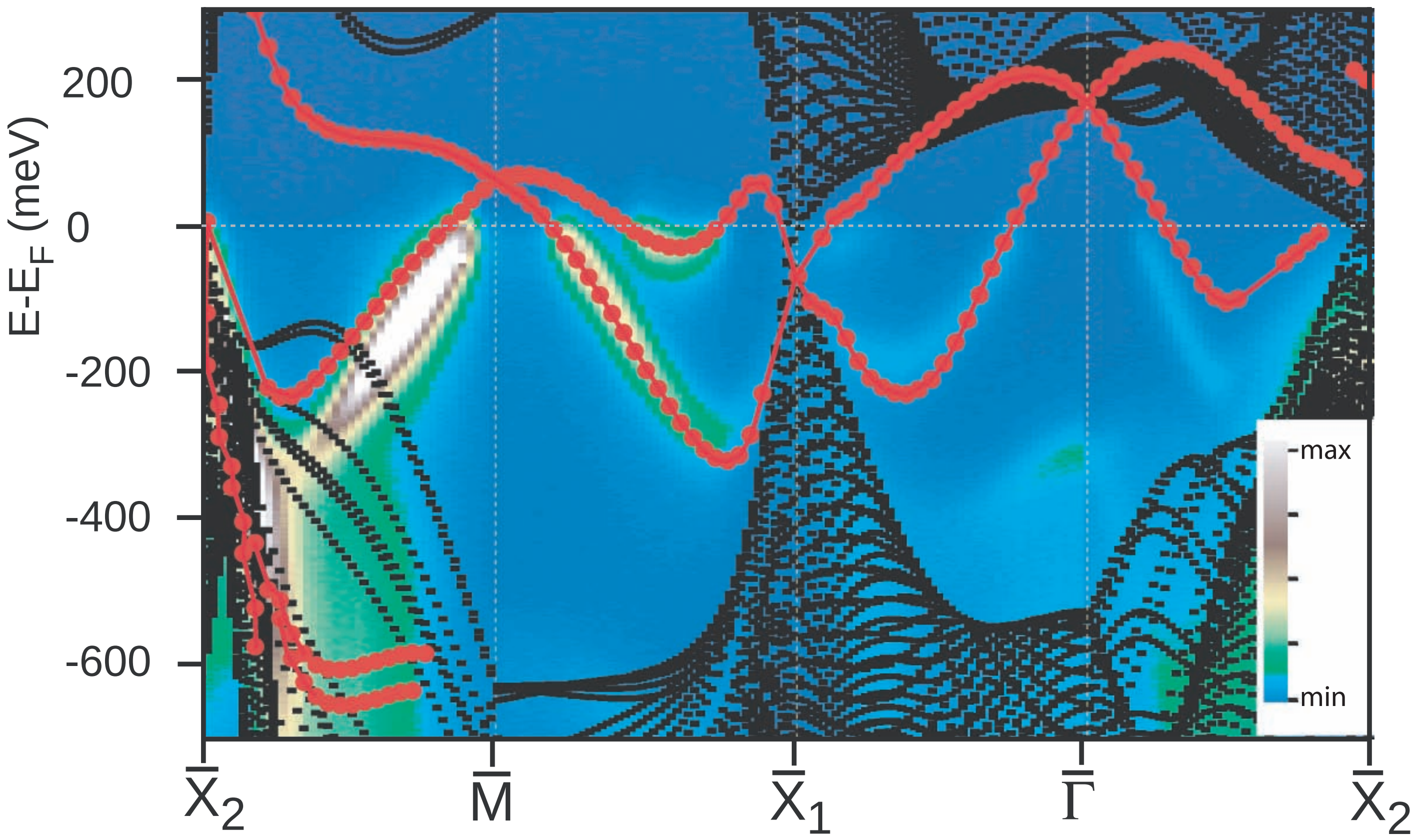
Be(10$\bar{1}$0)

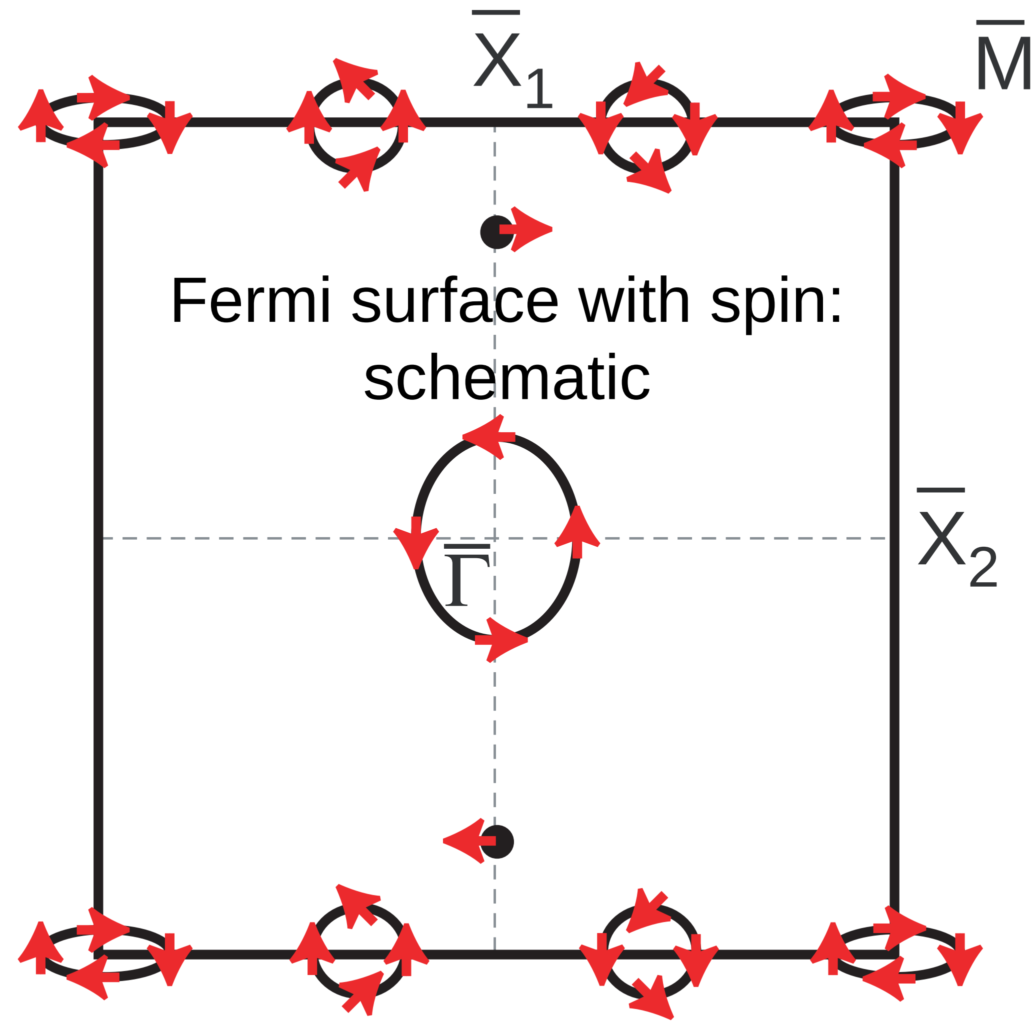


Ph. Hofmann, B.G. Briner, M. Doering, H.-P. Rust, E.W. Plummer and A.M. Bradshaw Phys. Rev. Lett. 79, 265 (1997).
B.G. Briner, Ph. Hofmann, M. Doering, H.-P. Rust, E.W. Plummer and A.M. Bradshaw Europhys. Lett. 39, 67 (1997).
L. Ptersen,P.T. Sprunger, Ph. Hofmann, E. Lægsgaard, B.G. Briner, M. Doering, H.-P. Rust, A.M. Bradshaw F. Besenbacher and E.W. Plummer, Phys. Rev. B **57**, R6858 (1998).

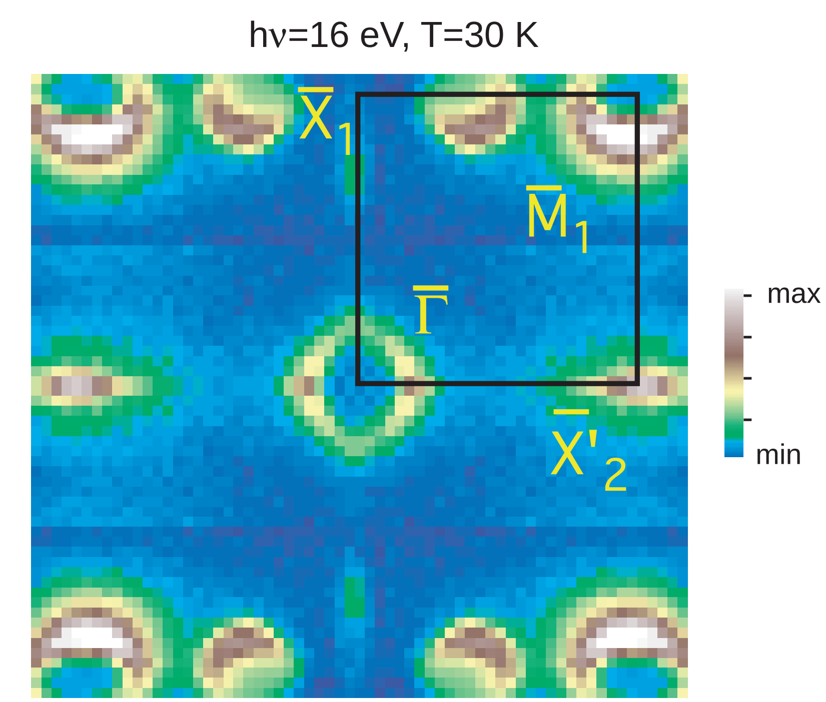
- A Fourier transformation of an STM image gives a direct image of the Fermi surface.
- In addition to this one sees the points corresponding to the FT of the lattice.

Bi(110) fermi surface and spin direction



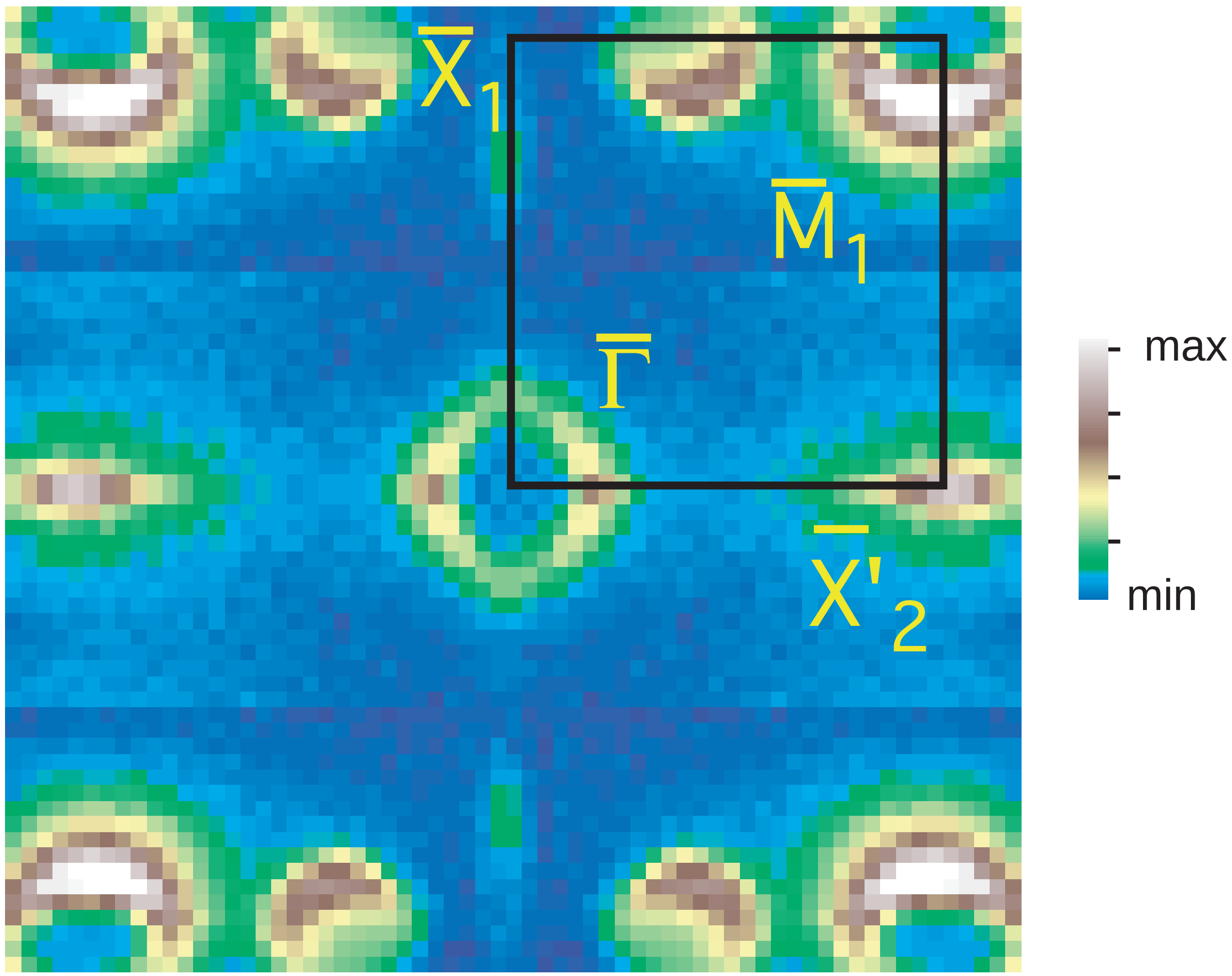


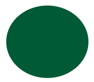
Fermi surface: experiment



waves on Bi(110)?

hν=16 eV, T=30 K

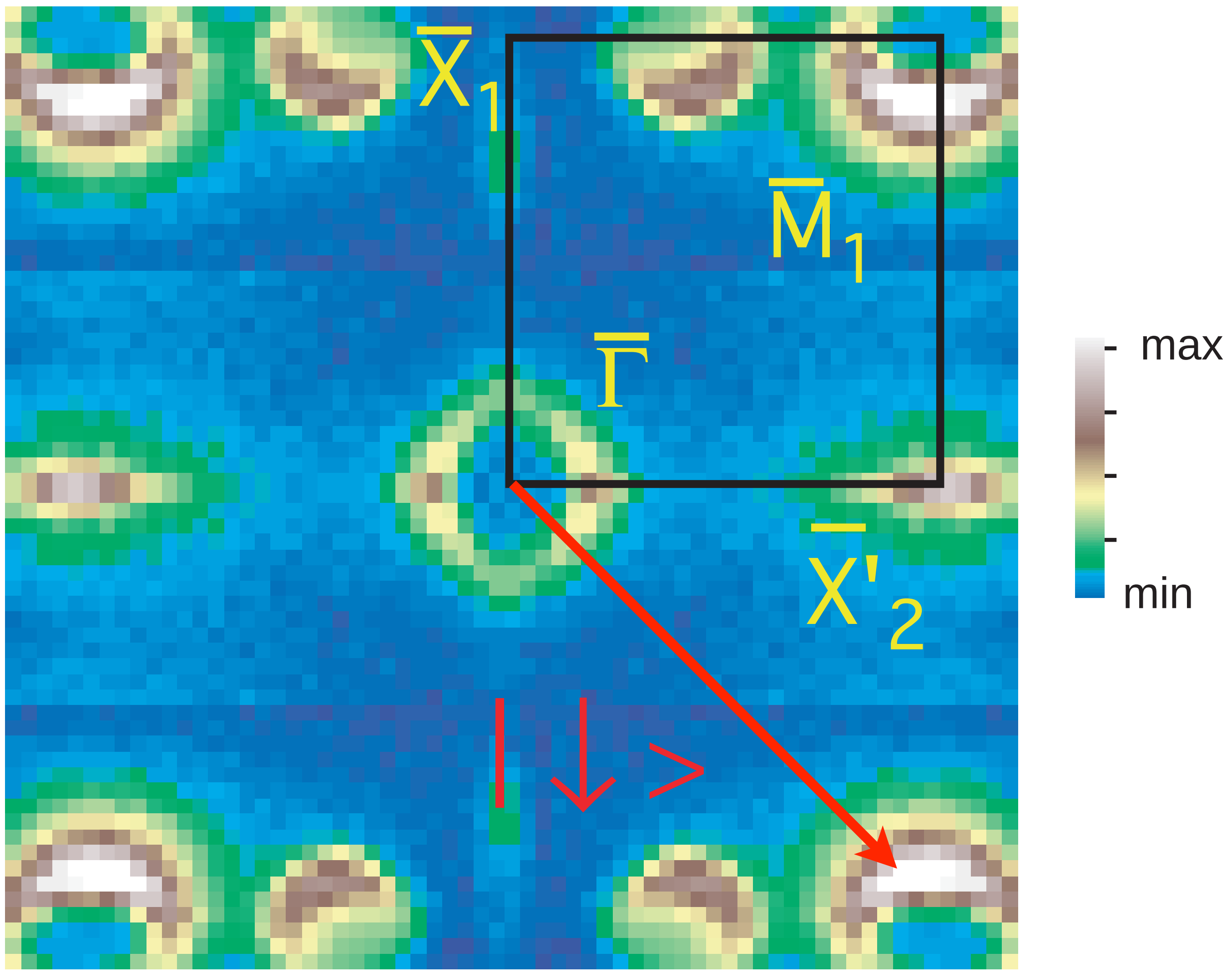


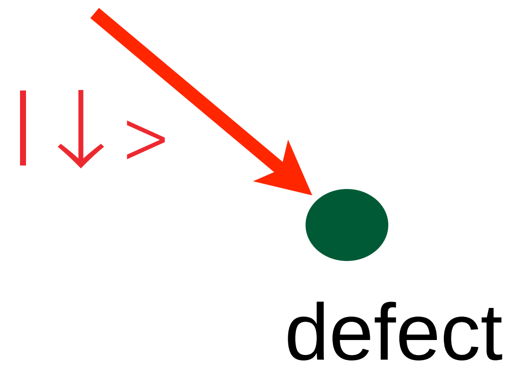


- “normal waves” not possible without spin-flip

waves on Bi(110)?

hν=16 eV, T=30 K

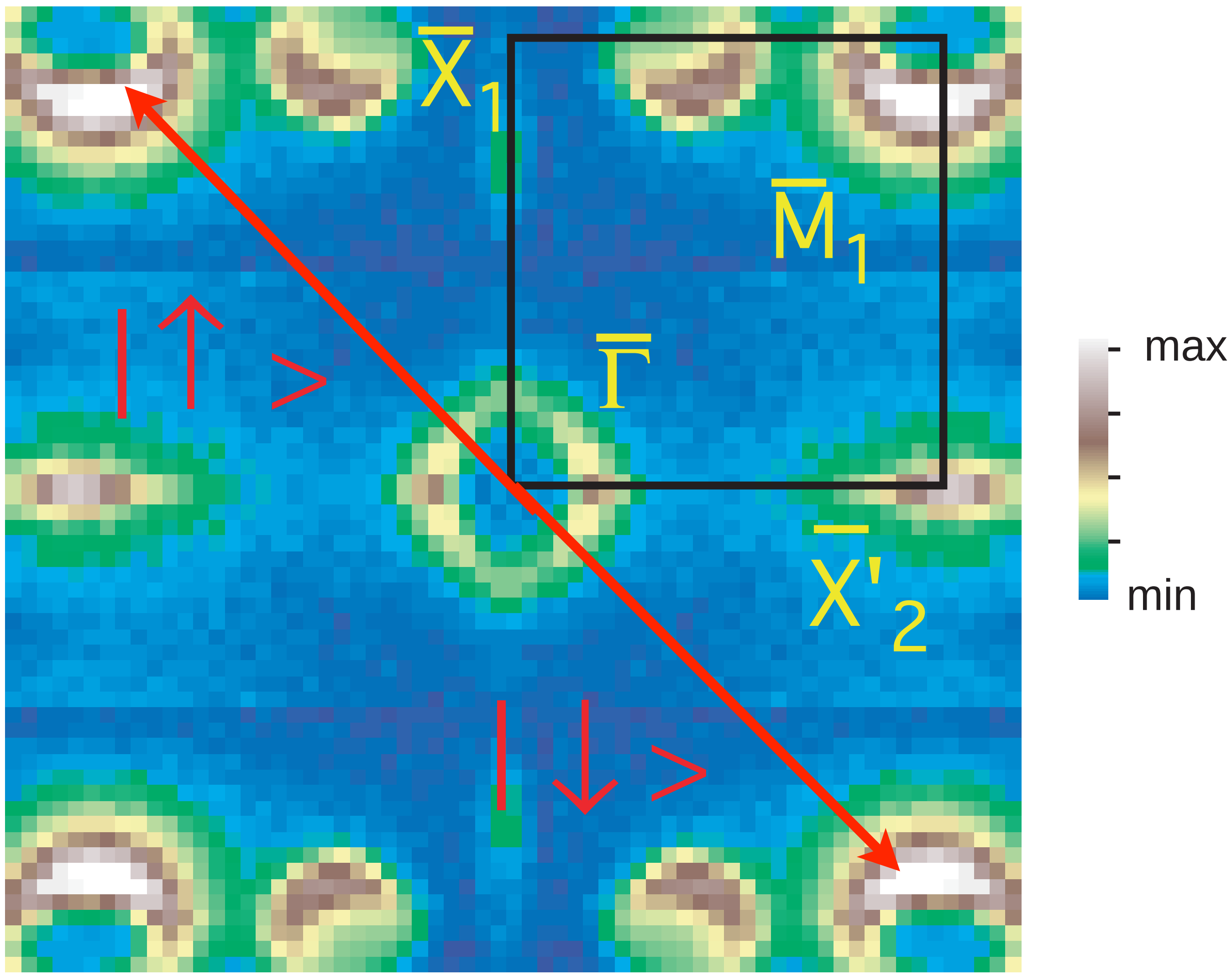


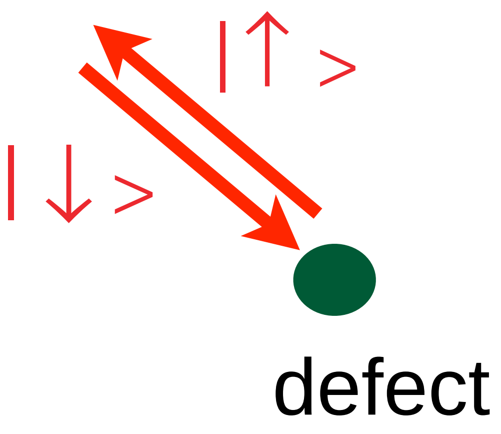


- “normal waves” not possible without spin-flip

waves on Bi(110)?

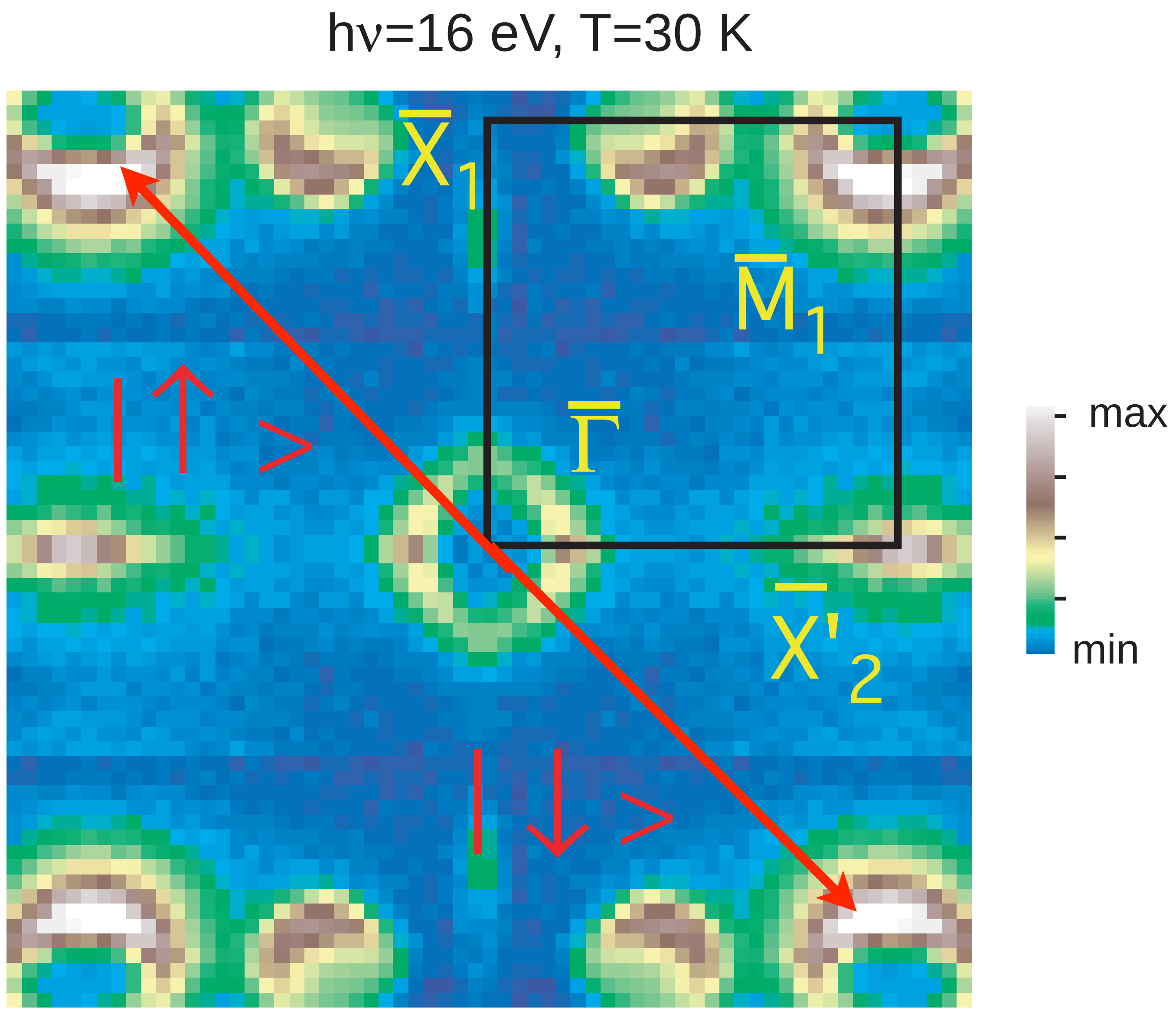
hν=16 eV, T=30 K

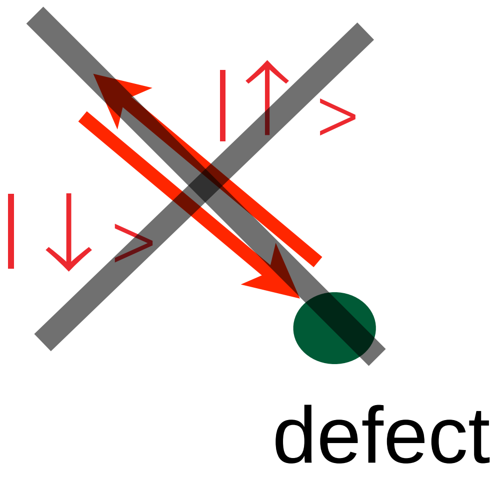




- “normal waves” not possible without spin-flip

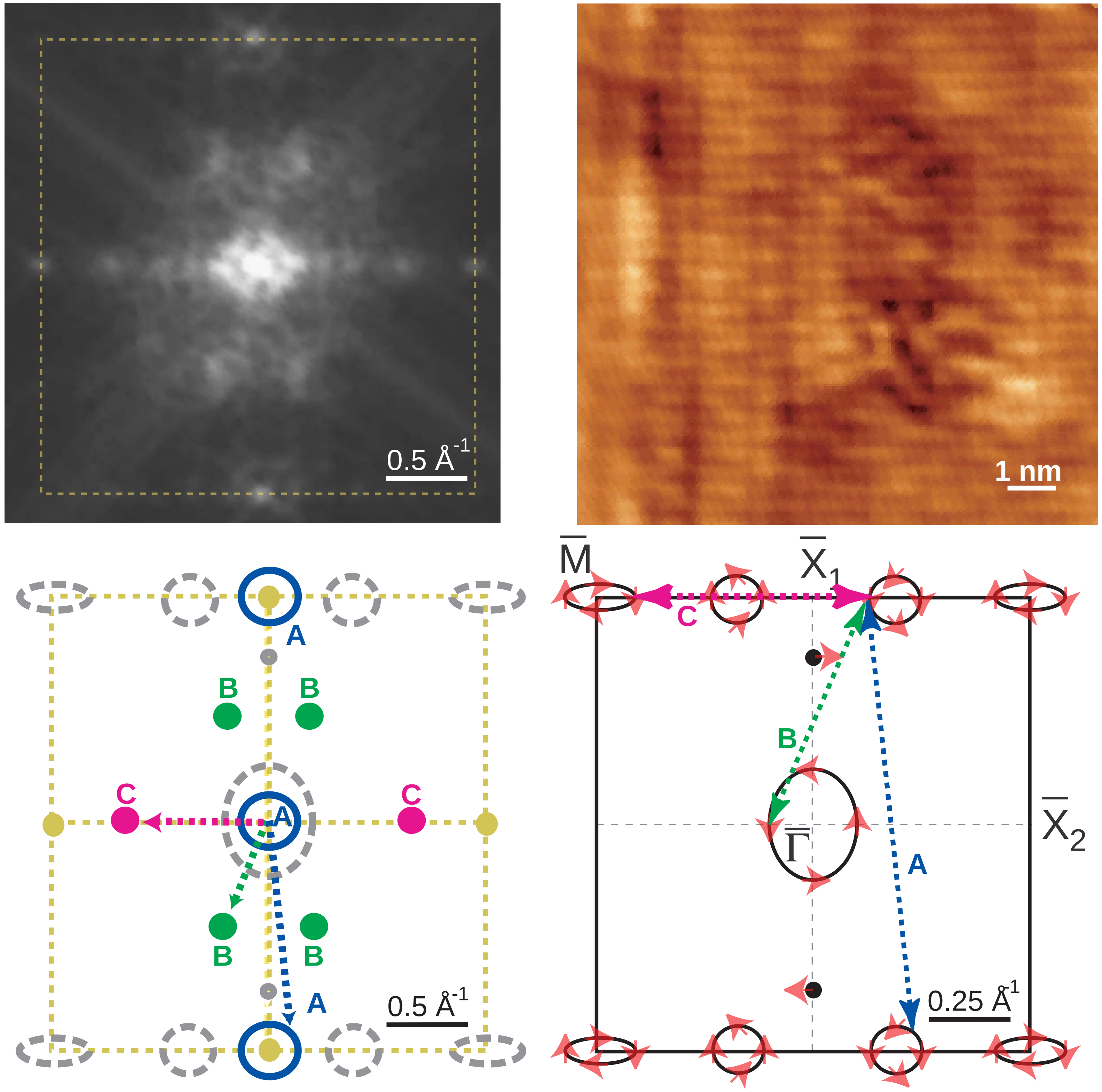
waves on Bi(110)?





- “normal waves” not possible without spin-flip

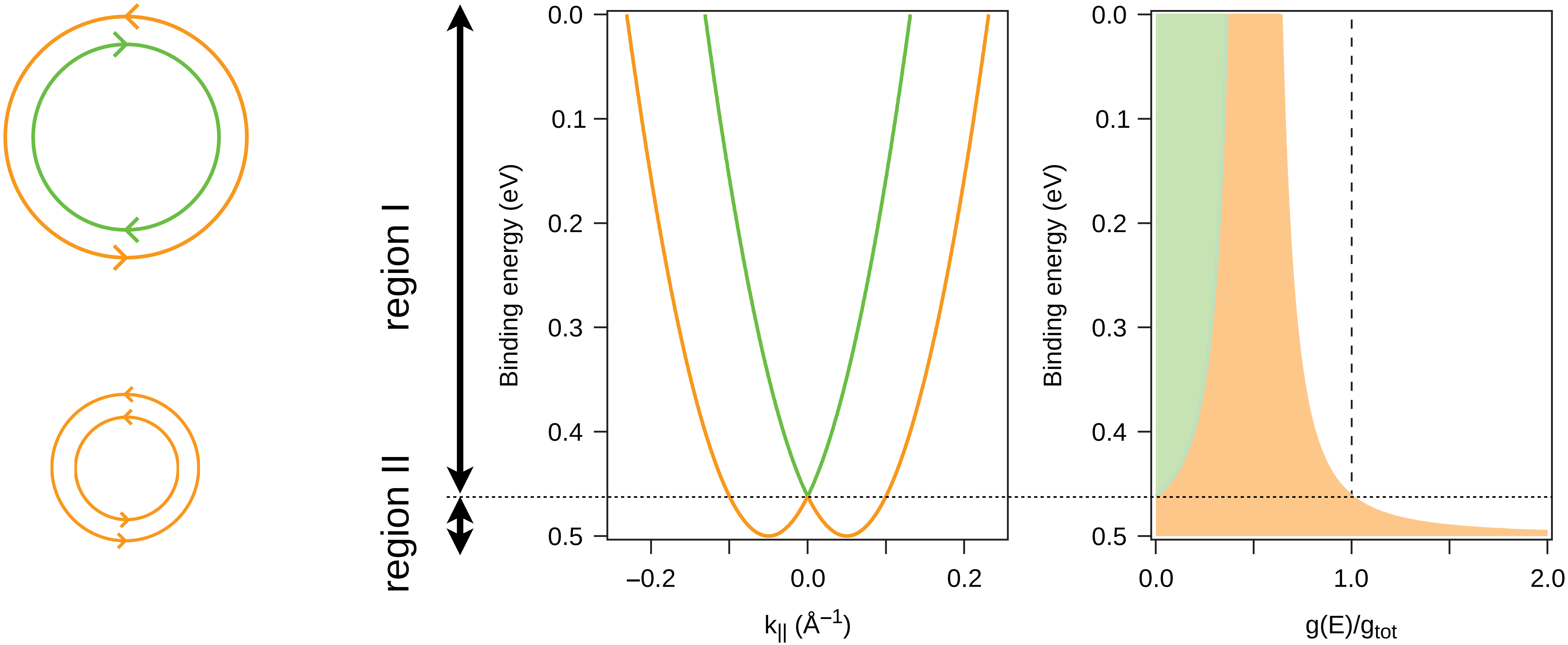
spectroscopic images



J. I. Pascual et al. , Physical Review Letters **93**, 196802 (2004)

electron-electron scattering in a Rashba system: detailed theory / experiment

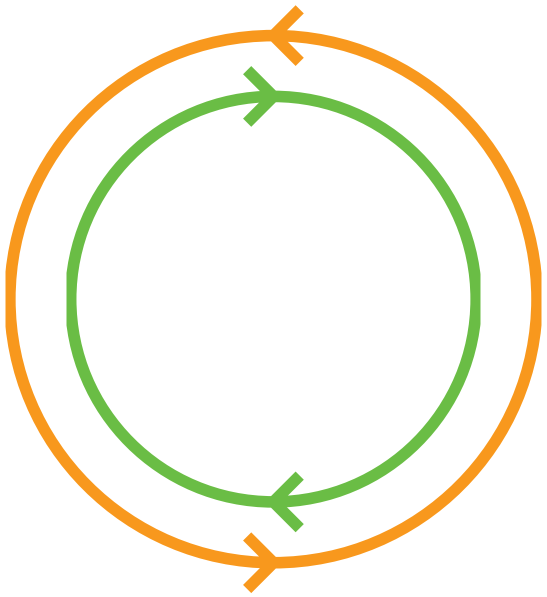
density of states

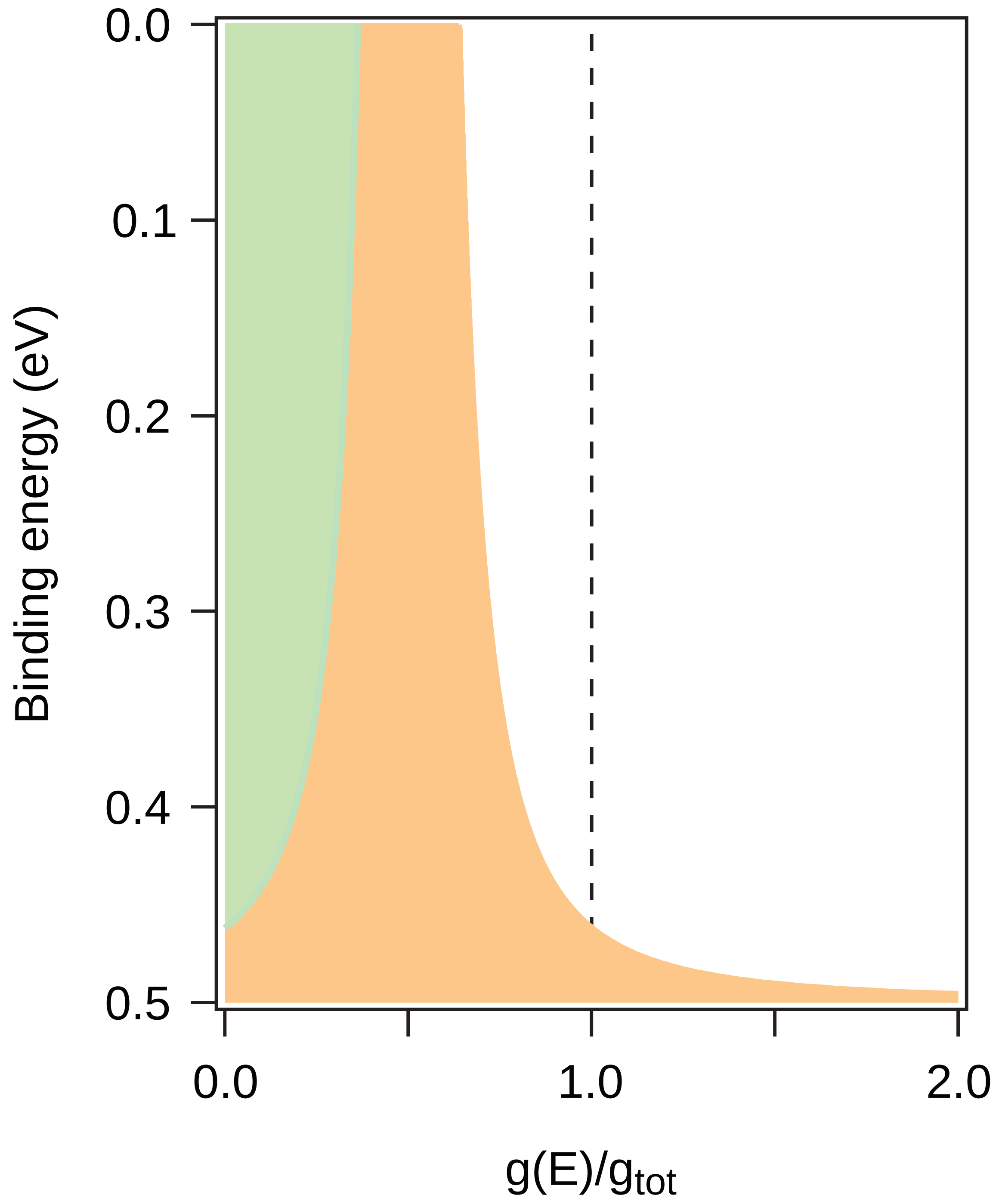


no SOI
$$g(E) = \frac{|m^*|}{\pi\hbar^2}$$

finite SOI
$$g(E) = \frac{|m^*|}{2\pi\hbar^2} \pm \frac{k_0}{2\pi}\sqrt{\frac{2|m^*|}{\hbar^2}}\frac{1}{2\sqrt{E-E_0}}$$

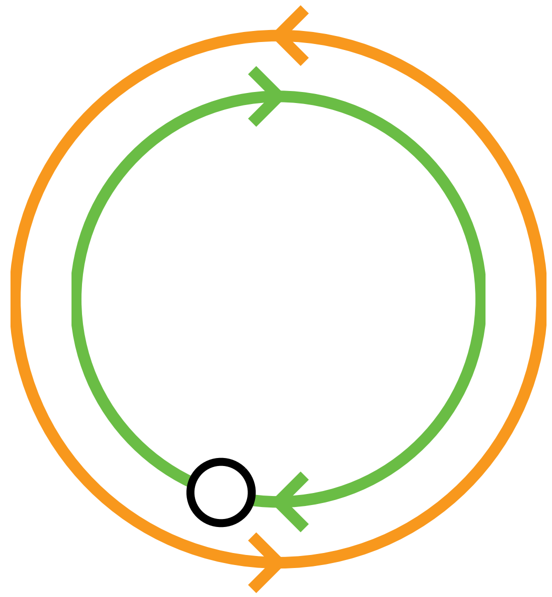
spin-dependent lifetimes?

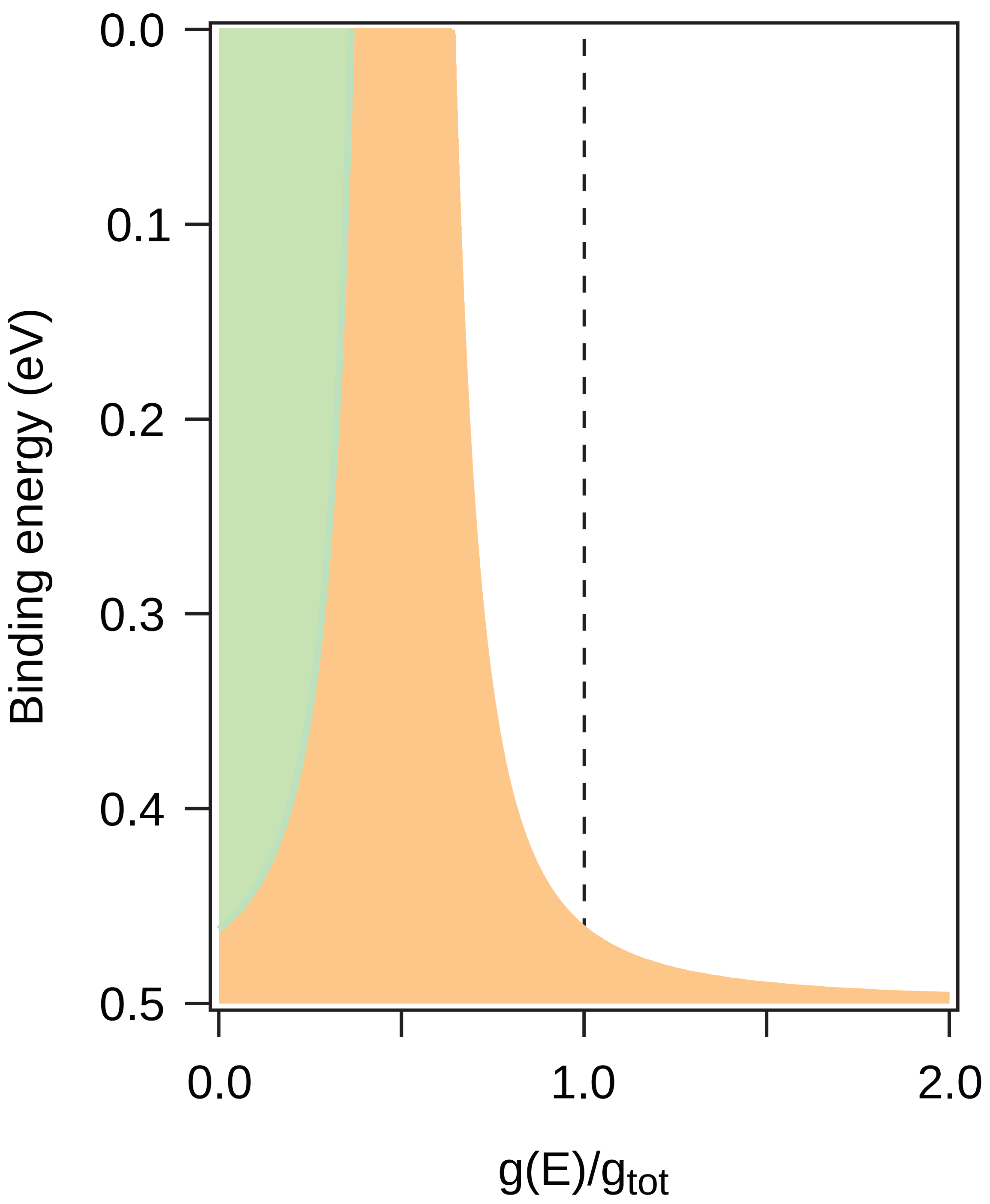




Different number of states with equal spin on both branches: Effect on photo-hole lifetime?

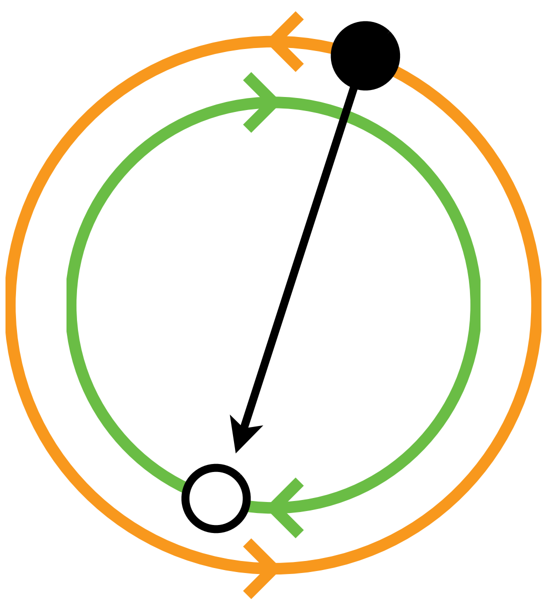
spin-dependent lifetimes?

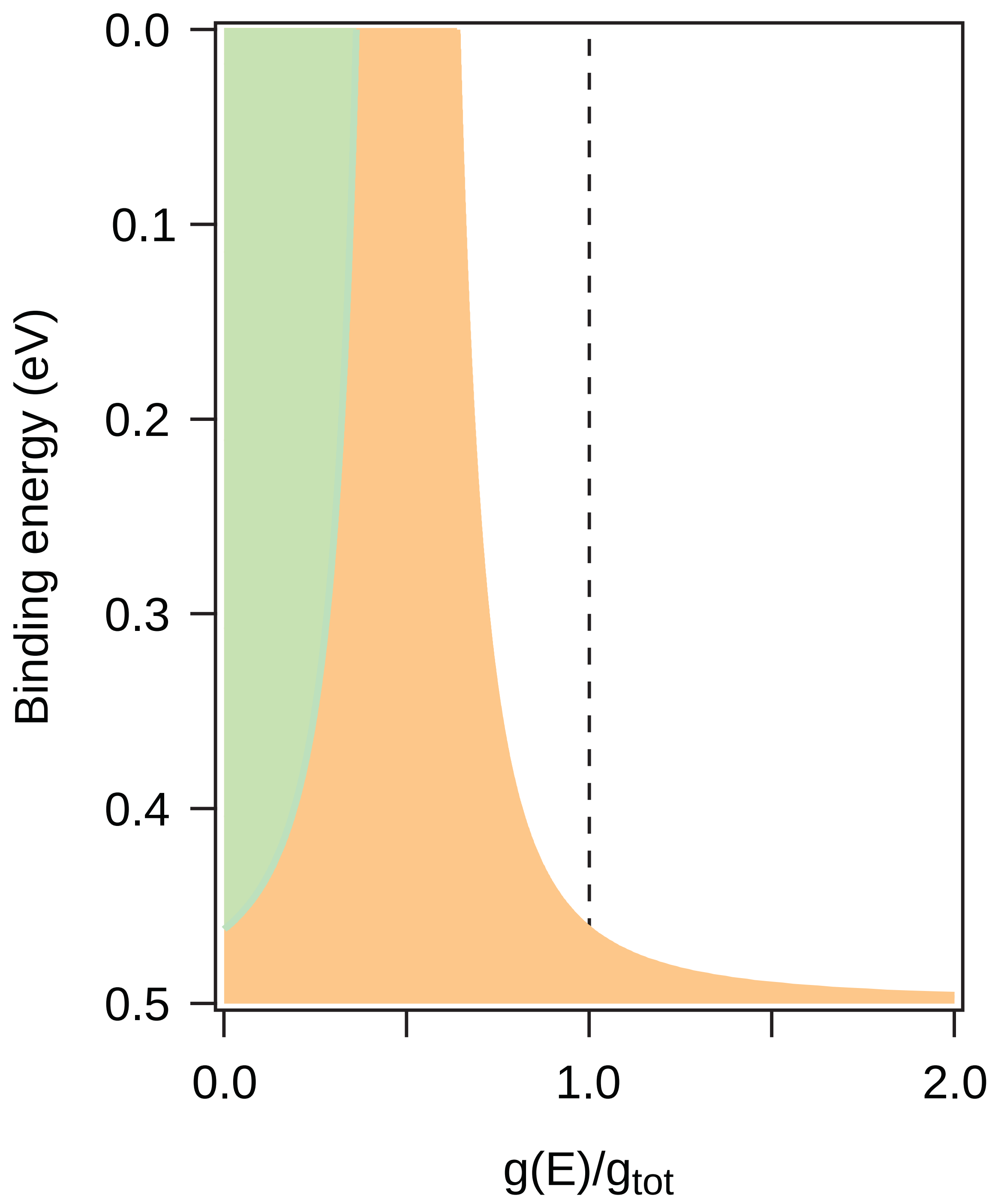




Different number of states with equal spin on both branches: Effect on photo-hole lifetime?

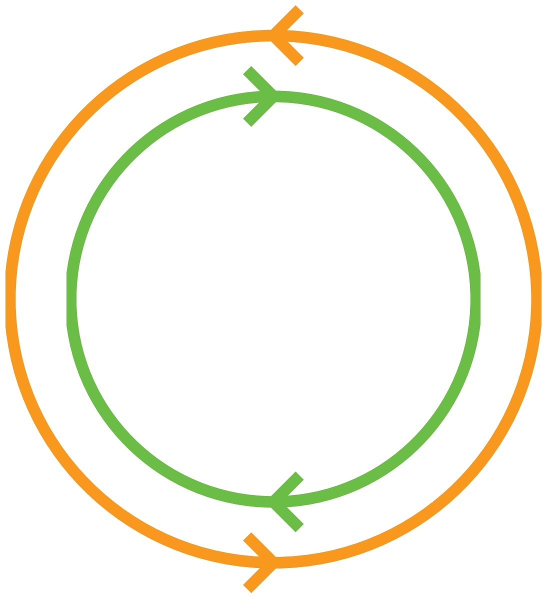
spin-dependent lifetimes?

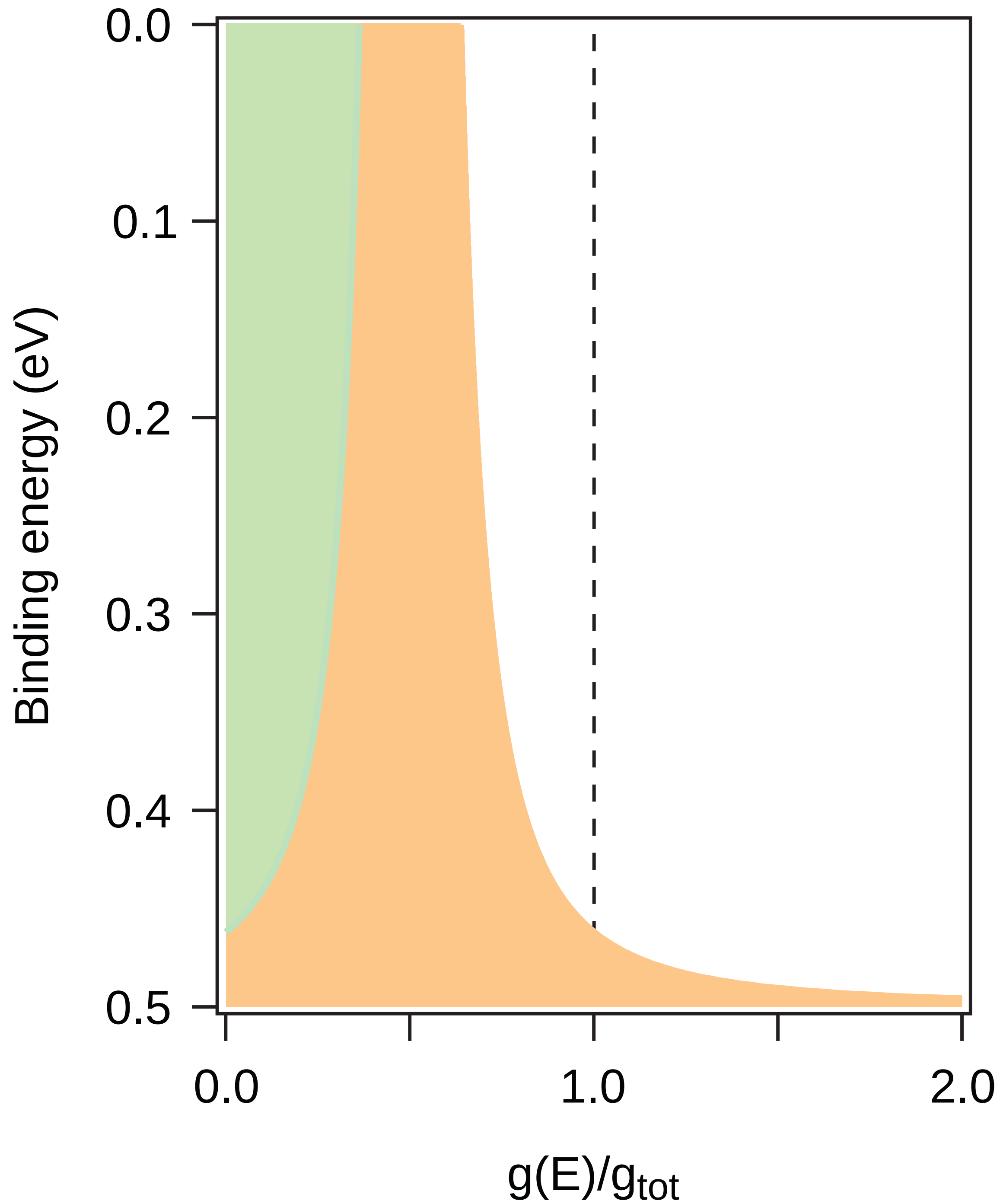




Different number of states with equal spin on both branches: Effect on photo-hole lifetime?

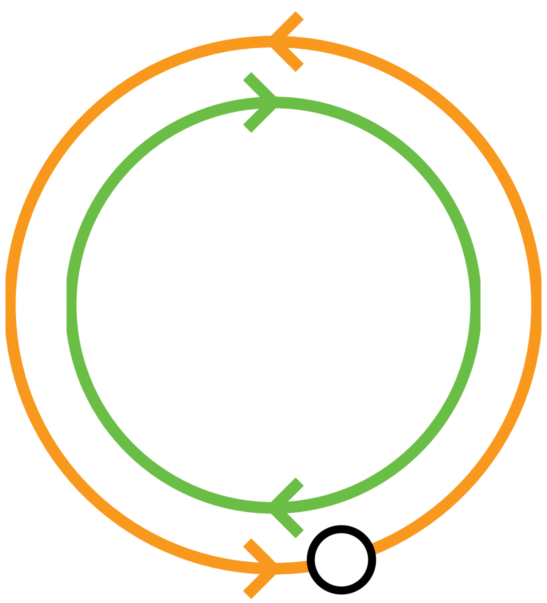
spin-dependent lifetimes?

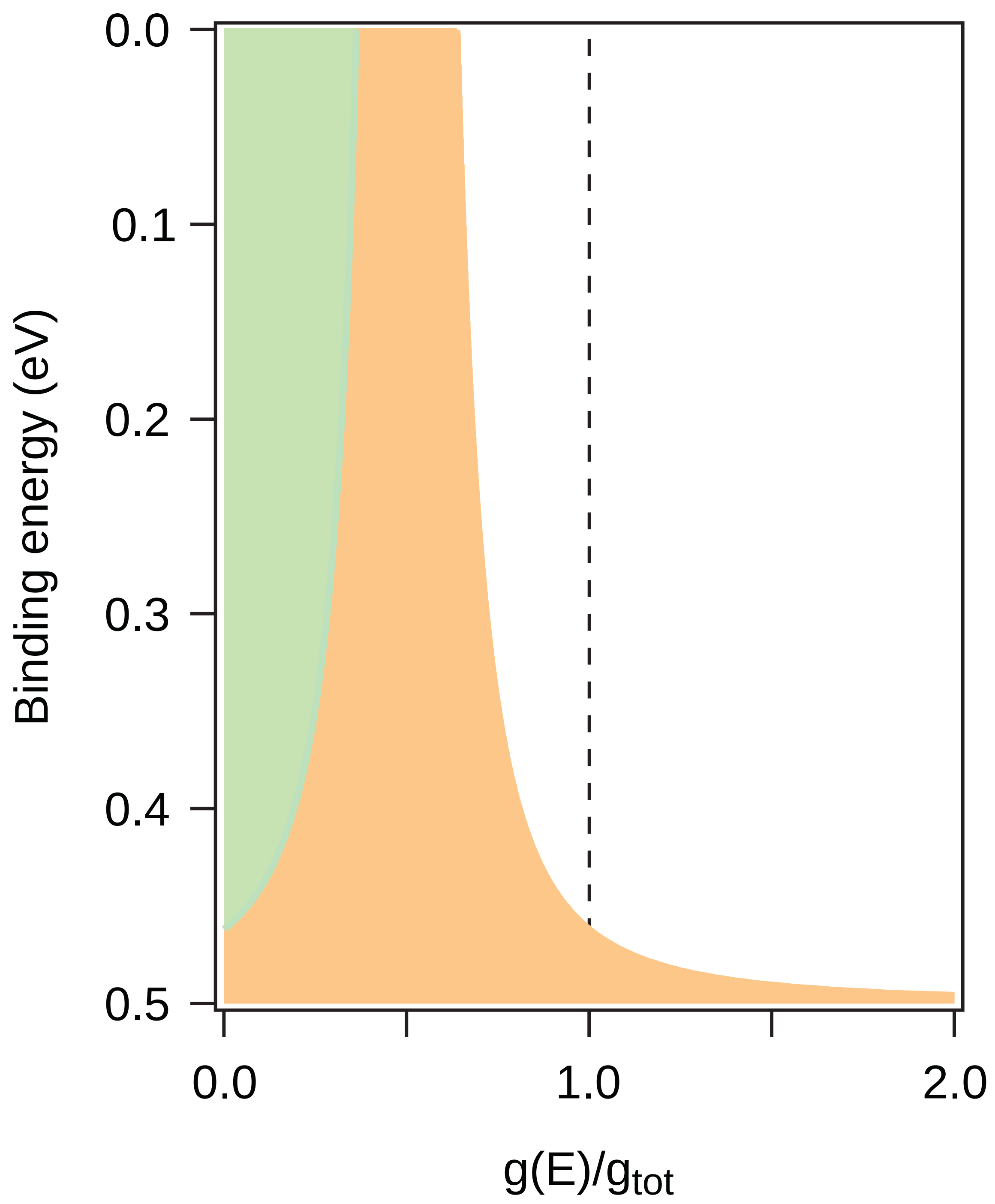




Different number of states with equal spin on both branches: Effect on photo-hole lifetime?

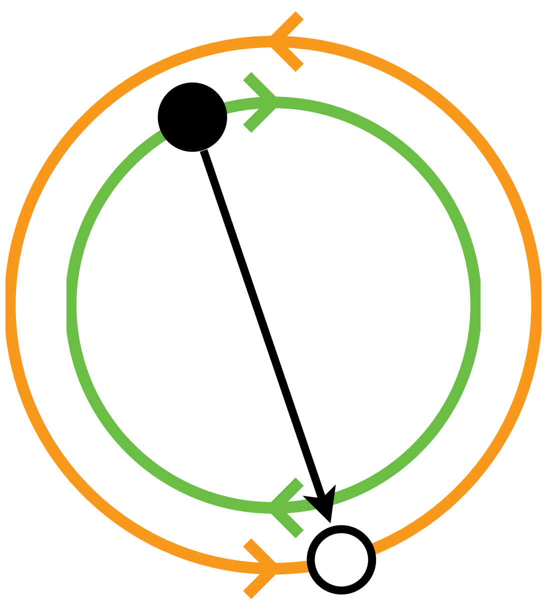
spin-dependent lifetimes?

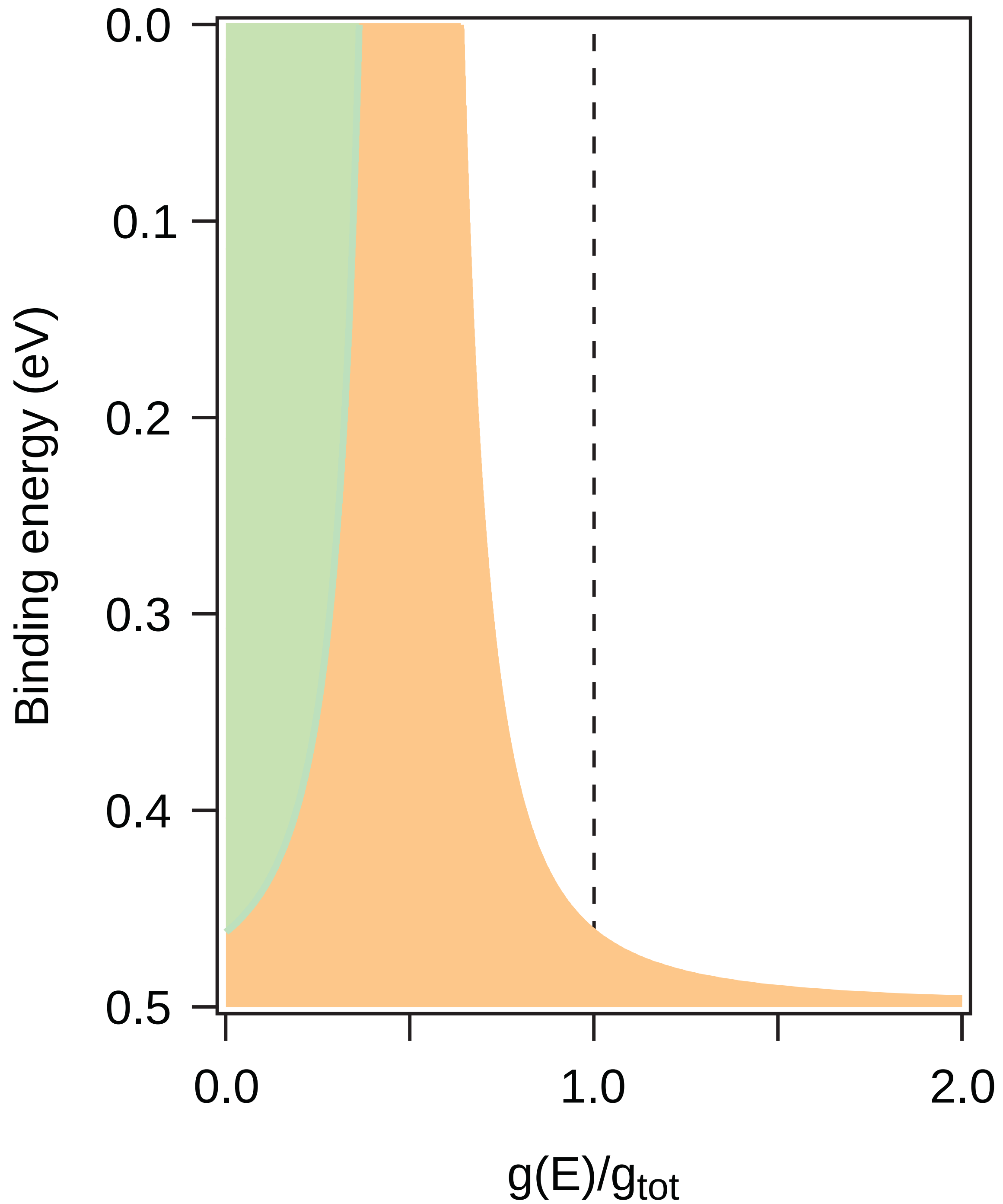




Different number of states with equal spin on both branches: Effect on photo-hole lifetime?

spin-dependent lifetimes?



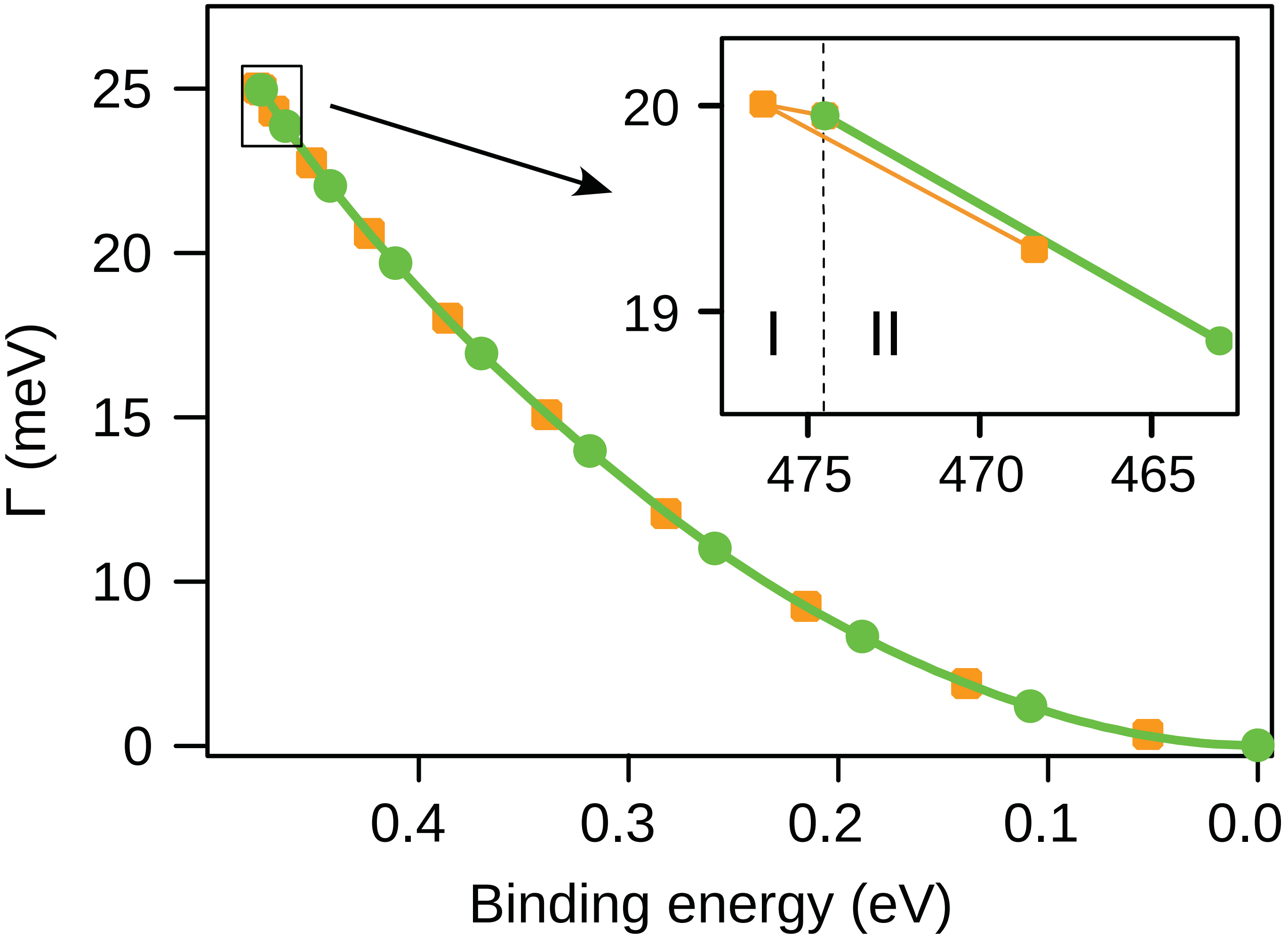


Different number of states with equal spin on both branches: Effect on photo-hole lifetime?

theory: GW approximation

GW theory confirms unequal contributions from branches

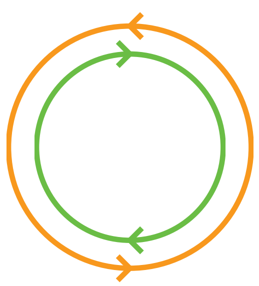
Negligible differences between branch lifetimes

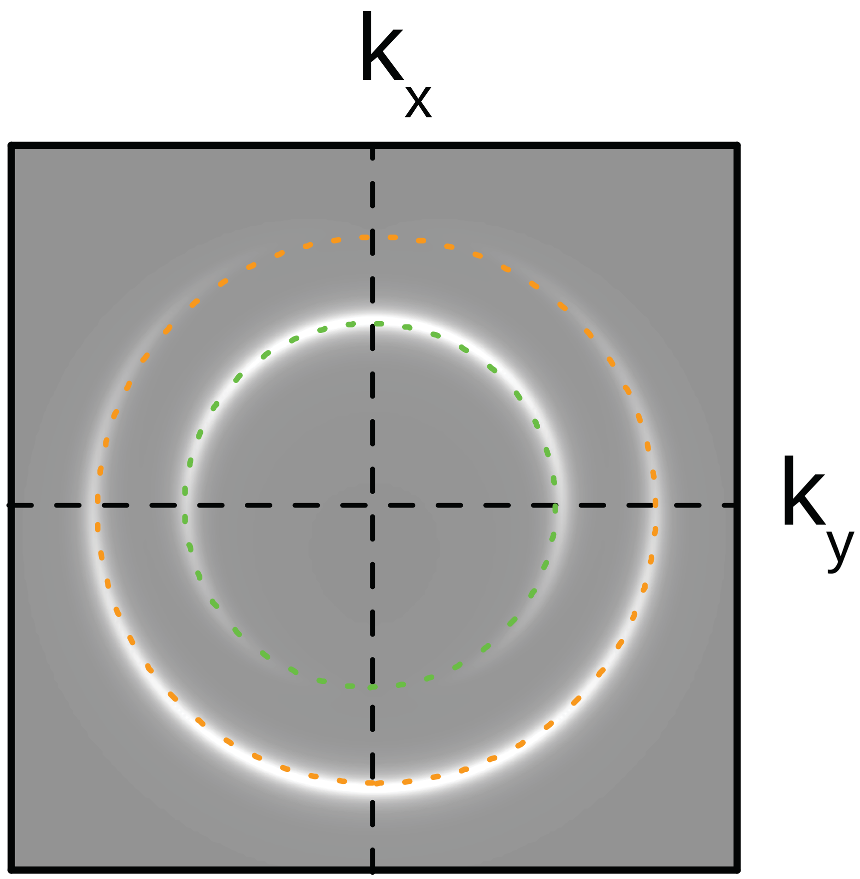


I. A. Nechaev et al. PRB **80**, 113402 (2009)

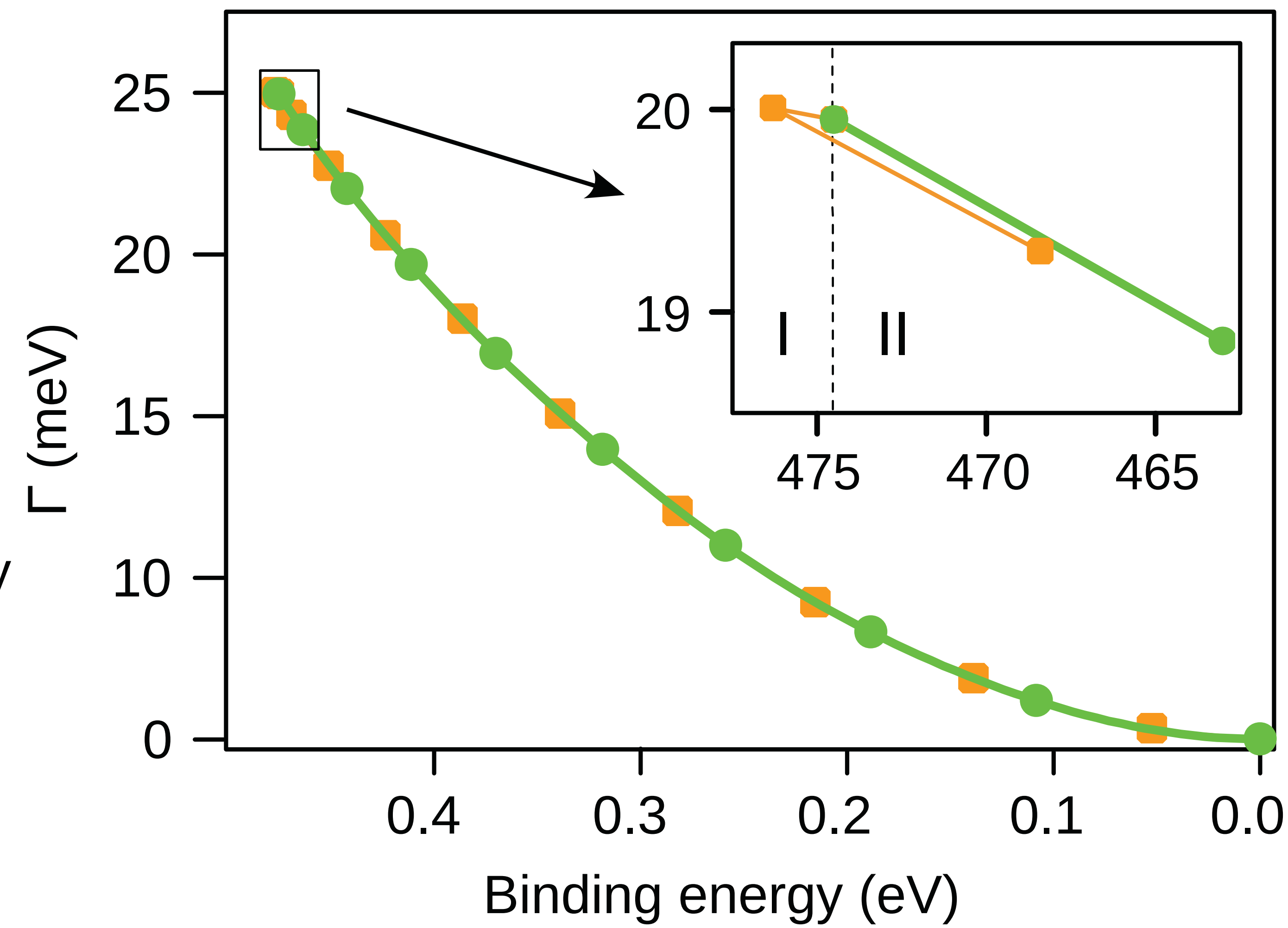
theory: GW approximation

Negligible differences between branch lifetimes





GW theory confirms unequal contributions from branches



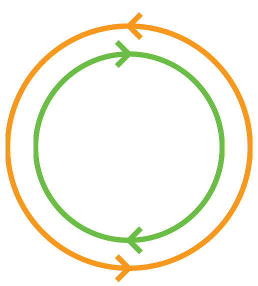
$$\Gamma_{\omega,\mathbf{k}} = -2\sum_{n's'}\int dz dz' M_{nn'}(z,z') \times \int \frac{d\mathbf{q}}{(2\pi)^2} F^{ss'}_{\mathbf{k},\mathbf{q}} f^{s'}_{\mathbf{q}n'} \theta(E^{s'}_{\mathbf{q}n'}-\omega)\times \quad \mathrm{Im}W(z,z';\mathbf{k}-\mathbf{q},\omega-E^{s'}_{\mathbf{q}n'})$$

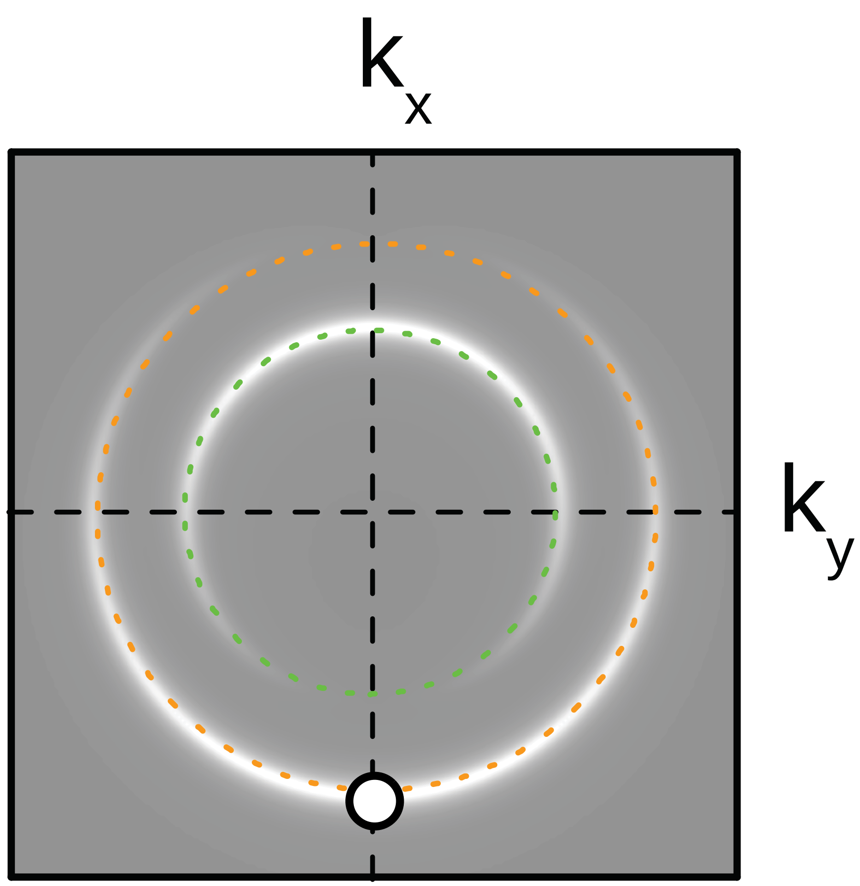
I. A. Nechaev et al. PRB **80**, 113402 (2009)

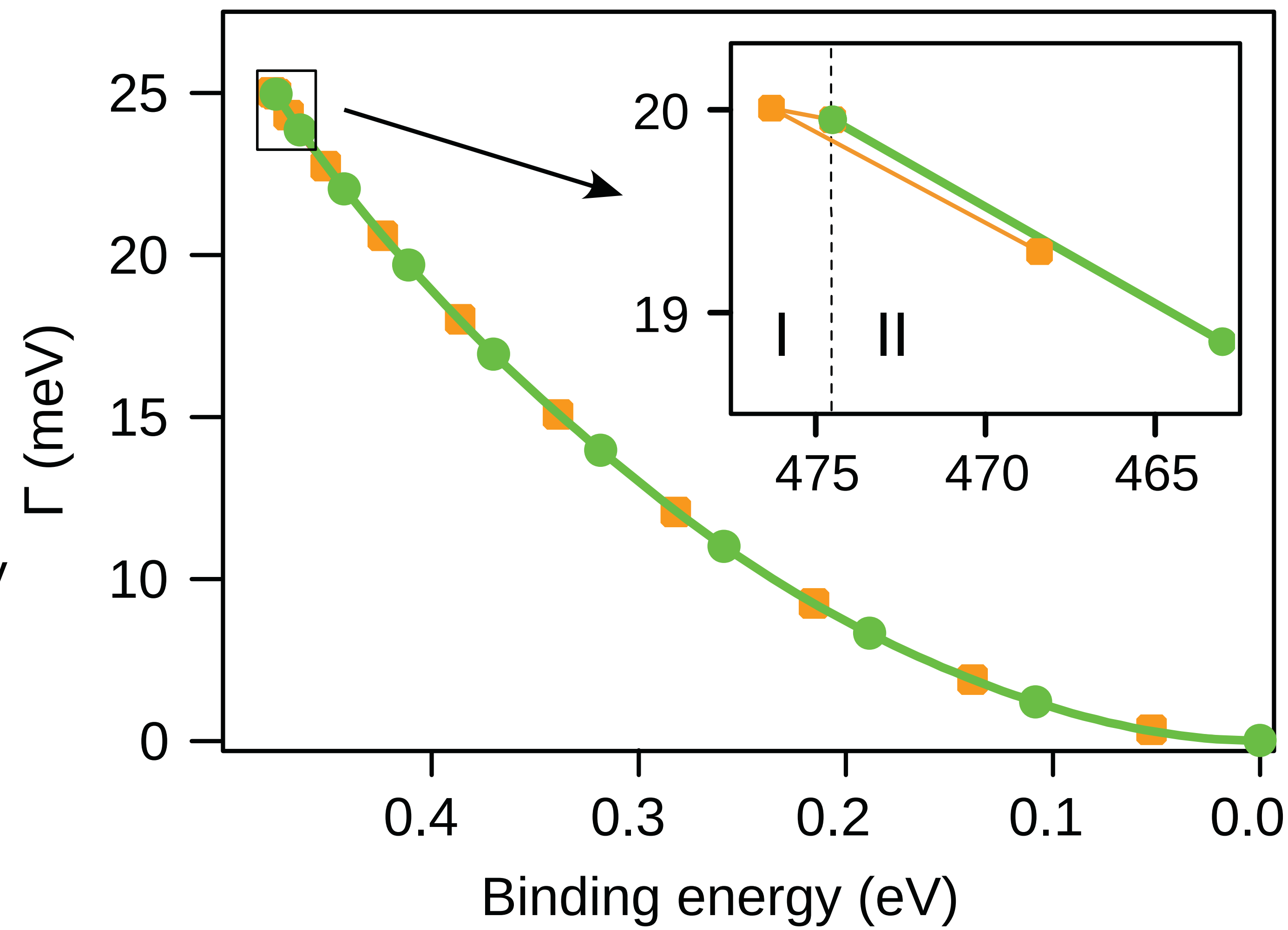
theory: GW approximation

GW theory confirms unequal contributions from branches

Negligible differences between branch lifetimes







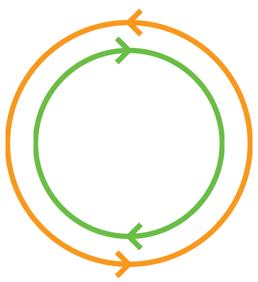
$$\Gamma_{\omega,\mathbf{k}} = -2\sum_{n's'}\int dz dz' M_{nn'}(z,z') \times \int \frac{d\mathbf{q}}{(2\pi)^2} F^{ss'}_{\mathbf{k},\mathbf{q}} f^{s'}_{\mathbf{q}n'} \theta(E^{s'}_{\mathbf{q}n'}-\omega)\times \quad \mathrm{Im}W(z,z';\mathbf{k}-\mathbf{q},\omega-E^{s'}_{\mathbf{q}n'})$$

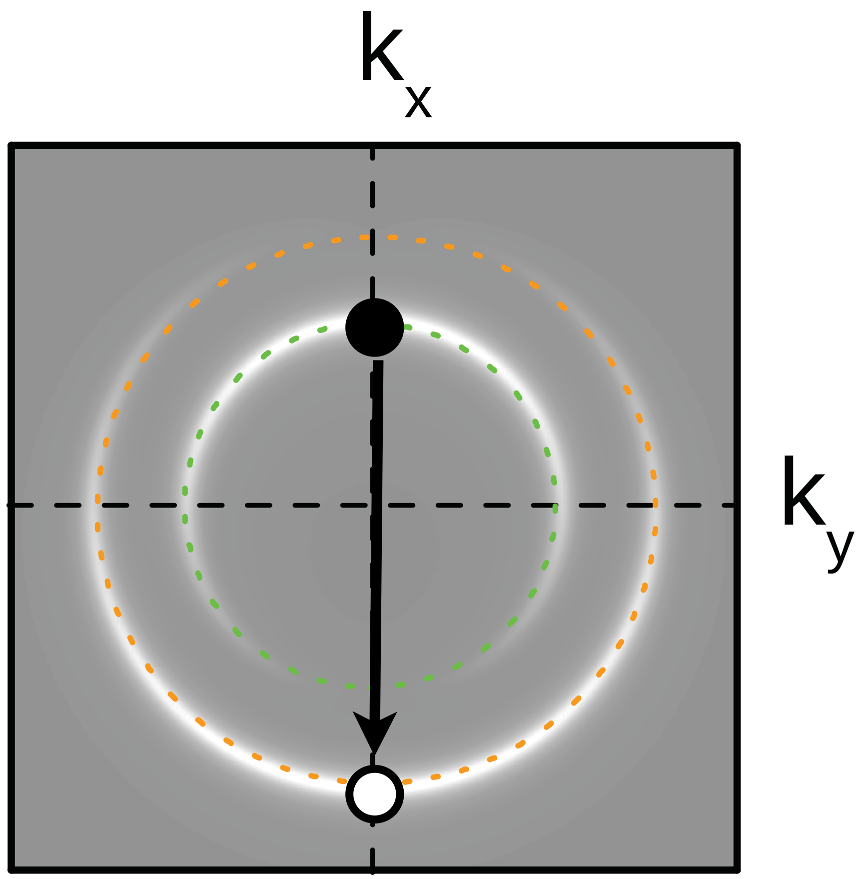
I. A. Nechaev et al. PRB **80**, 113402 (2009)

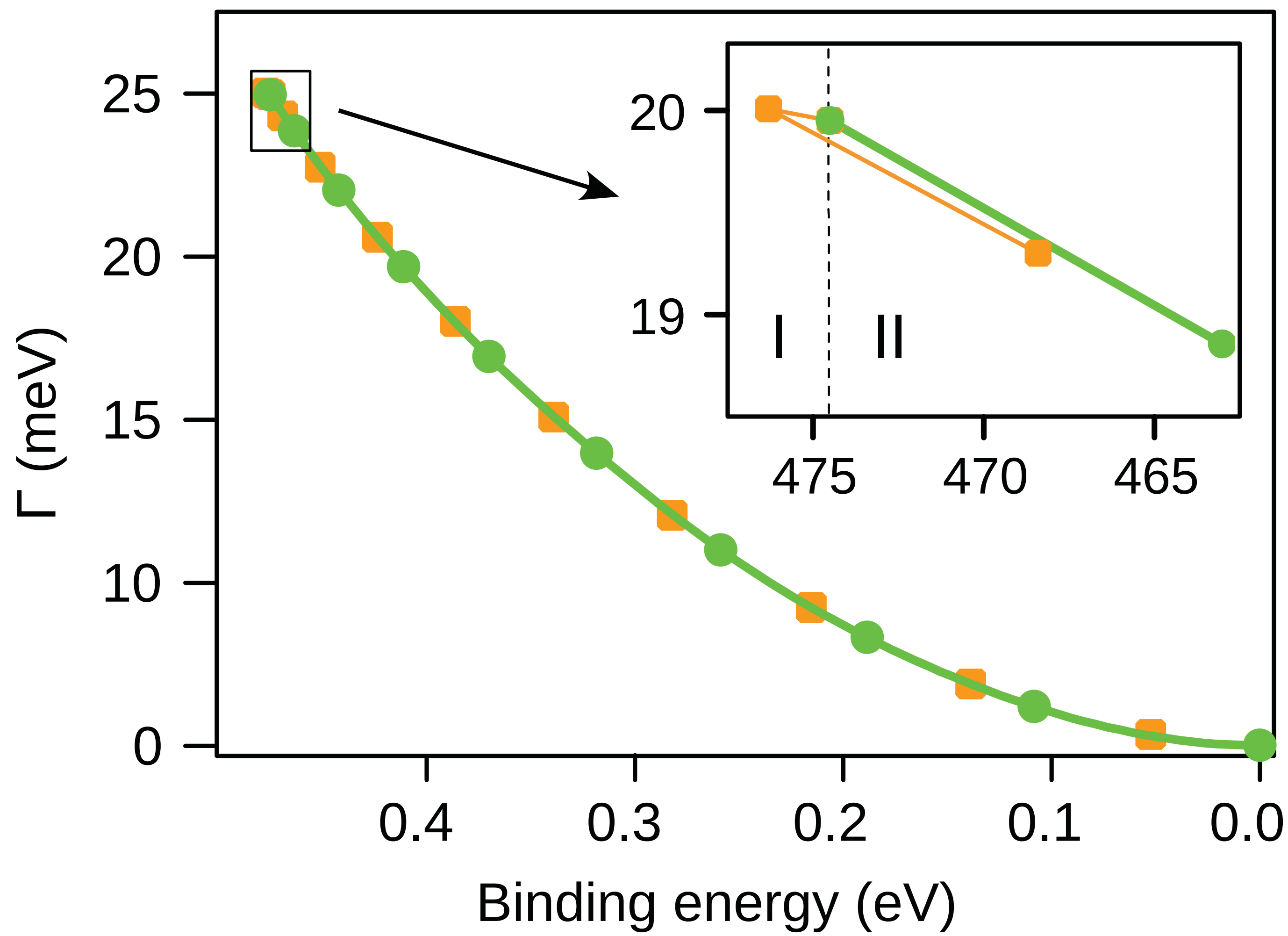
theory: GW approximation

GW theory confirms unequal contributions from branches

Negligible differences between branch lifetimes







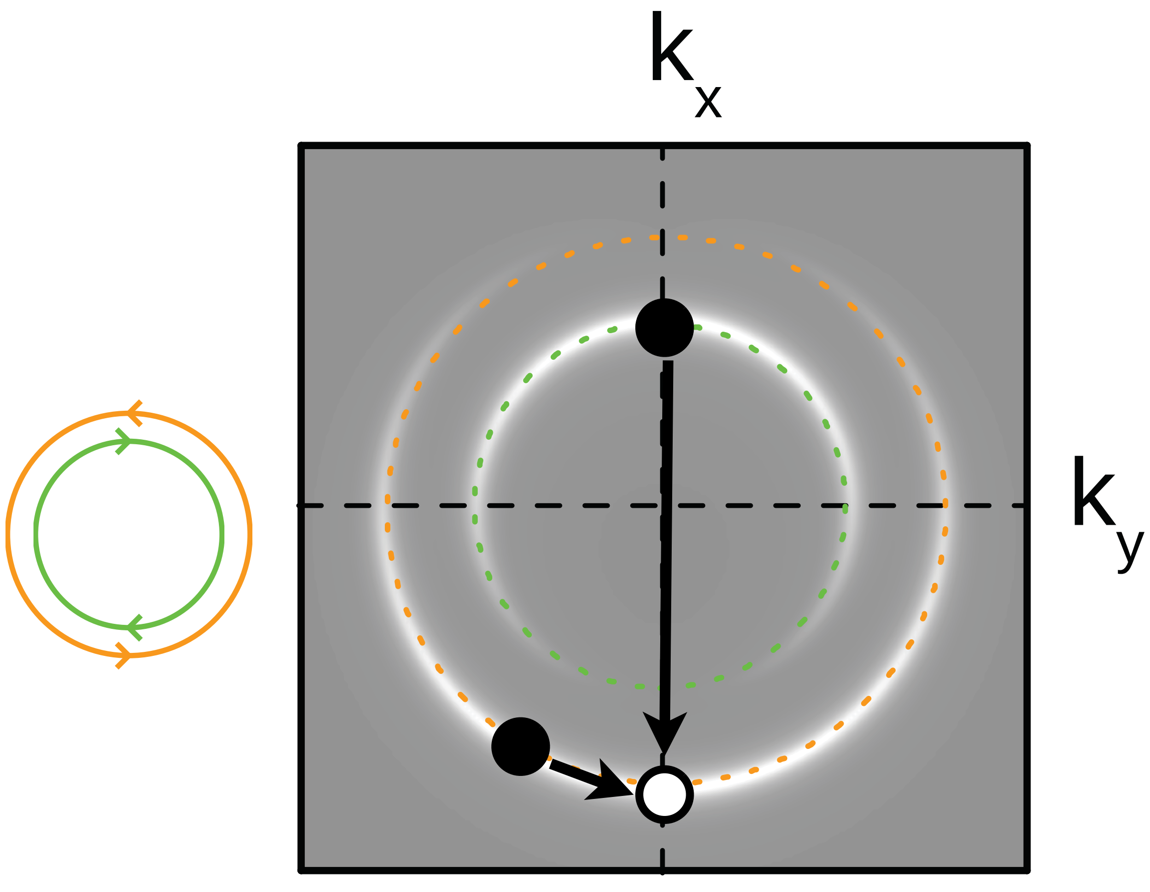
$$\Gamma_{\omega,\mathbf{k}} = -2\sum_{n's'}\int dz dz' M_{nn'}(z,z') \times \int \frac{d\mathbf{q}}{(2\pi)^2} F^{ss'}_{\mathbf{k},\mathbf{q}} f^{s'}_{\mathbf{q}n'} \theta(E^{s'}_{\mathbf{q}n'}-\omega)\times \quad \mathrm{Im}W(z,z';\mathbf{k}-\mathbf{q},\omega-E^{s'}_{\mathbf{q}n'})$$

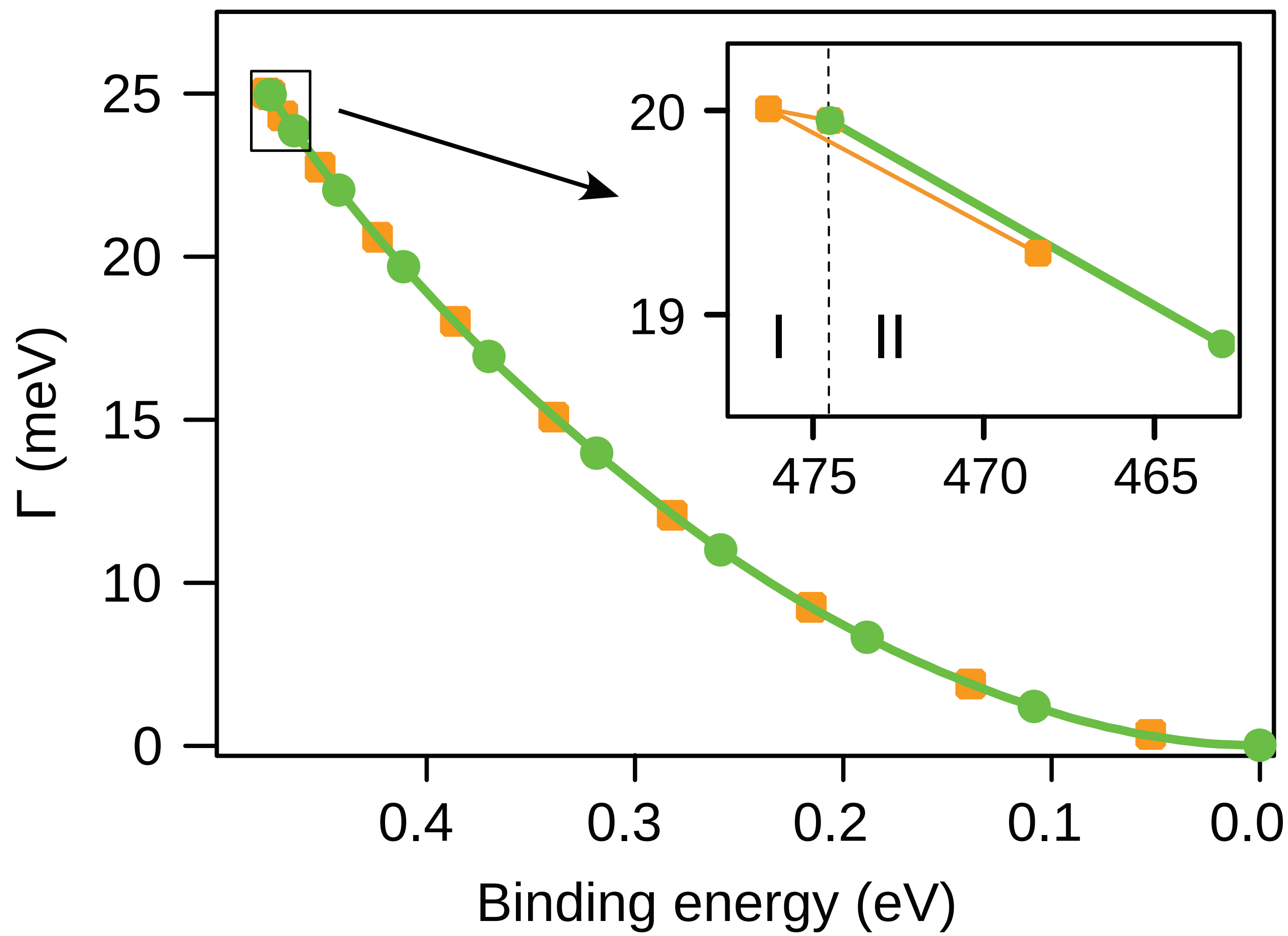
I. A. Nechaev et al. PRB **80**, 113402 (2009)

theory: GW approximation

GW theory confirms unequal contributions from branches

Negligible differences between branch lifetimes





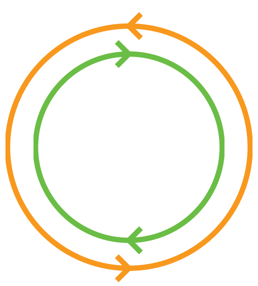
$$\Gamma_{\omega,\mathbf{k}} = -2\sum_{n's'}\int dz dz' M_{nn'}(z,z') \times \int \frac{d\mathbf{q}}{(2\pi)^2} F^{ss'}_{\mathbf{k},\mathbf{q}} f^{s'}_{\mathbf{q}n'} \theta(E^{s'}_{\mathbf{q}n'}-\omega)\times \quad \mathrm{Im}W(z,z';\mathbf{k}-\mathbf{q},\omega-E^{s'}_{\mathbf{q}n'})$$

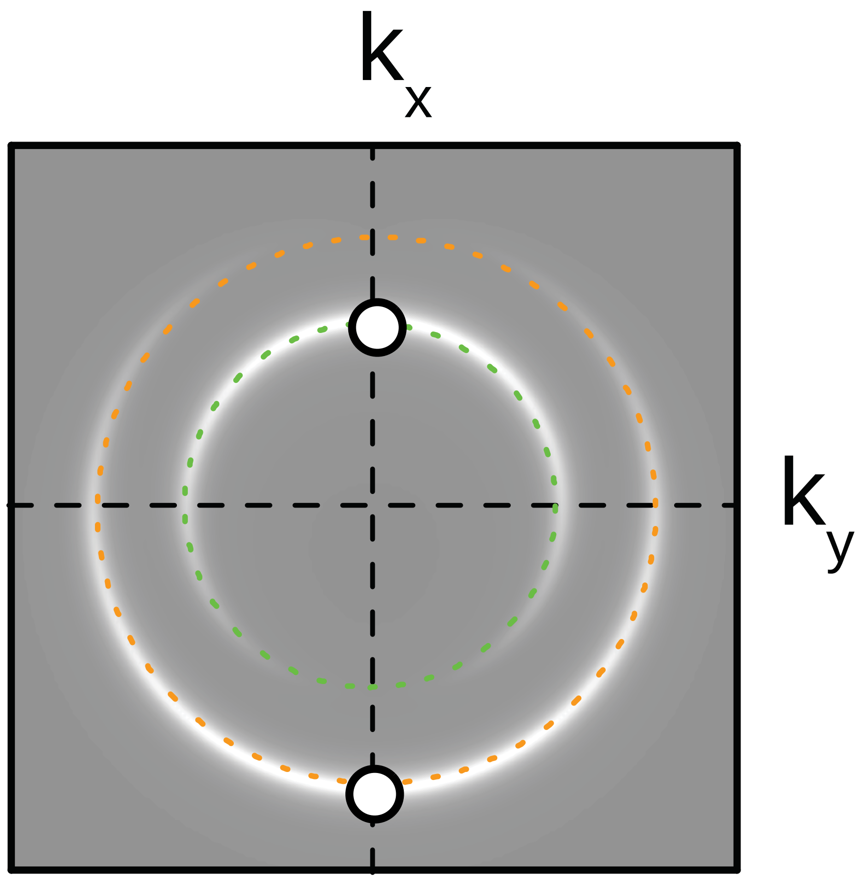
I. A. Nechaev et al. PRB **80**, 113402 (2009)

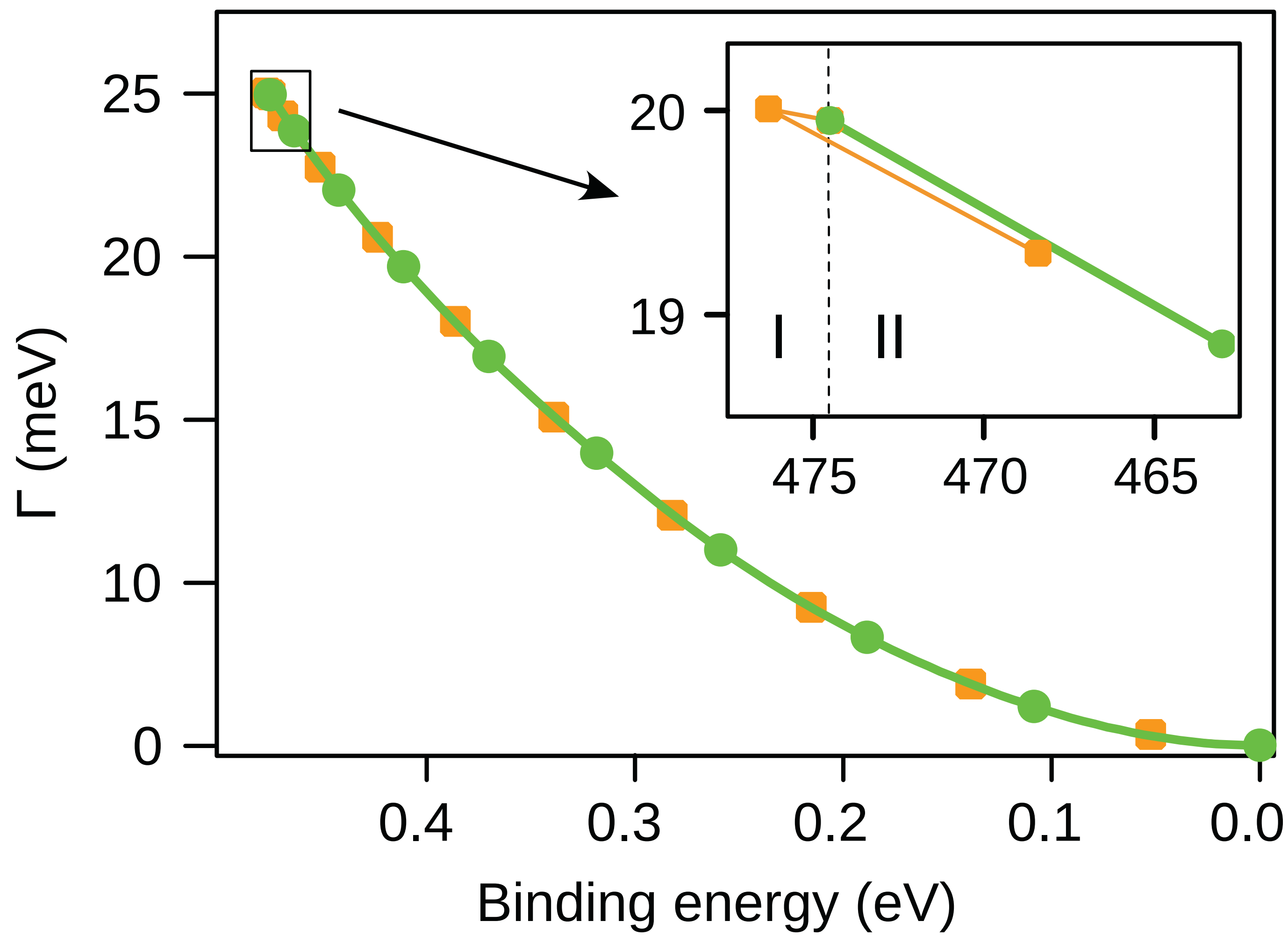
theory: GW approximation

GW theory confirms unequal contributions from branches

Negligible differences between branch lifetimes





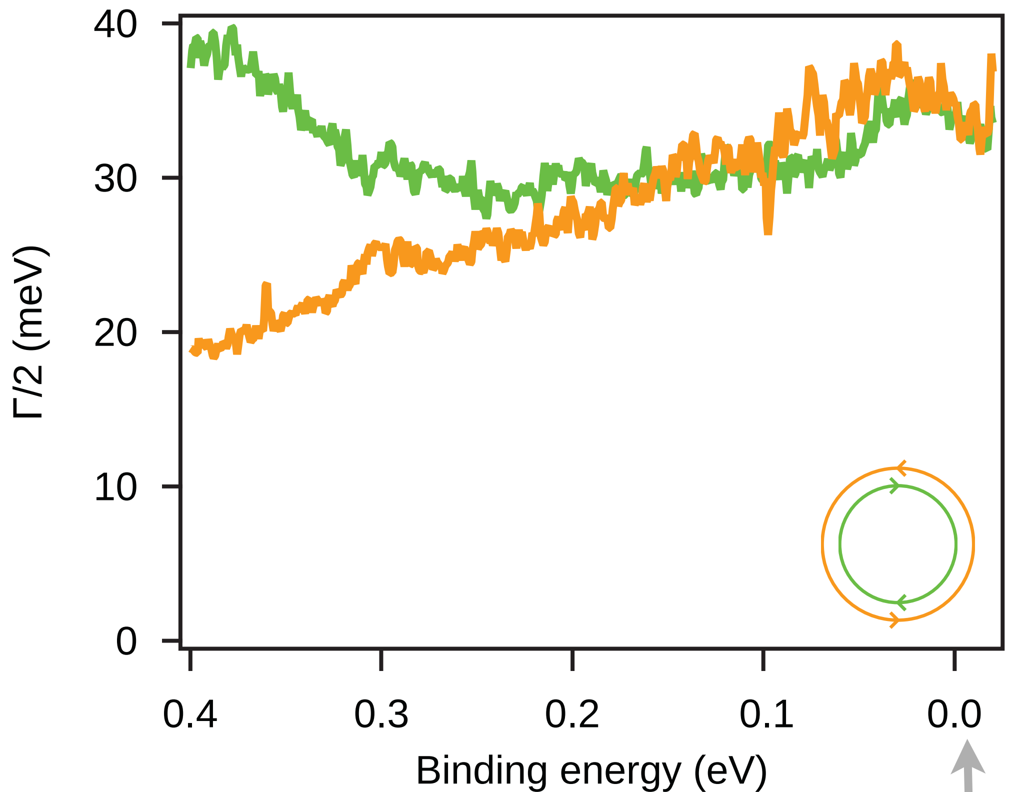


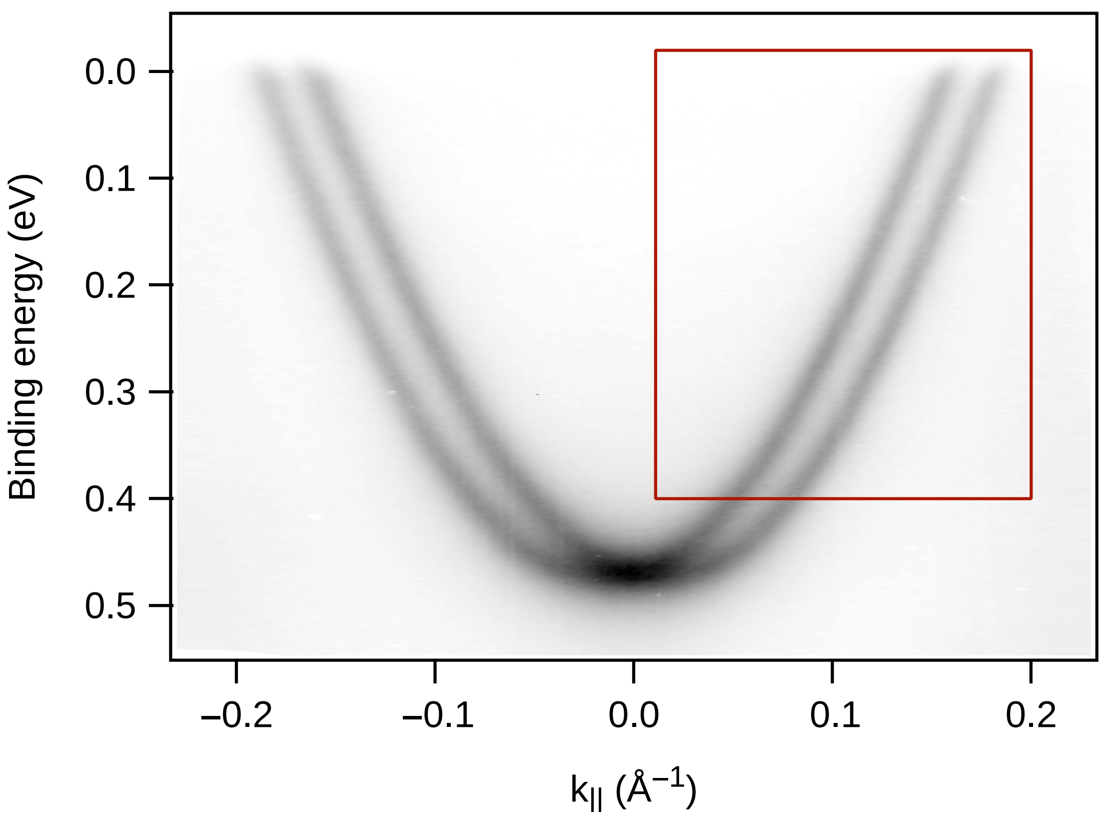
$$\Gamma_{\omega,\mathbf{k}} = -2\sum_{n's'}\int dz dz' M_{nn'}(z,z') \times \int \frac{d\mathbf{q}}{(2\pi)^2} F^{ss'}_{\mathbf{k},\mathbf{q}} f^{s'}_{\mathbf{q}n'} \theta(E^{s'}_{\mathbf{q}n'} - \omega)\times \quad \mathrm{Im}W(z,z';\mathbf{k}-\mathbf{q},\omega - E^{s'}_{\mathbf{q}n'})$$

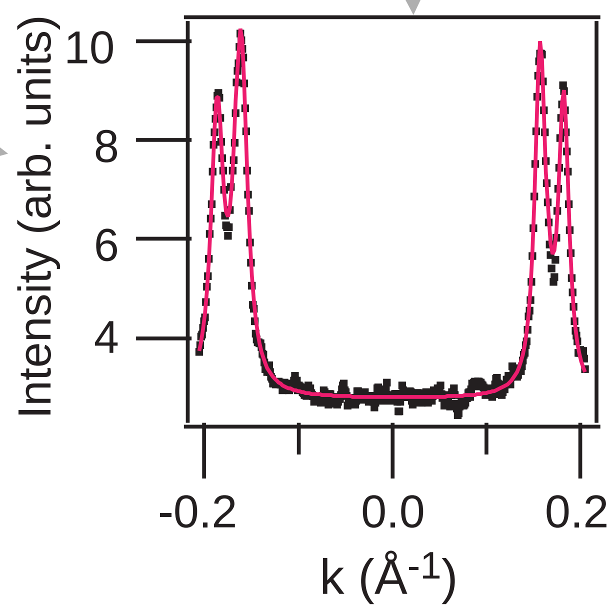
I. A. Nechaev et al. PRB **80**, 113402 (2009)

experiment

MDC fitting suggests decrease of inner-state lifetime with increasing BE





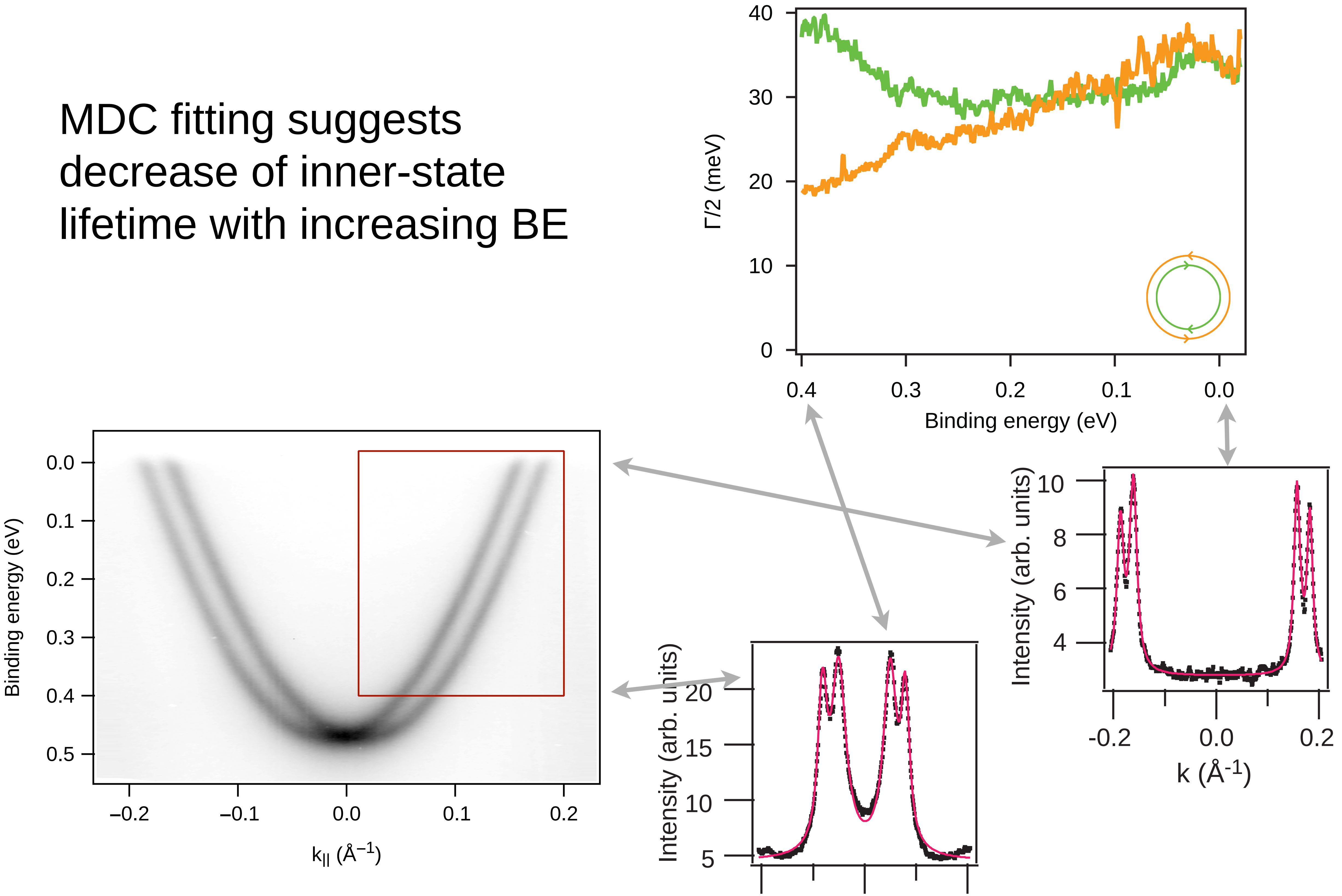


SGM-3 @ ASTRD

ΔE < 10 meV, Δk < 0.004 $Å^{-1}$

experiment

MDC fitting suggests decrease of inner-state lifetime with increasing BE



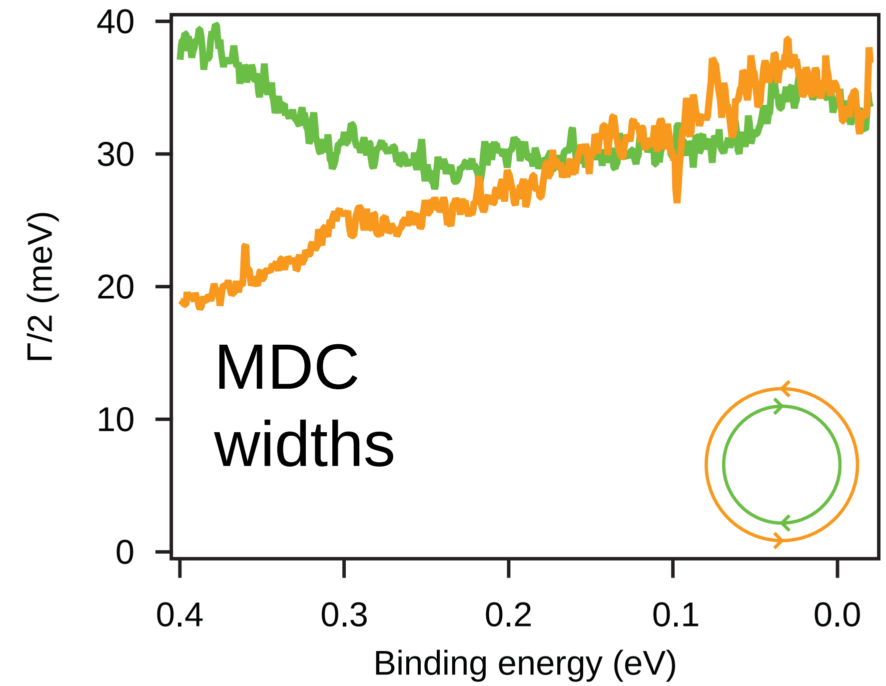
SGM-3 @ ASTRD

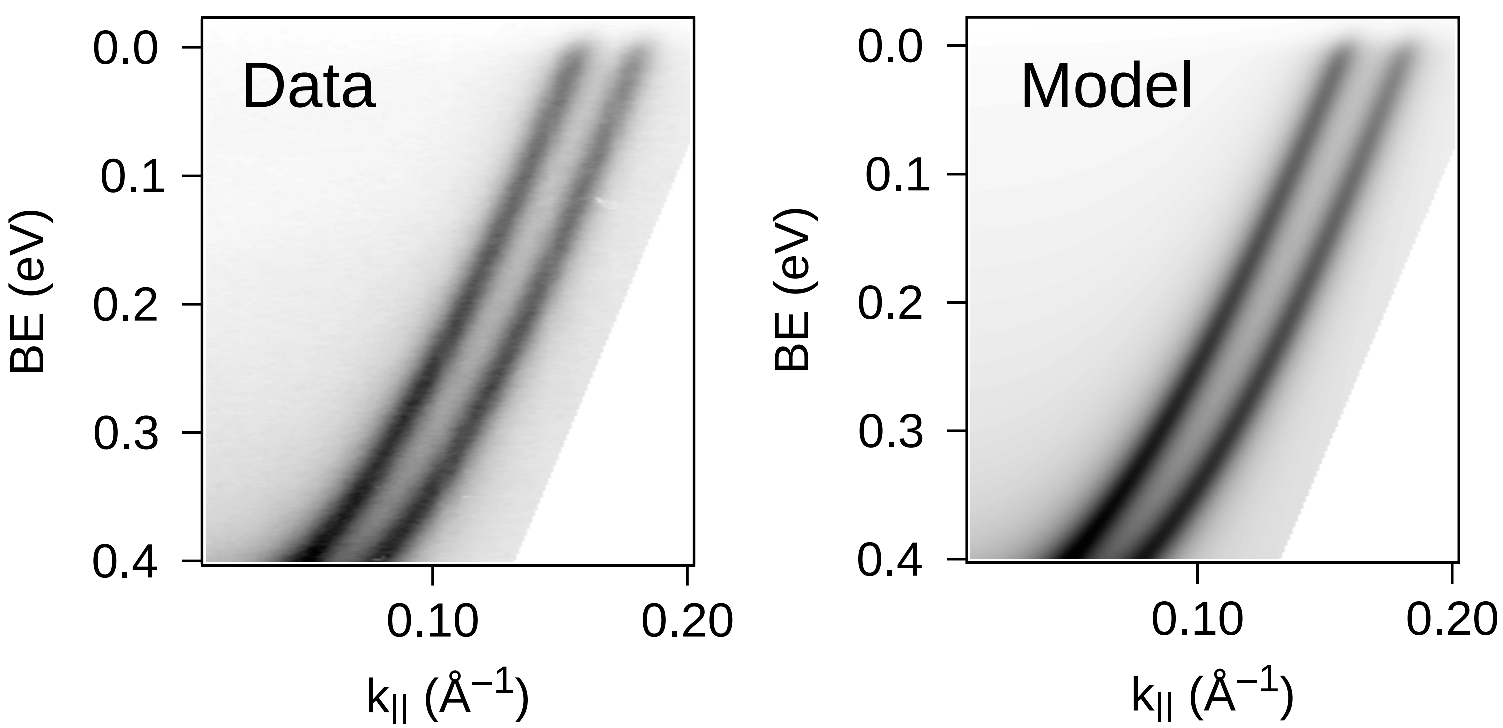
ΔE < 10 meV, Δk < 0.004 Å^{-1}

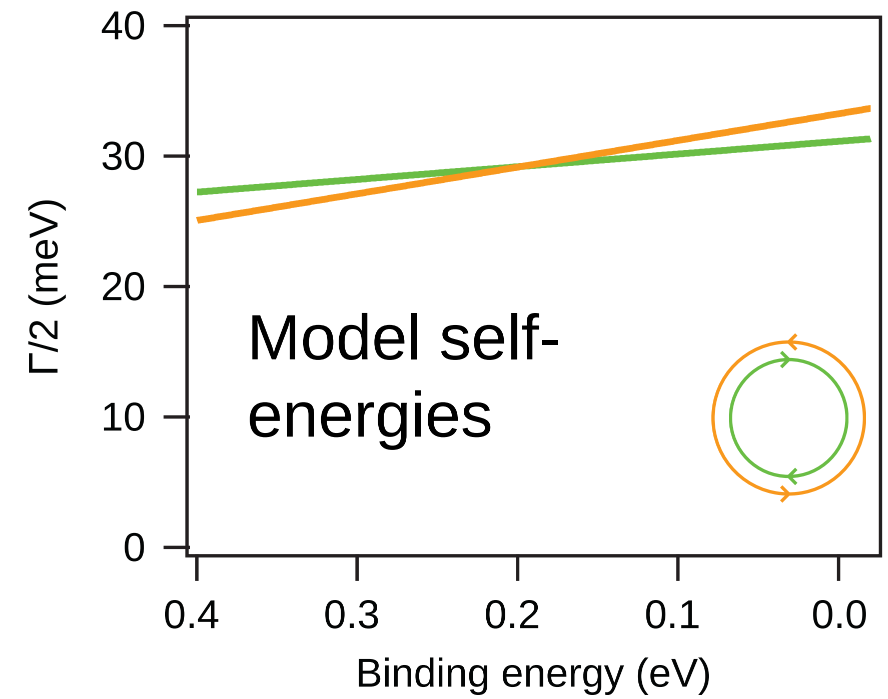
experiment

Solution: 2-D fits

- Calculate spectral function from simple self-energy
- Account for broadening

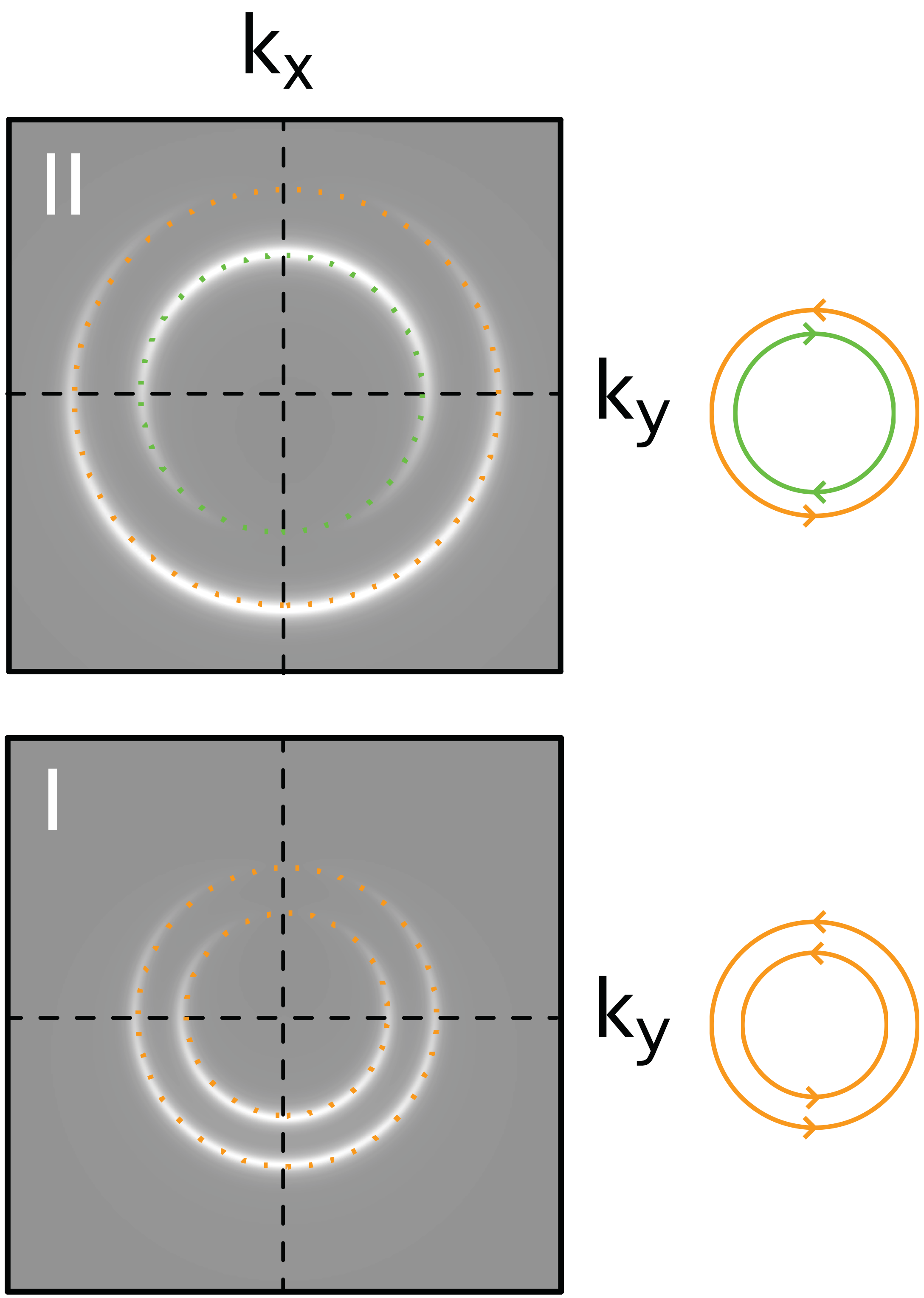


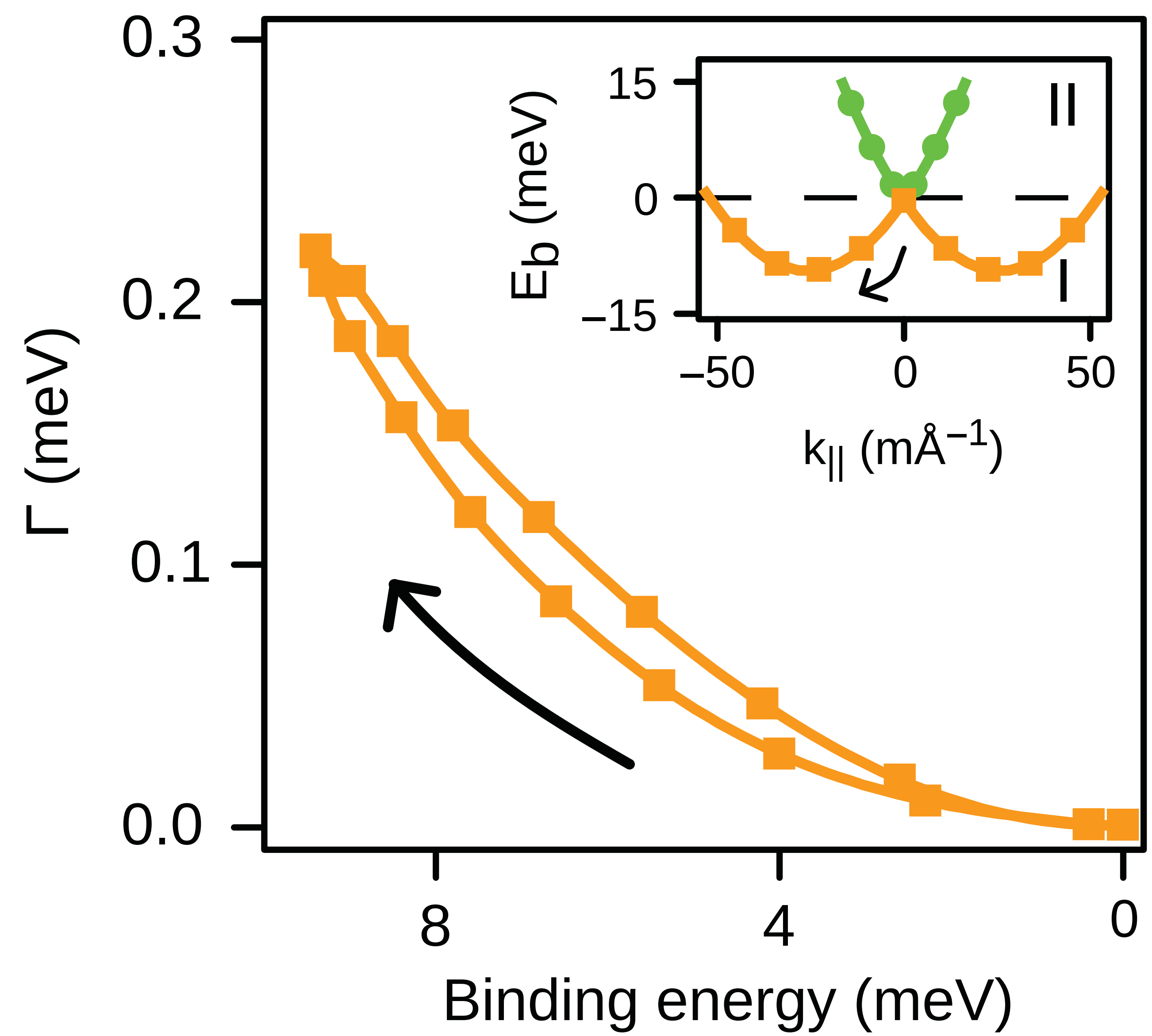




I. A. Nechaev et al. PRB **80**, 113402 (2009)

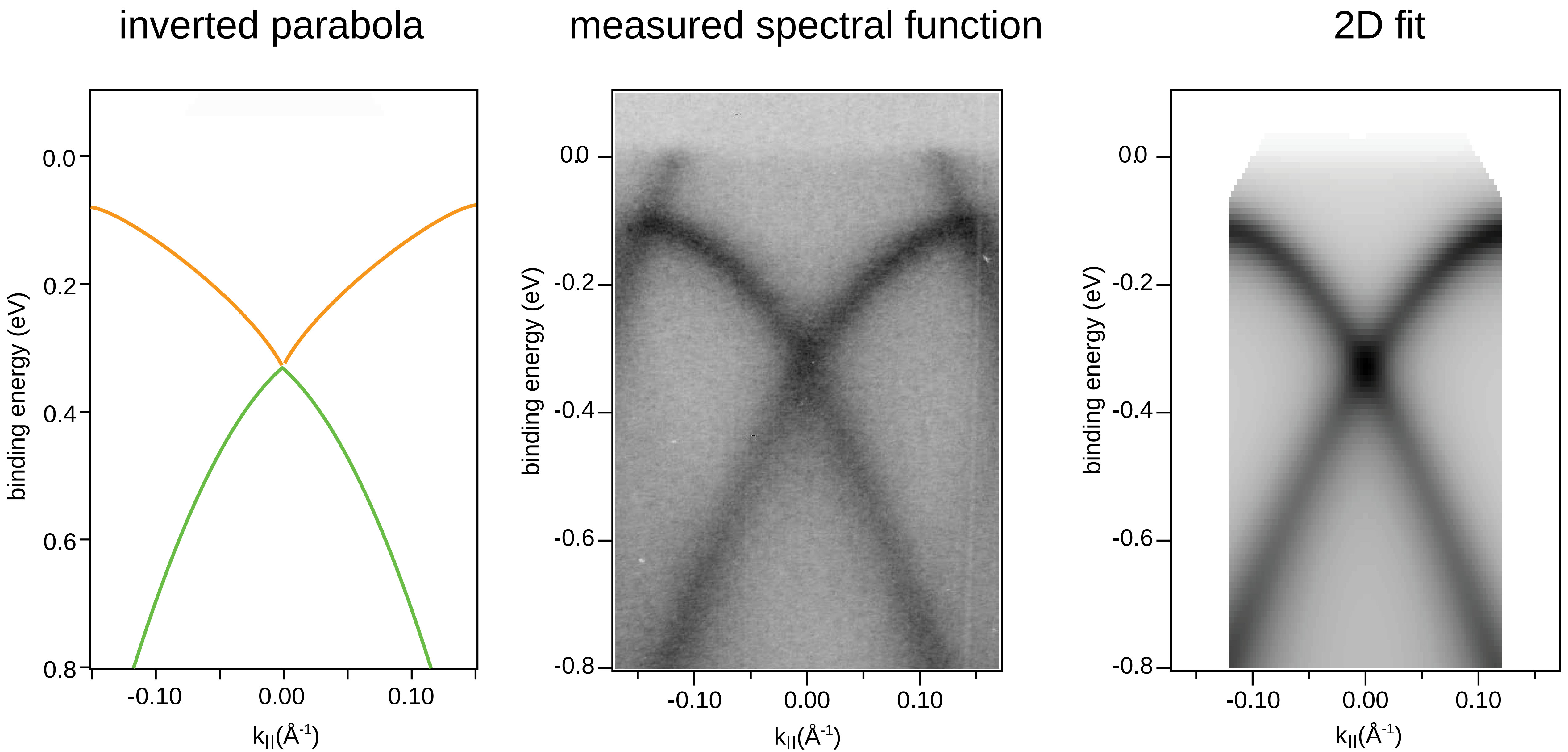
the situation in region I





I. A. Nechaev et al. PRB **80**, 113402 (2009)

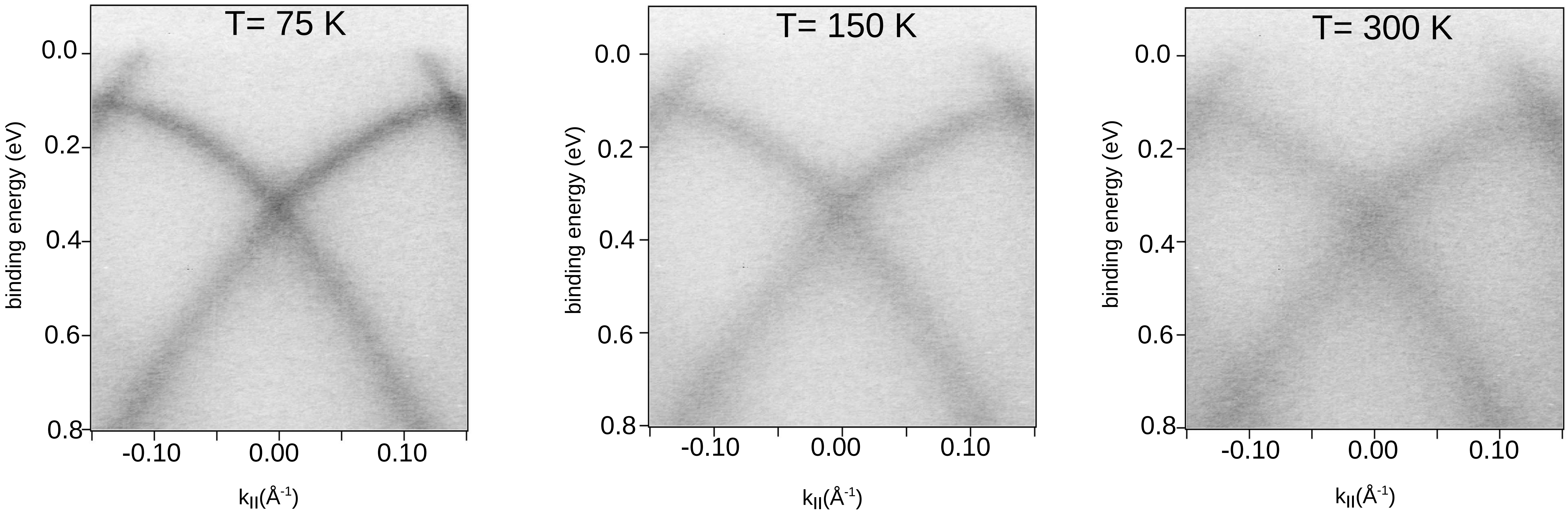
Bi/Ag(111) surface alloy: a better example?



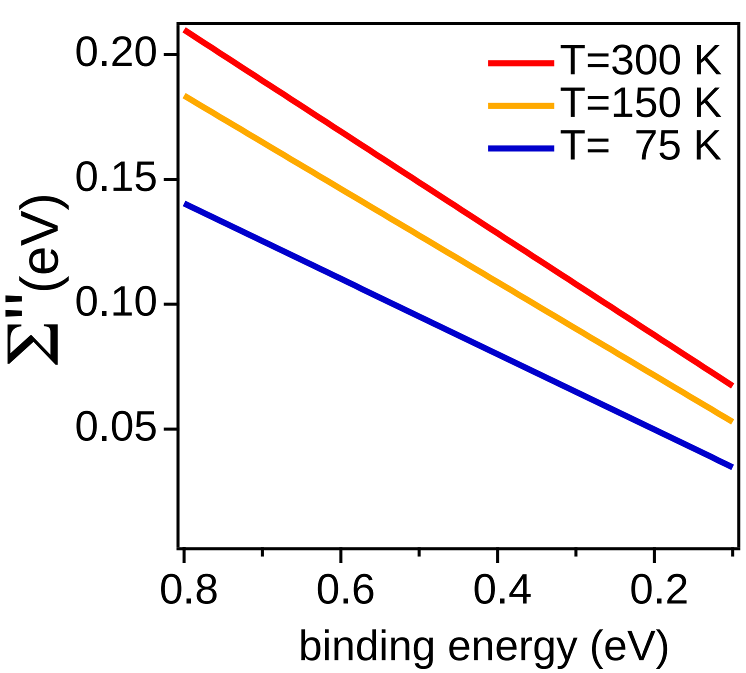
C. R. Ast, J. Henk et al. Phys. Rev. Lett. 98, 186807 (2007)
F. Meier et al. Phys. Rev. B 77, 165431 (2008)
G. Bihlmayer et al., Phys. Rev. B 75, 195414 (2007)

enhanced electron-phonon coupling:
E. Cappelluti et al. Physical Review B **76**, 085334 (2007)

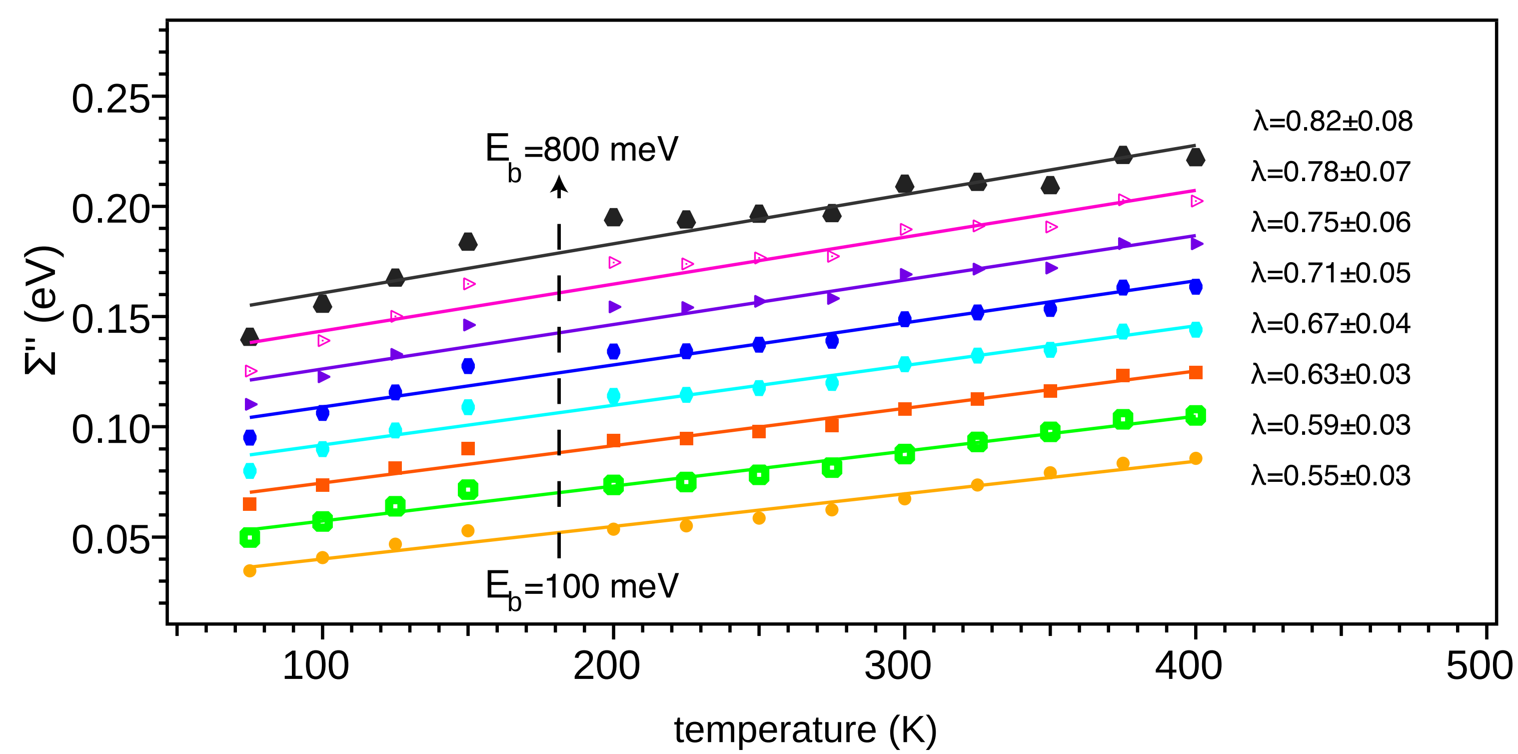
Bi/Ag(111) temperature dependence



resulting self-energy

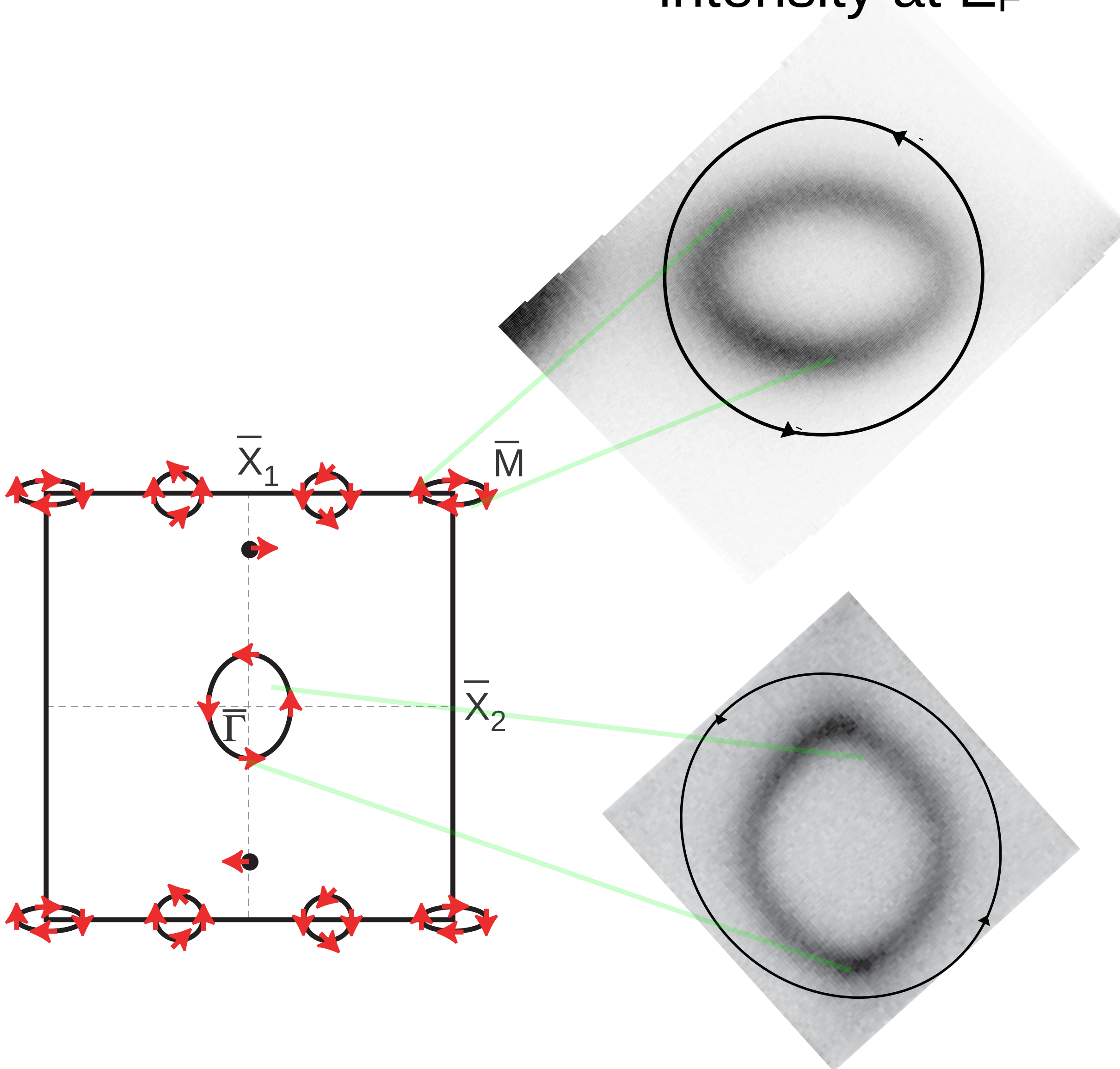


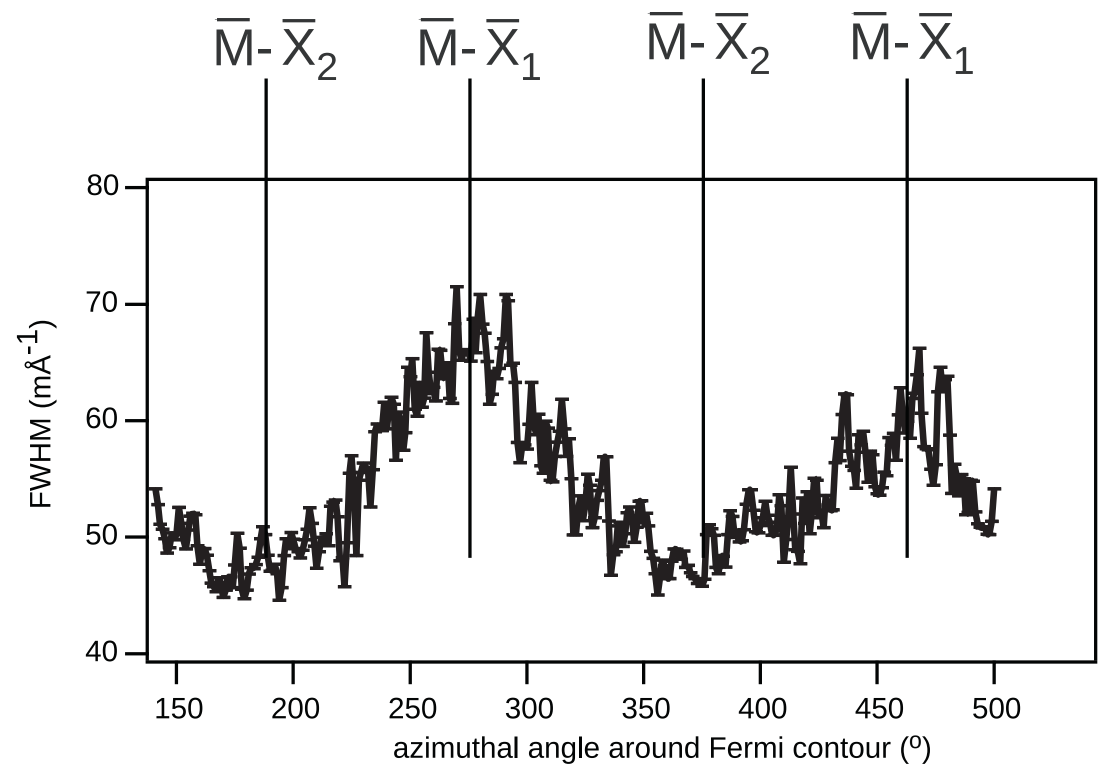
temperature dependence

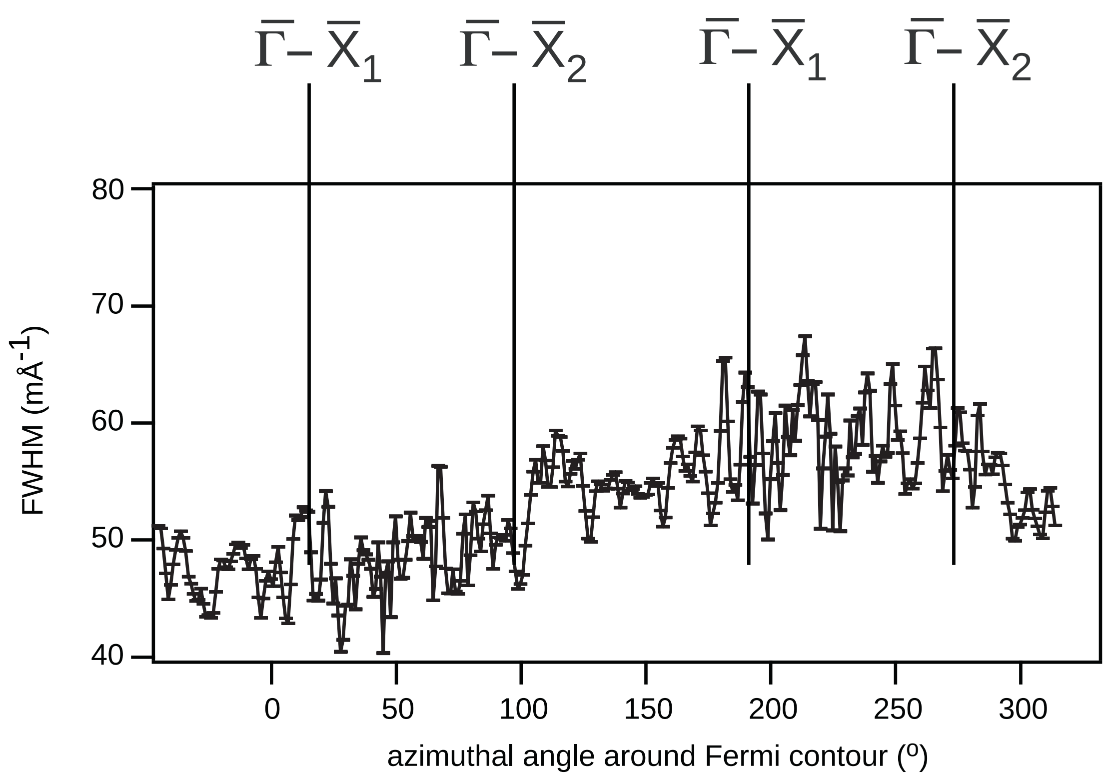


strong lifetime variations on Bi(110)

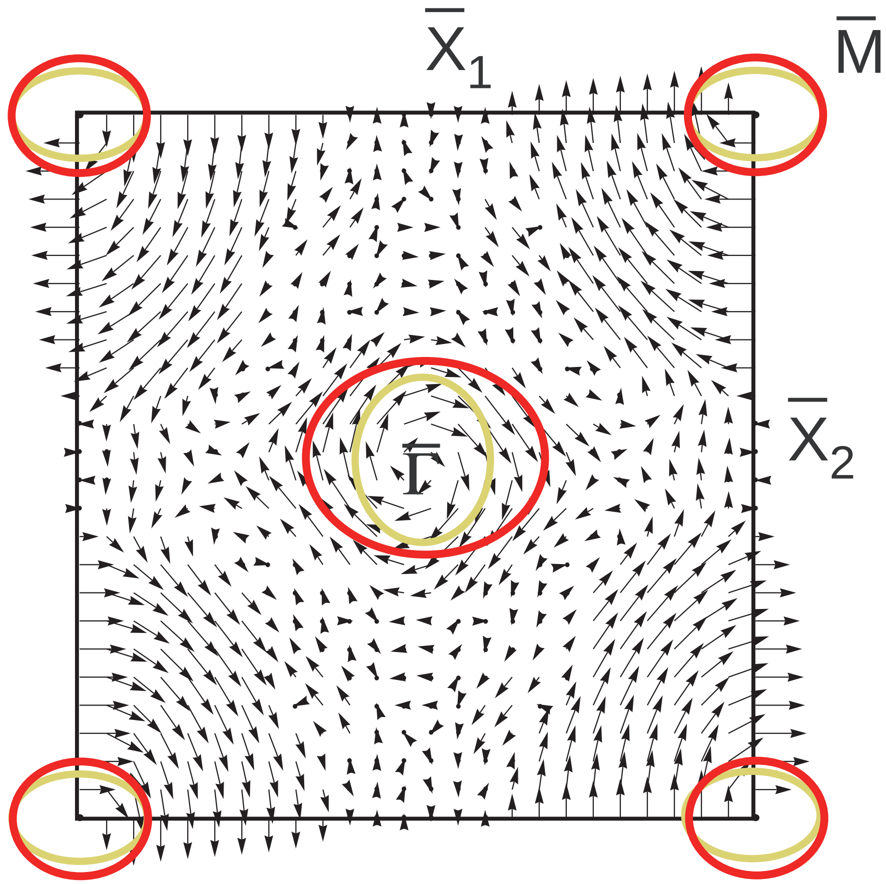
photoemission intensity at E_F

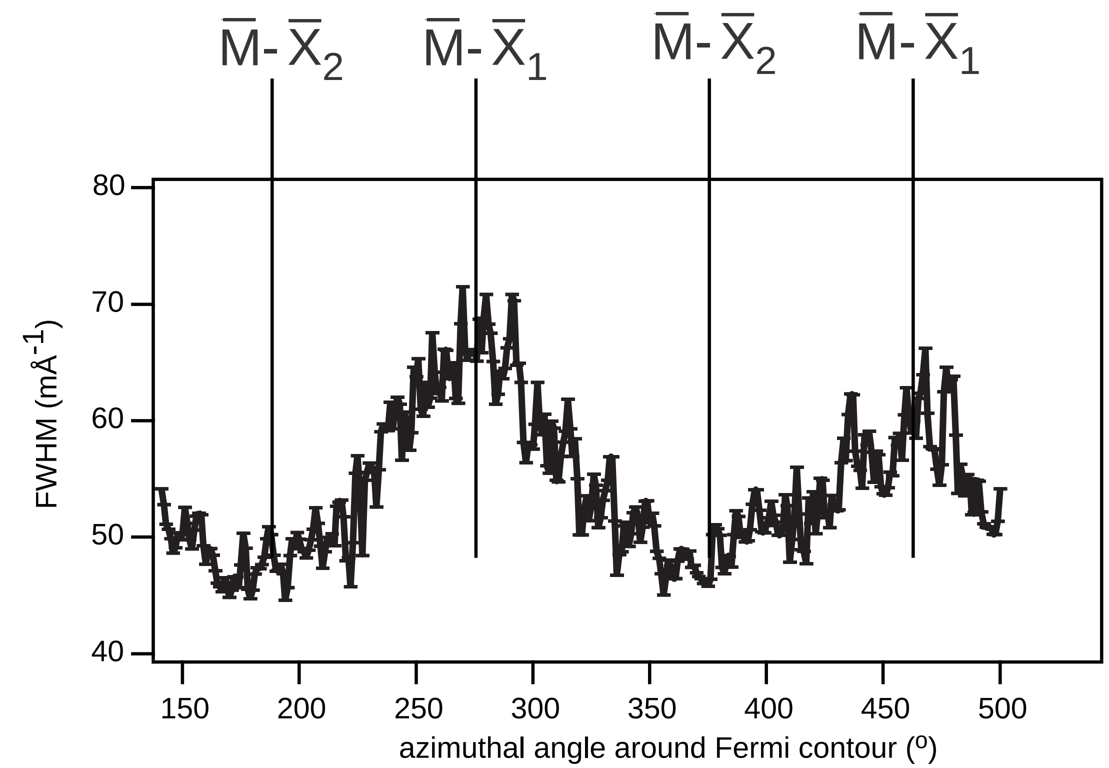




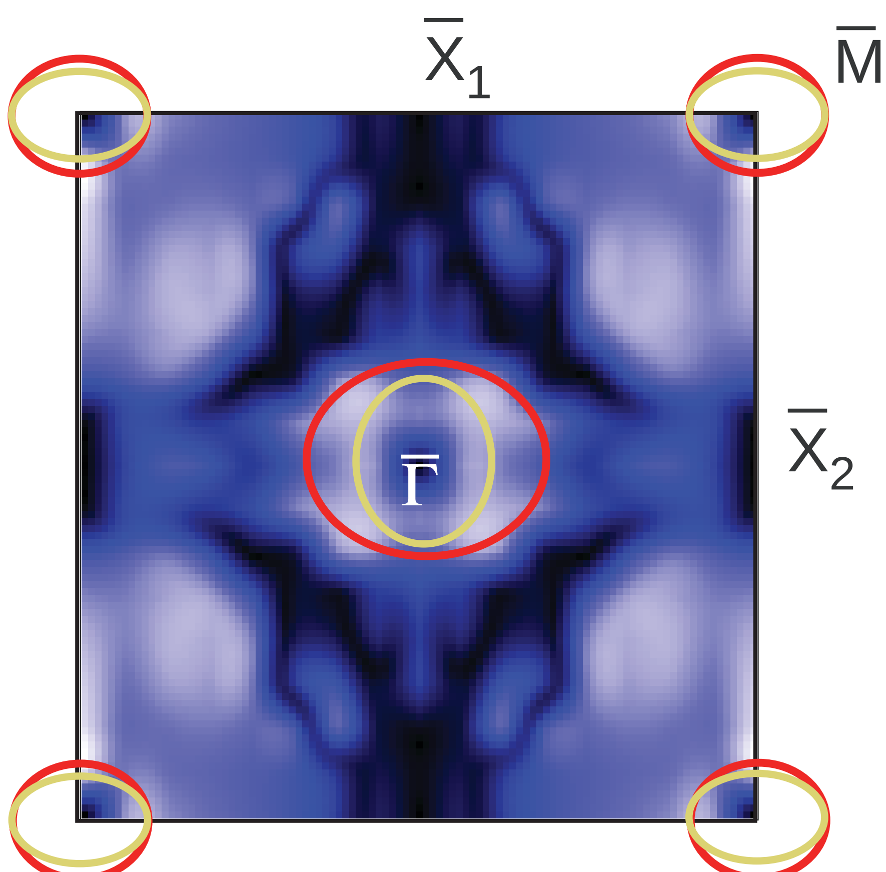


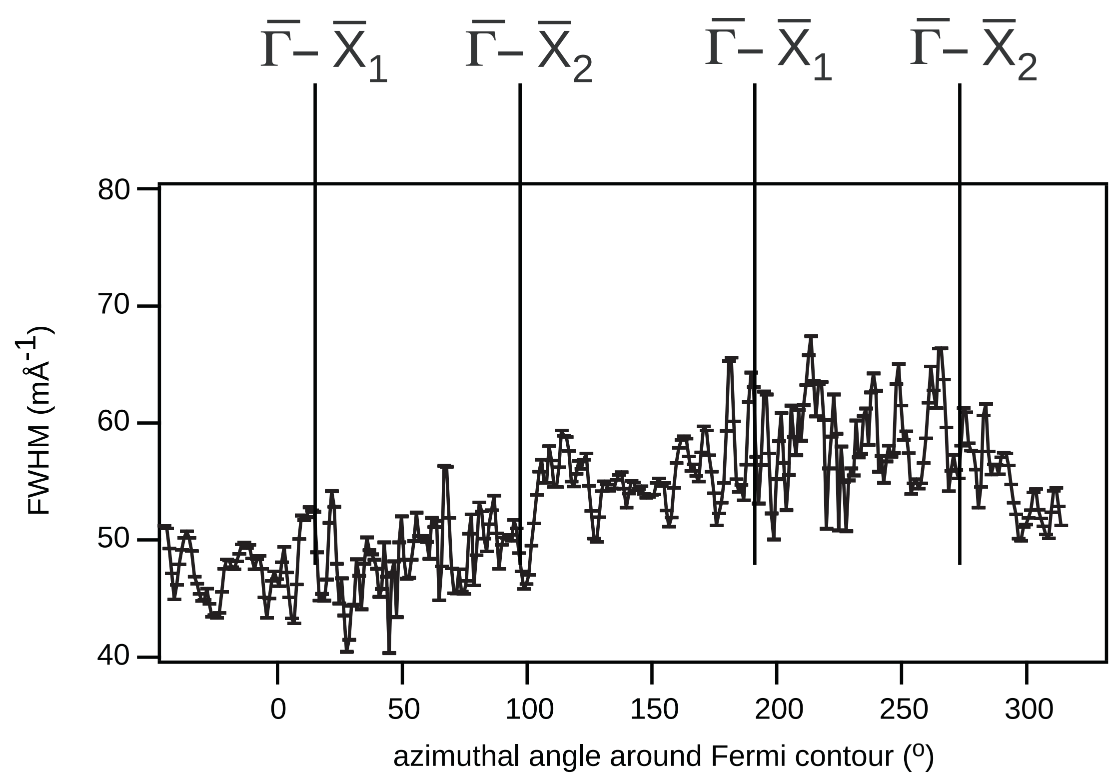
calculated spin polarization
with exp and theo Fermi contour





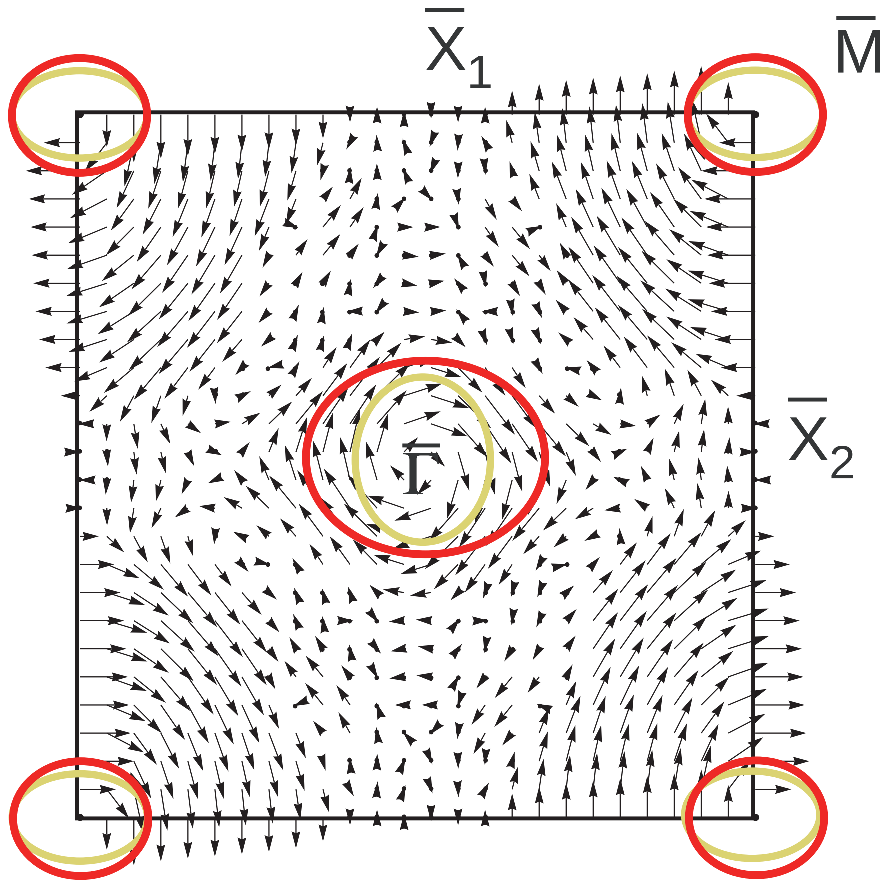
calculated spin polarization (modulus)



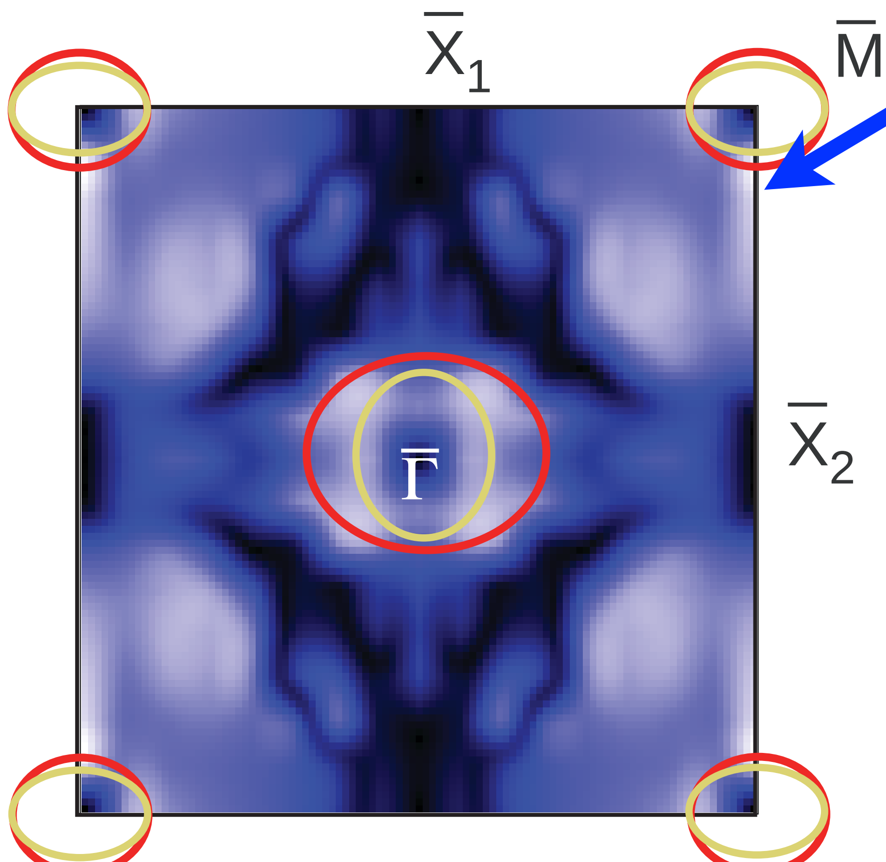


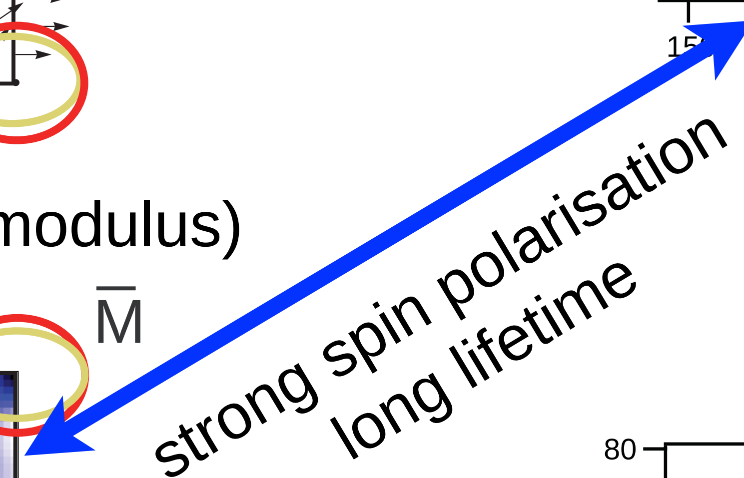
calculation: A. Eiguren

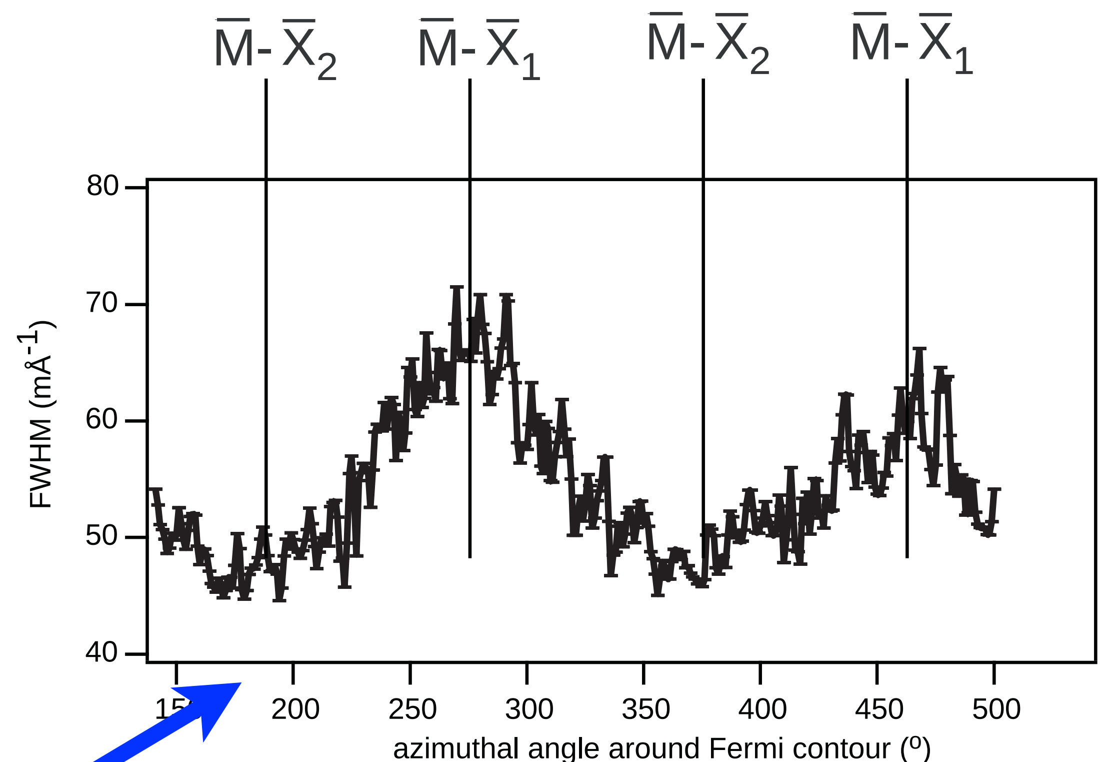
calculated spin polarization
with exp and theo Fermi contour

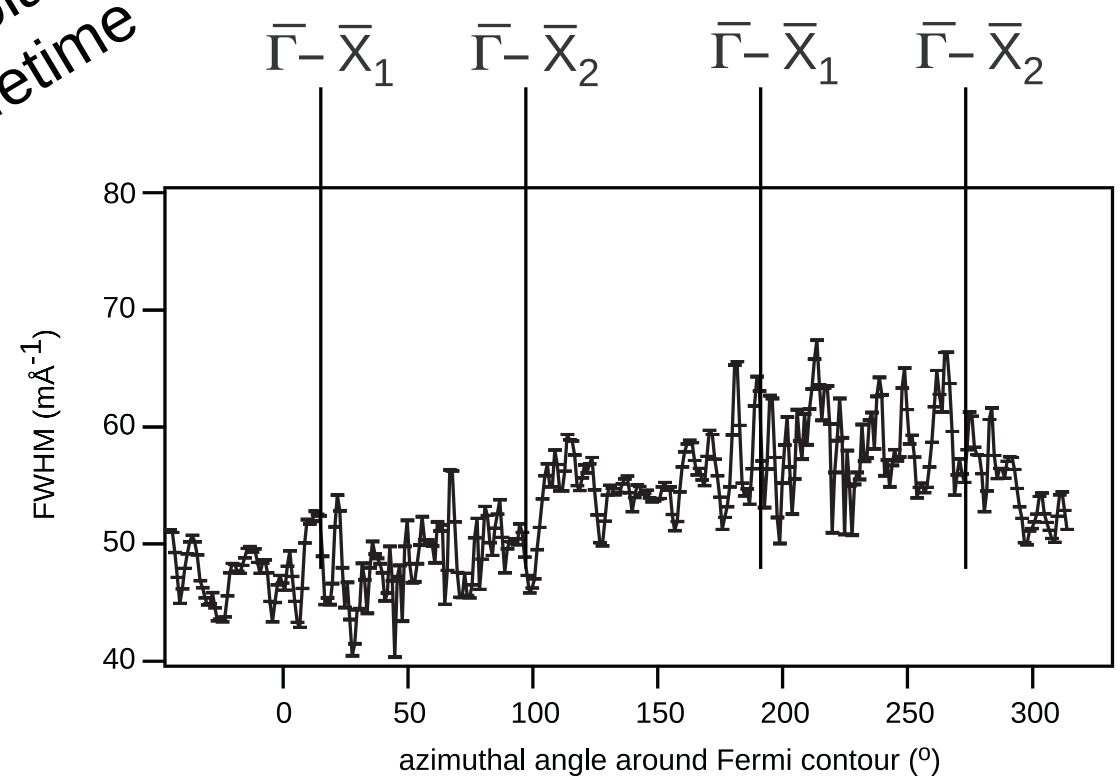


calculated spin polarization (modulus)









calculation: A. Eiguren

some conclusions

- Very strong impact on quasiparticle interference.
- Lifetimes in Rashba systems independent of branch of dispersion on Au(111).
- No increase of electron-phonon coupling near the van Hove singularity of Bi/Ag(111).
- Strong lifetime effects on the Fermi surface elements of Bi(110). Qualitative agreement with calculated spin polarisation degree. Strong spin polarisation corresponds to long lifetime of the state.

Collaborators and funding

Institute for Storage Ring Facilities
University of Aarhus

Marco Bianchi
Dandan Guan
Emile Rienks
Maria Fuglsang Jensen

Zhejiang University, Hangzhou
Shining Bao

Inst. of Strength Physics
and Mat. Science
Russian Academy of Sciences,
Tomsk
Yu. M. Koroteev

Fritz-Haber-Institut der MPG, Berlin
Gustavo Ceballos
Martin Hansmann
Hans-Peter Rust
Karsten Horn

DIPC Donostia/San Sebastian
Ilya Nechaev
(also Kostroma State University, Russia)
Slava Silkin
Eugene Chulkov
Pedro Echenique

Freie Universität, Berlin
Nacho Pascual
Isabel Fernandez-Torrente
Patricio Häberle
Manuel Ugeda

Forschungszentrum Jülich
Gustav Bihlmayer
Stefan Blügel

University of the Basque Country
Asier Eiguren

Universität Zürich / Swiss Light Source
Paul Scherrer Institut
Fabian Meier
Jürg Osterwalder

The Danish National Research Council
Lundbeck Foundation
The Carlsberg Foundation
Ikerbasque Foundation
The Spanish Ministry for Science and Technology

spin polarisation

operator

$$S^2 = S_x^2 + S_y^2 + S_z^2 = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

expectation value

$$\langle S^2 \rangle = \frac{3}{4}\hbar^2$$

spin polarisation (modulus)

$$\langle S_x \rangle^2 + \langle S_y \rangle^2 + \langle S_z \rangle^2$$

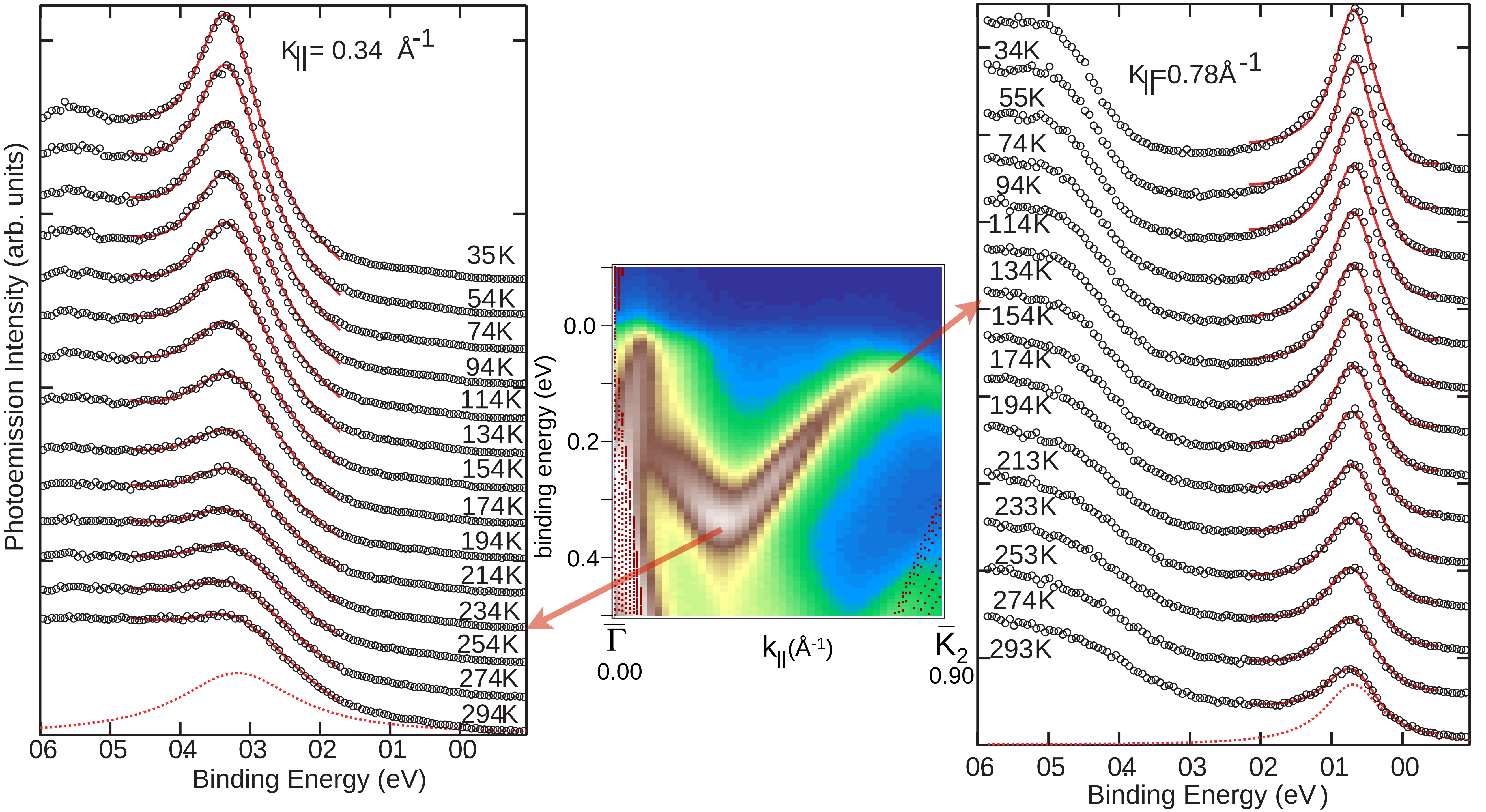
values

$$0 \ldots \frac{1}{4}\hbar^2$$

example for maximum polarisation: $\chi = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

here we use the Bloch spinor: $\chi = \begin{pmatrix} u_{\mathbf{k}}(\mathbf{r}) \\ v_{\mathbf{k}}(\mathbf{r}) \end{pmatrix} e^{i\mathbf{kr}}$

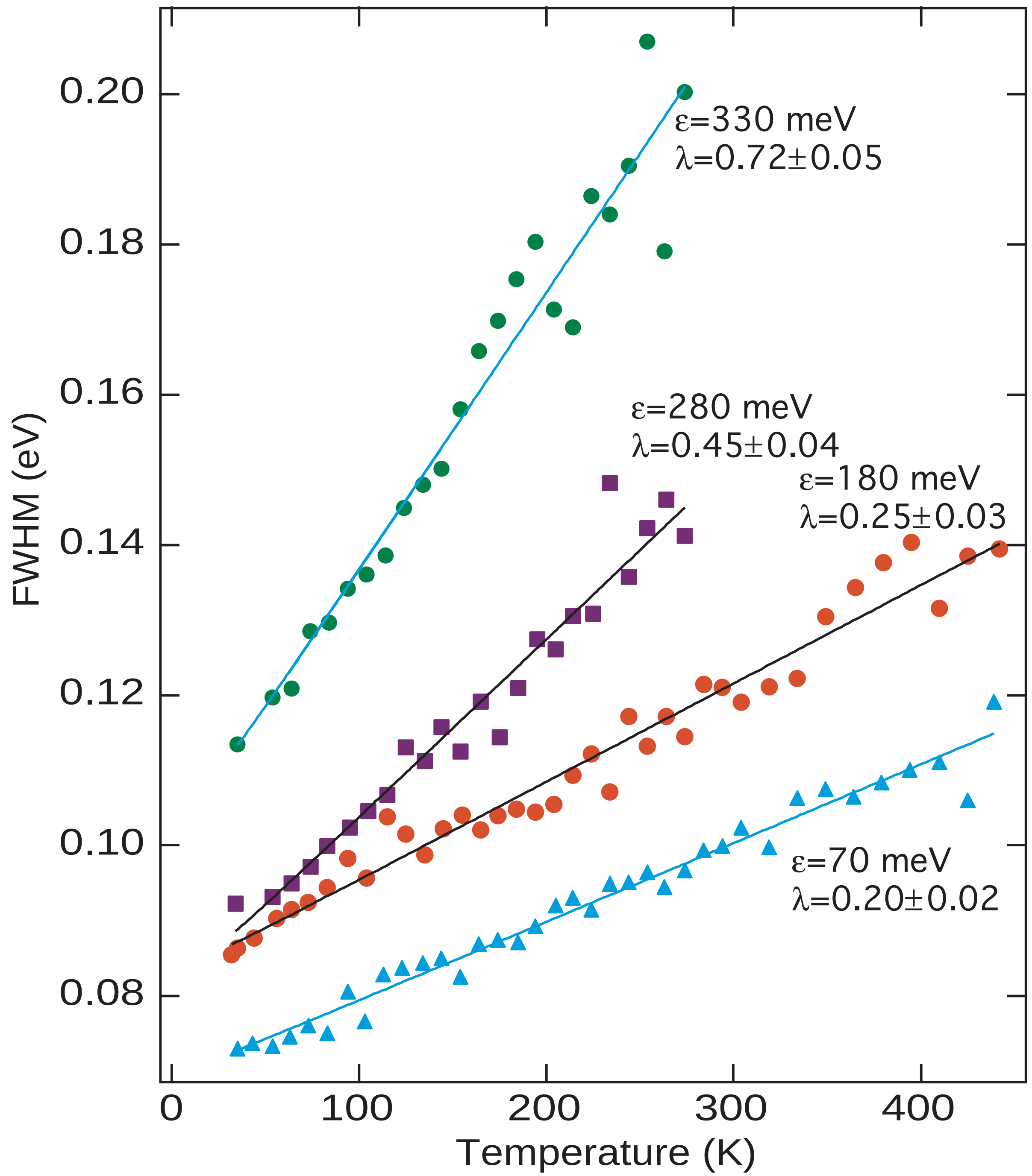
El-ph coupling on Bi(100)

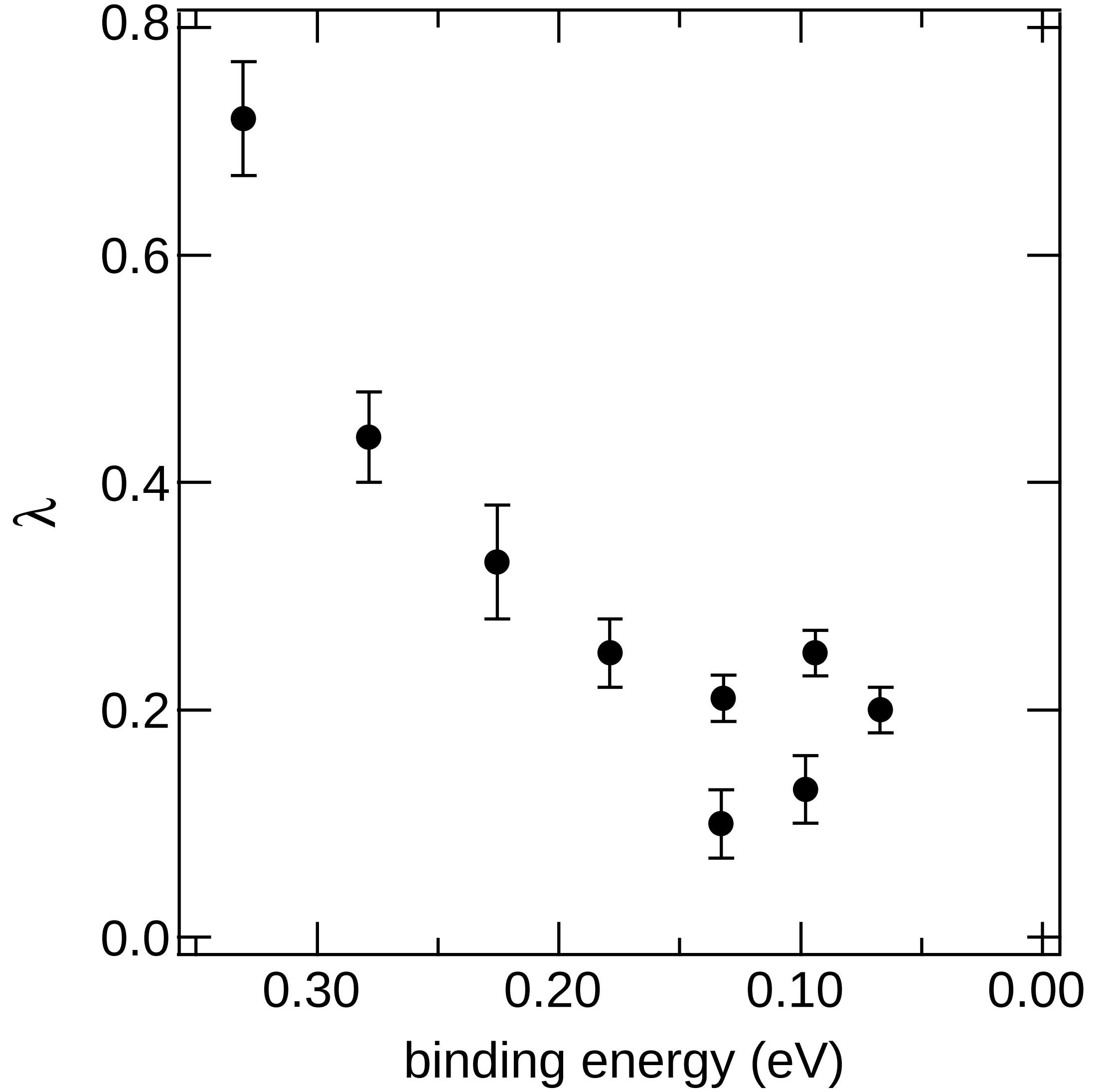


- markedly different T-dependence on different k-points

J. E. Gayone, S. V. Hoffmann, Z. Li and Ph. Hofmann, Physical Review Letters **91**, 127601 (2003).

El-ph coupling on Bi(100)

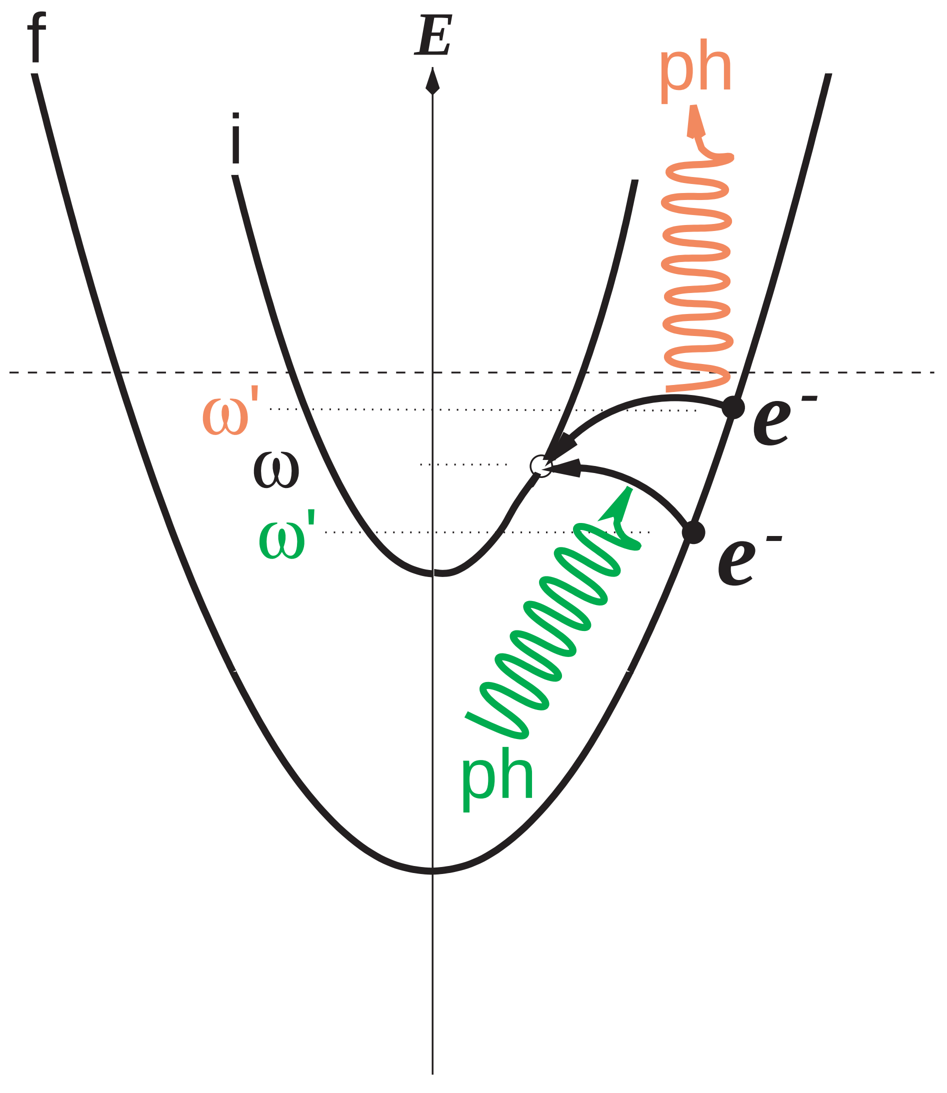


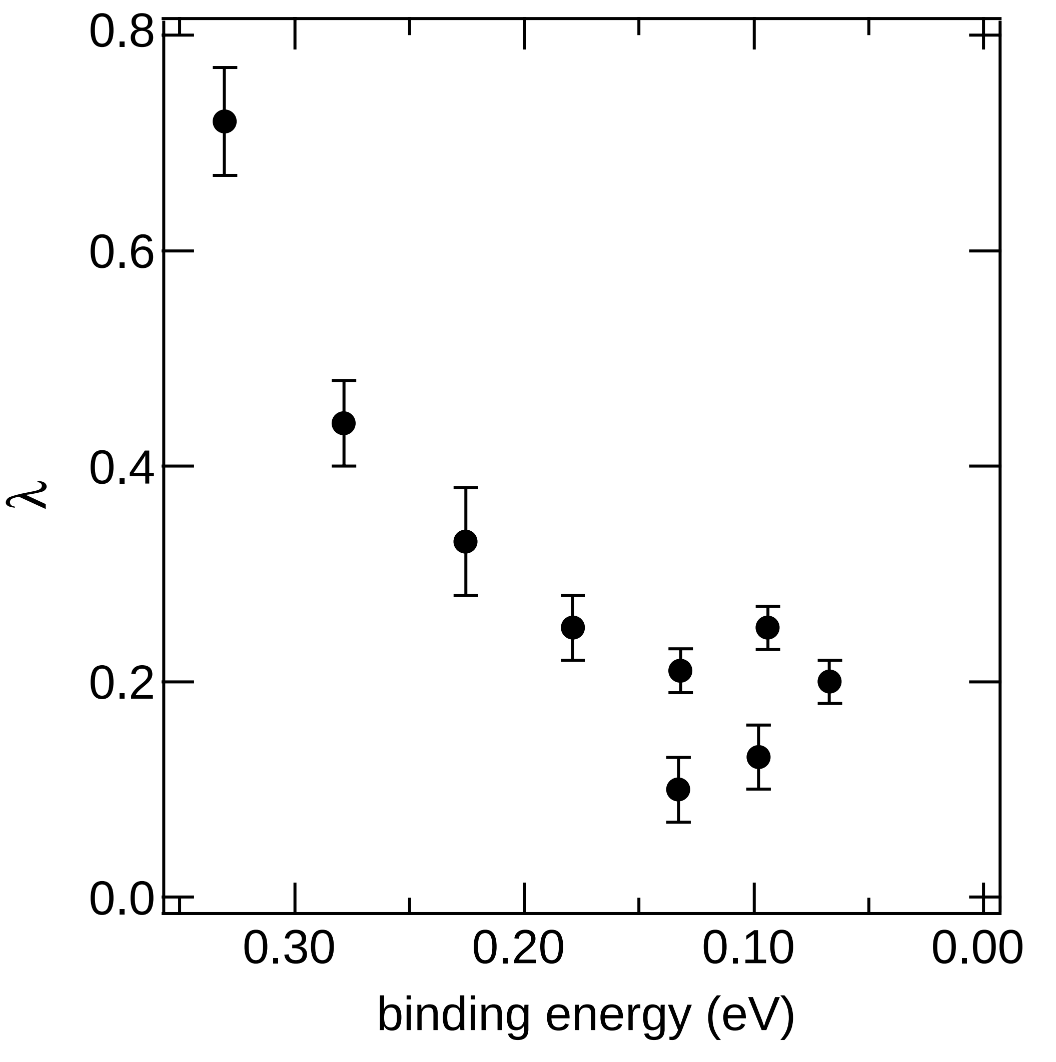


- The coupling parameter λ depends strongly on the binding energy.
- λ, measured in this way, cannot be interpreted as the mass-enhancement parameter at the Fermi level.

J. E. Gayone, S. V. Hoffmann, Z. Li and Ph. Hofmann, Physical Review Letters **91**, 127601 (2003).

Why is λ energy-dependent?

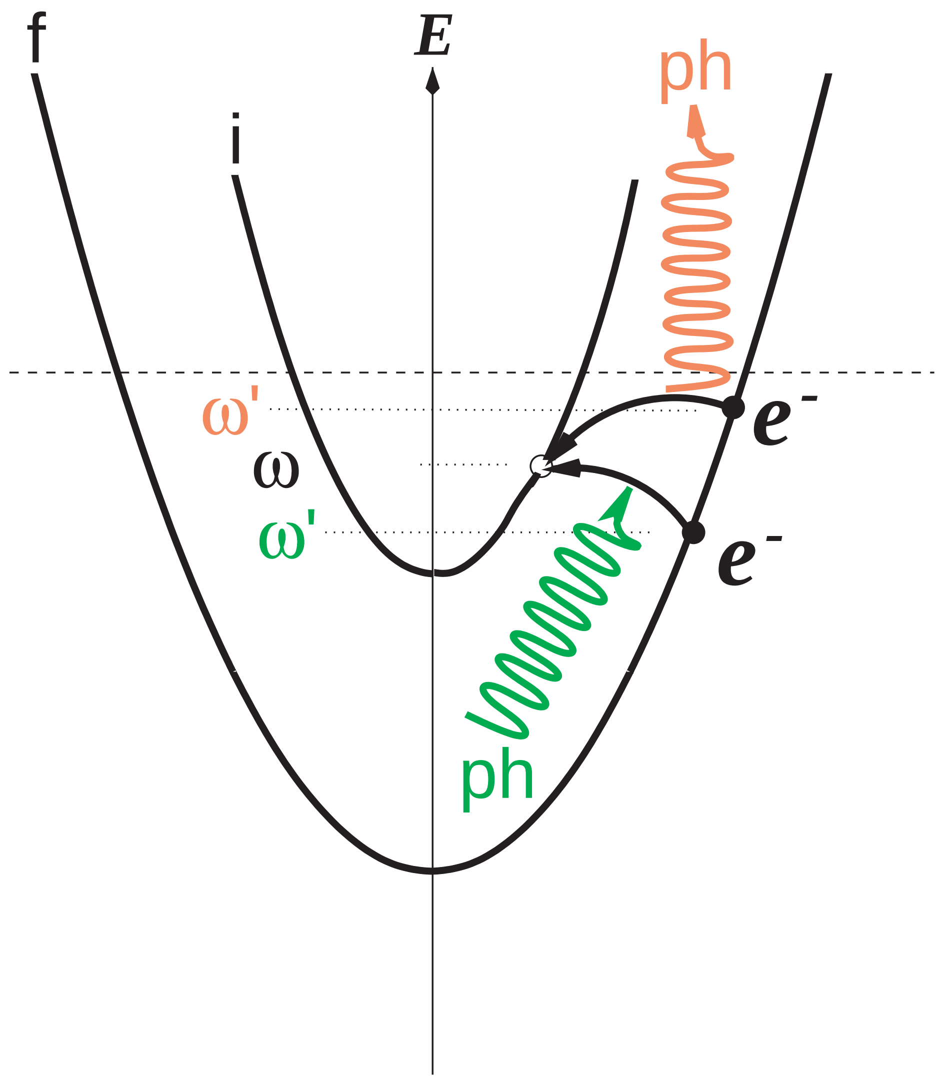


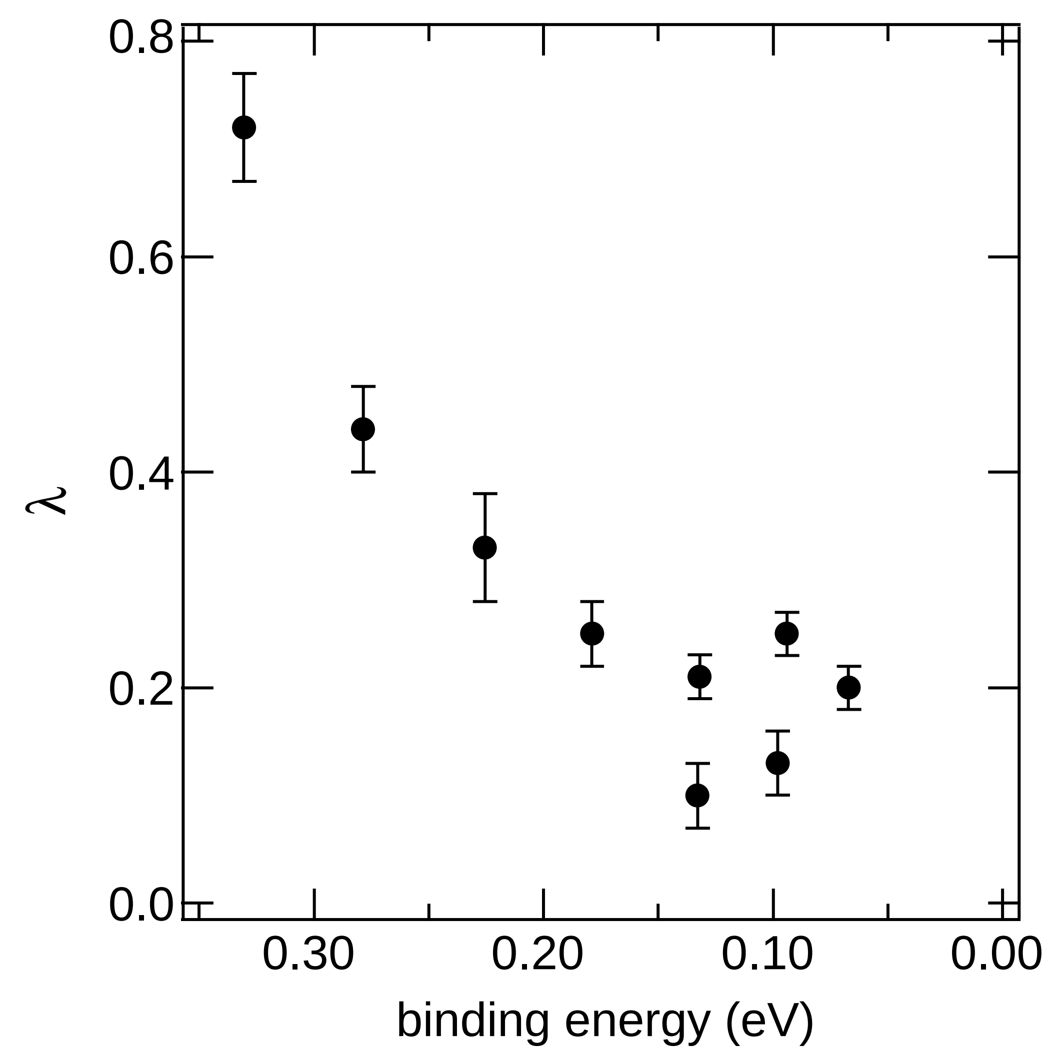


$$\alpha^2 F_{\vec{k}_i}(\omega) = \sum_{\vec{q},\nu,f} |g_{i,f}^{\vec{q},\nu}|^2 \delta(\omega - \omega_{\vec{q},\nu}) \delta(\epsilon_{\vec{k}_i} - \epsilon_{\vec{k}_f})$$

- The phonon energy window is small (≈10 meV)
- The bulk density of states is strongly energy dependent.
- This is reflected in a strong energy dependence of the inter-band scattering.

Why is λ energy-dependent?

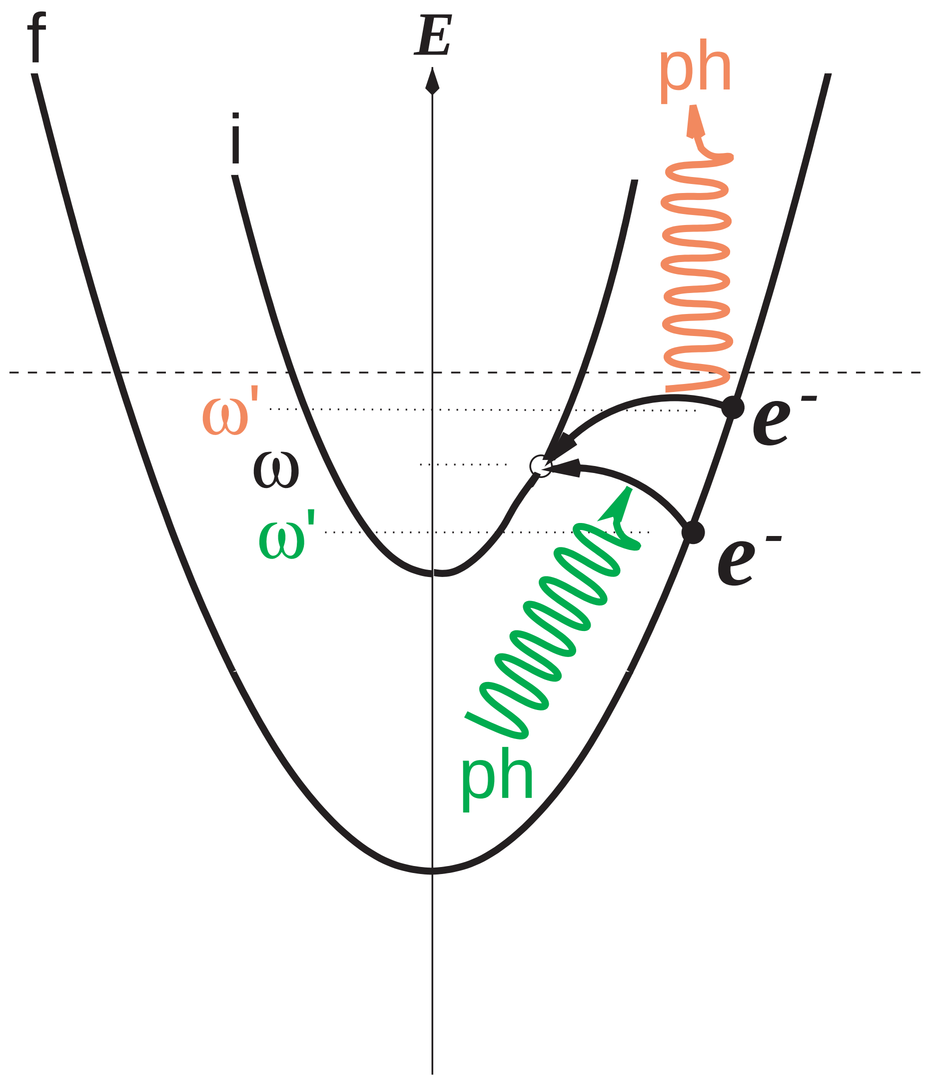


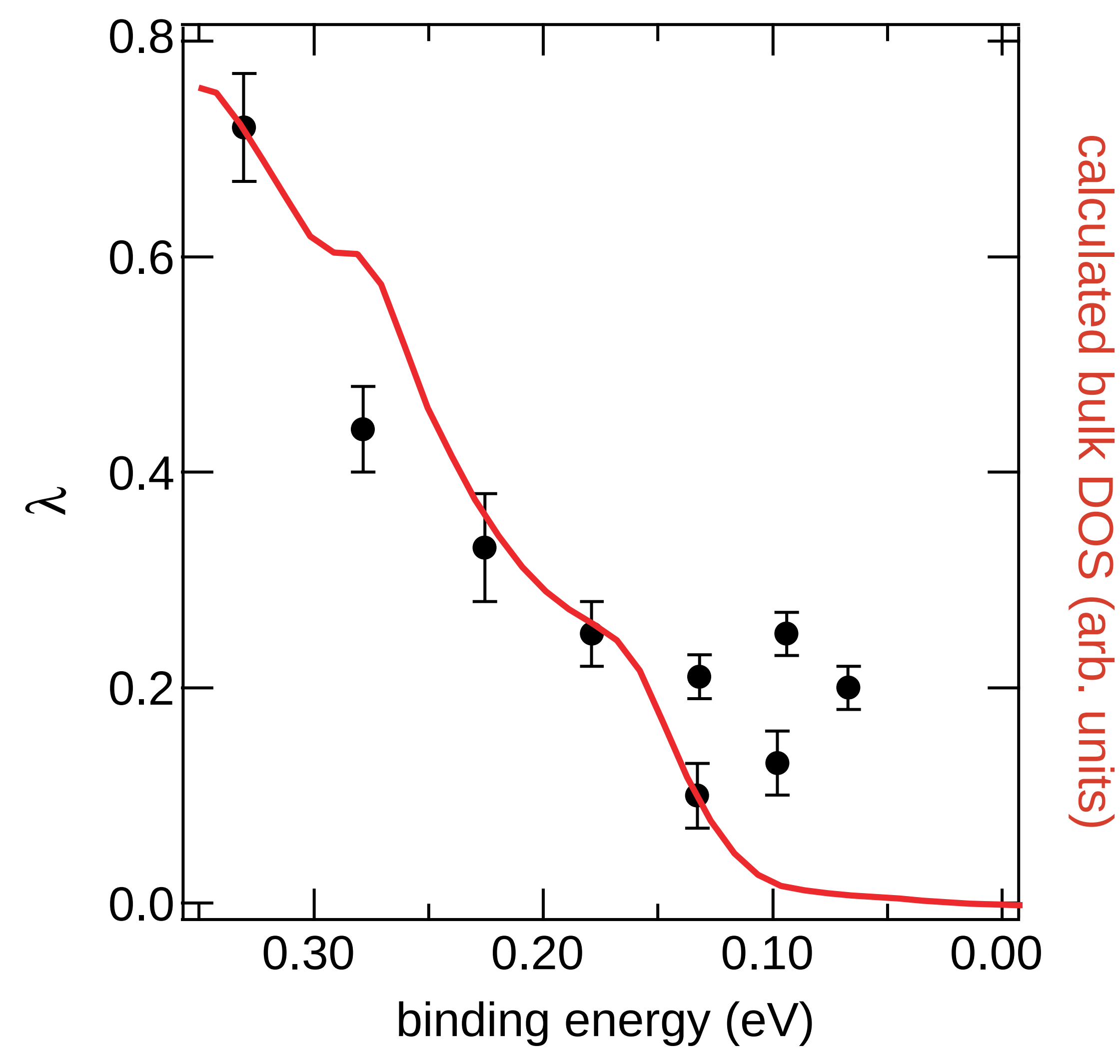


$$\alpha^2 F_{\vec{k}_i}(\omega) = \sum_{\vec{q},\nu,f} |g_{i,f}^{\vec{q},\nu}|^2 \delta(\omega - \omega_{\vec{q},\nu}) \delta(\epsilon_{\vec{k}_i} - \epsilon_{\vec{k}_f})$$

- The phonon energy window is small (≈10 meV)
- The bulk density of states is strongly energy dependent.
- This is reflected in a strong energy dependence of the inter-band scattering.

Why is λ energy-dependent?

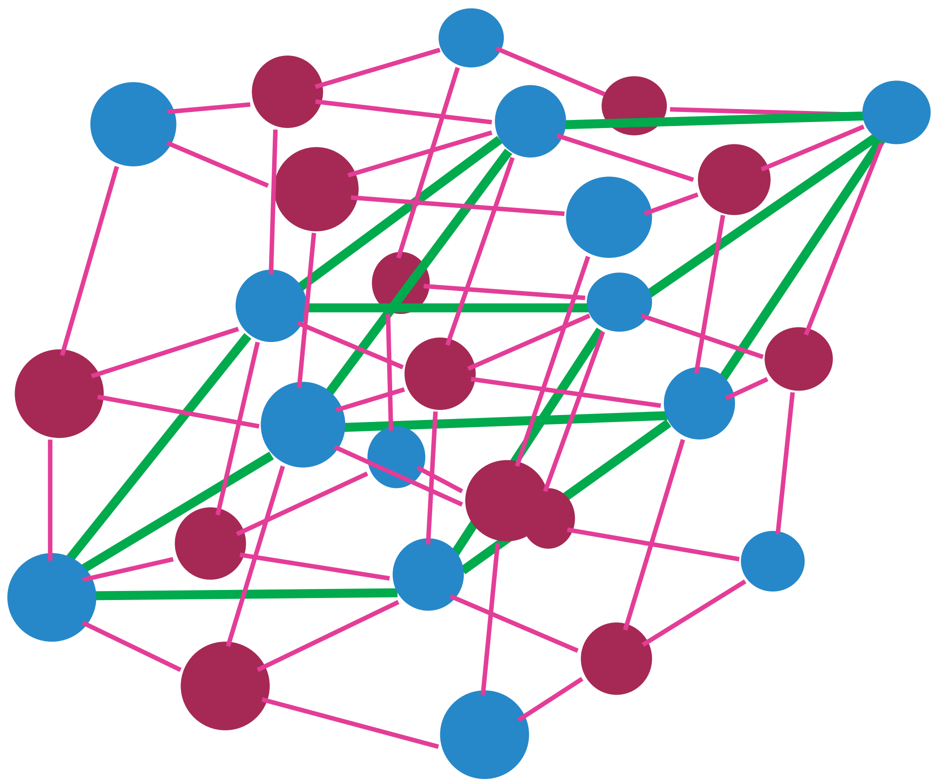


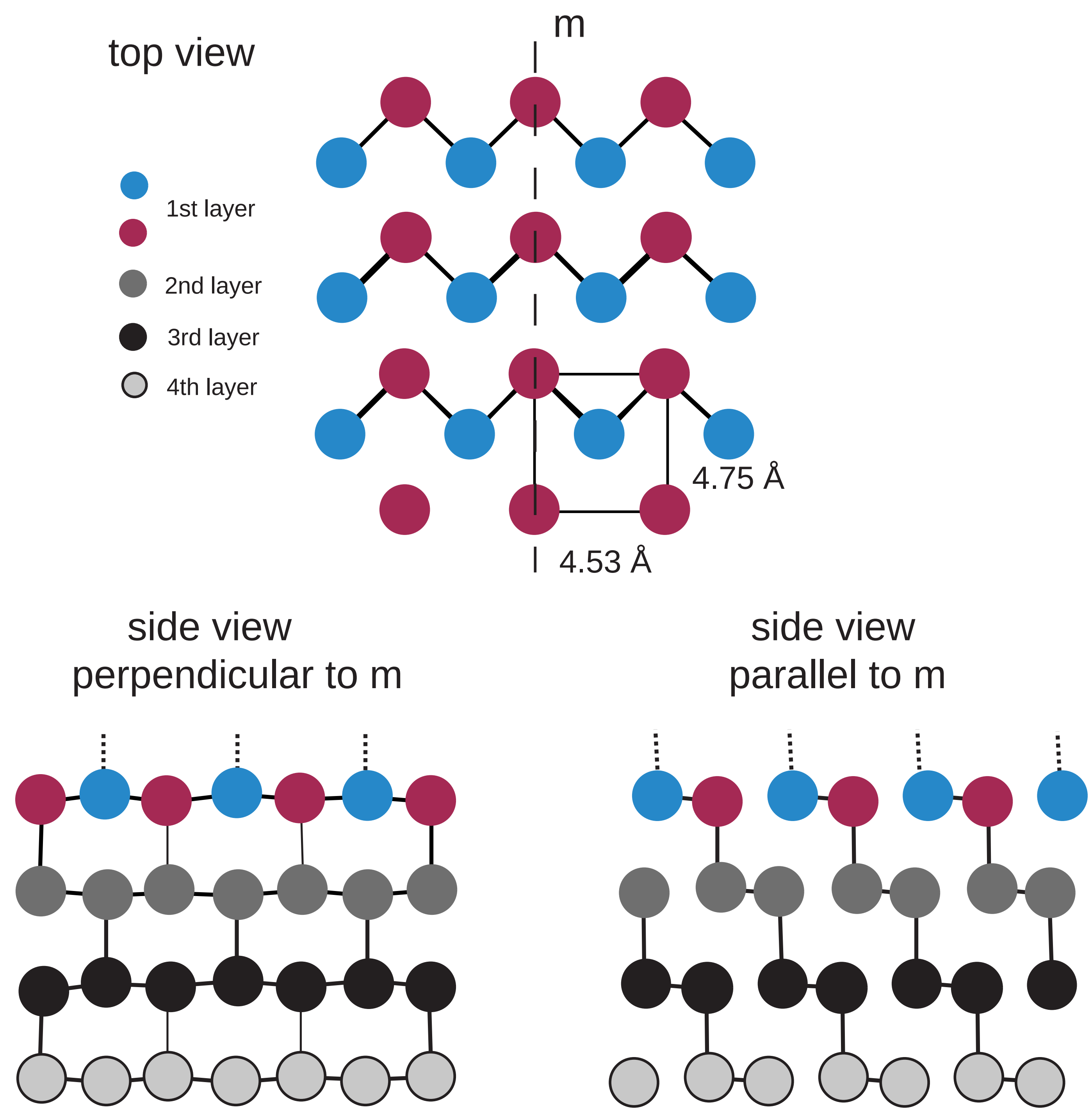


$$\alpha^2 F_{\vec{k}_i}(\omega) = \sum_{\vec{q},\nu,f} |g_{i,f}^{\vec{q},\nu}|^2 \delta(\omega - \omega_{\vec{q},\nu}) \delta(\epsilon_{\vec{k}_i} - \epsilon_{\vec{k}_f})$$

- The phonon energy window is small (≈10 meV)
- The bulk density of states is strongly energy dependent.
- This is reflected in a strong energy dependence of the inter-band scattering.

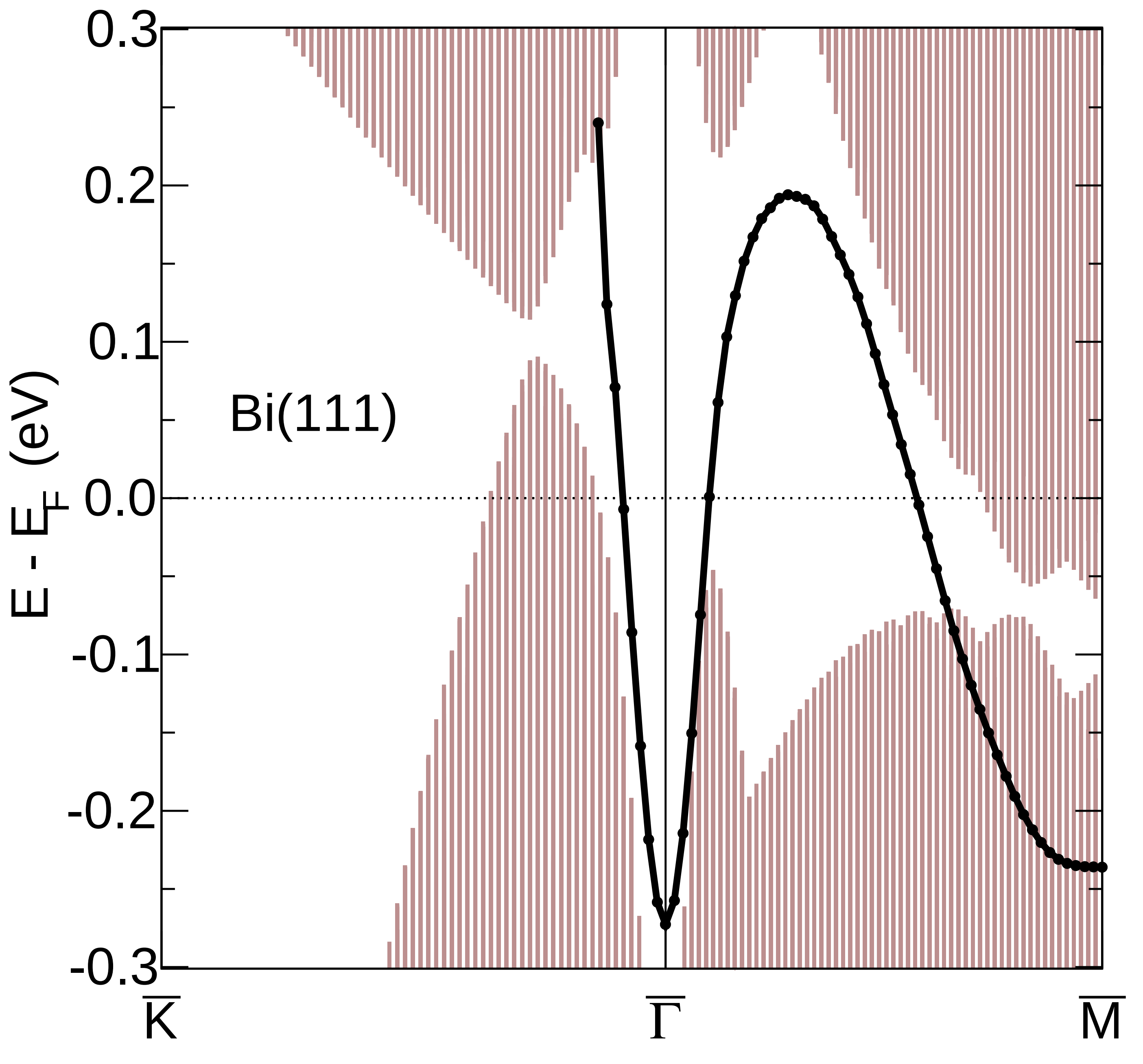
geometric structure of Bi(110)





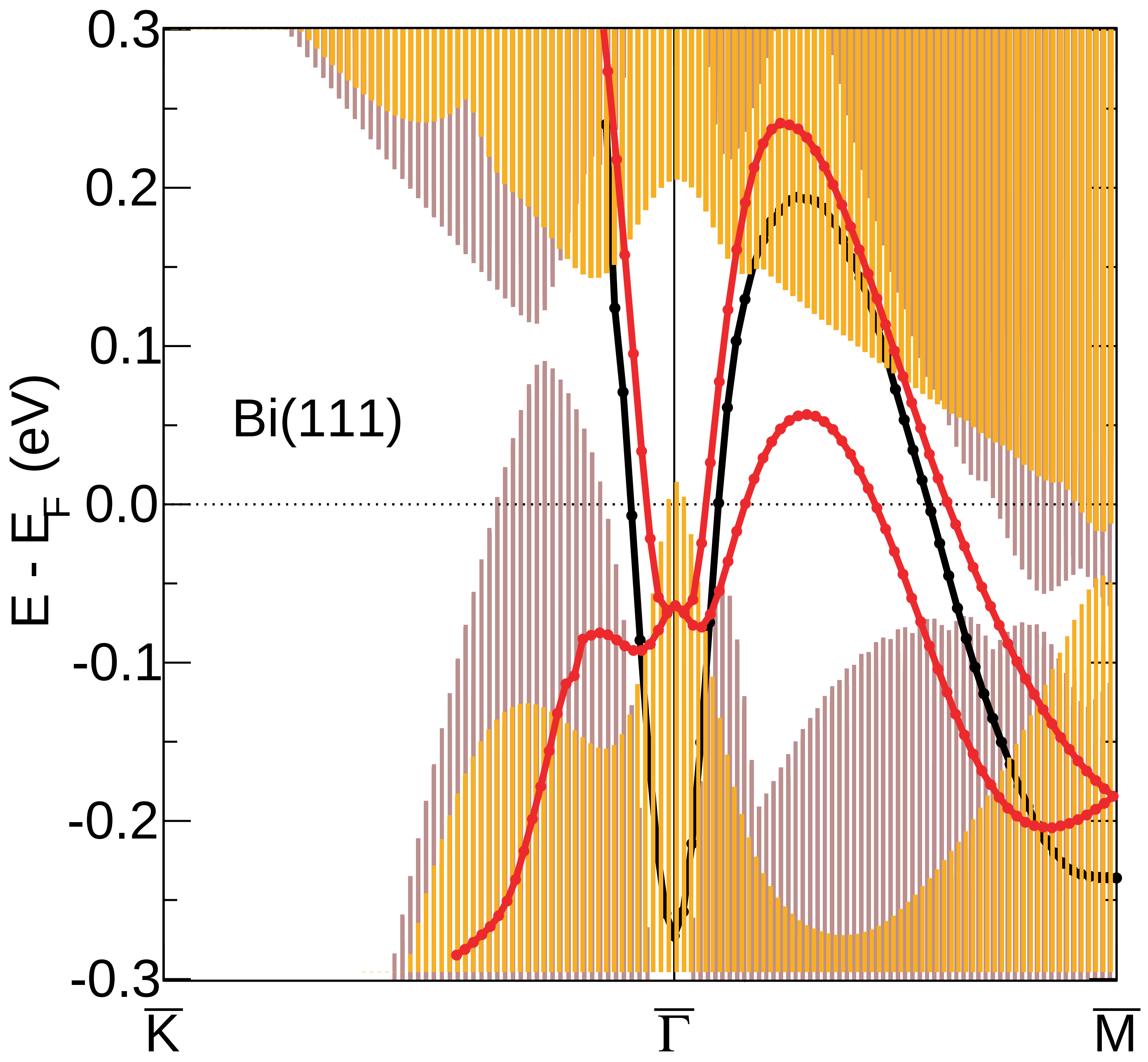
- one dangling bond per unit cell
- only one mirror plane
- no reconstruction

strong spin-orbit splitting on Bi surfaces



Yu. M. Koroteev, G. Bihlmayer, J. E. Gayone, E. V. Chulkov, S. Blügel, P. M. Echenique and Ph. Hofmann,
Physical Review Letters **93**, 046403 (2004).

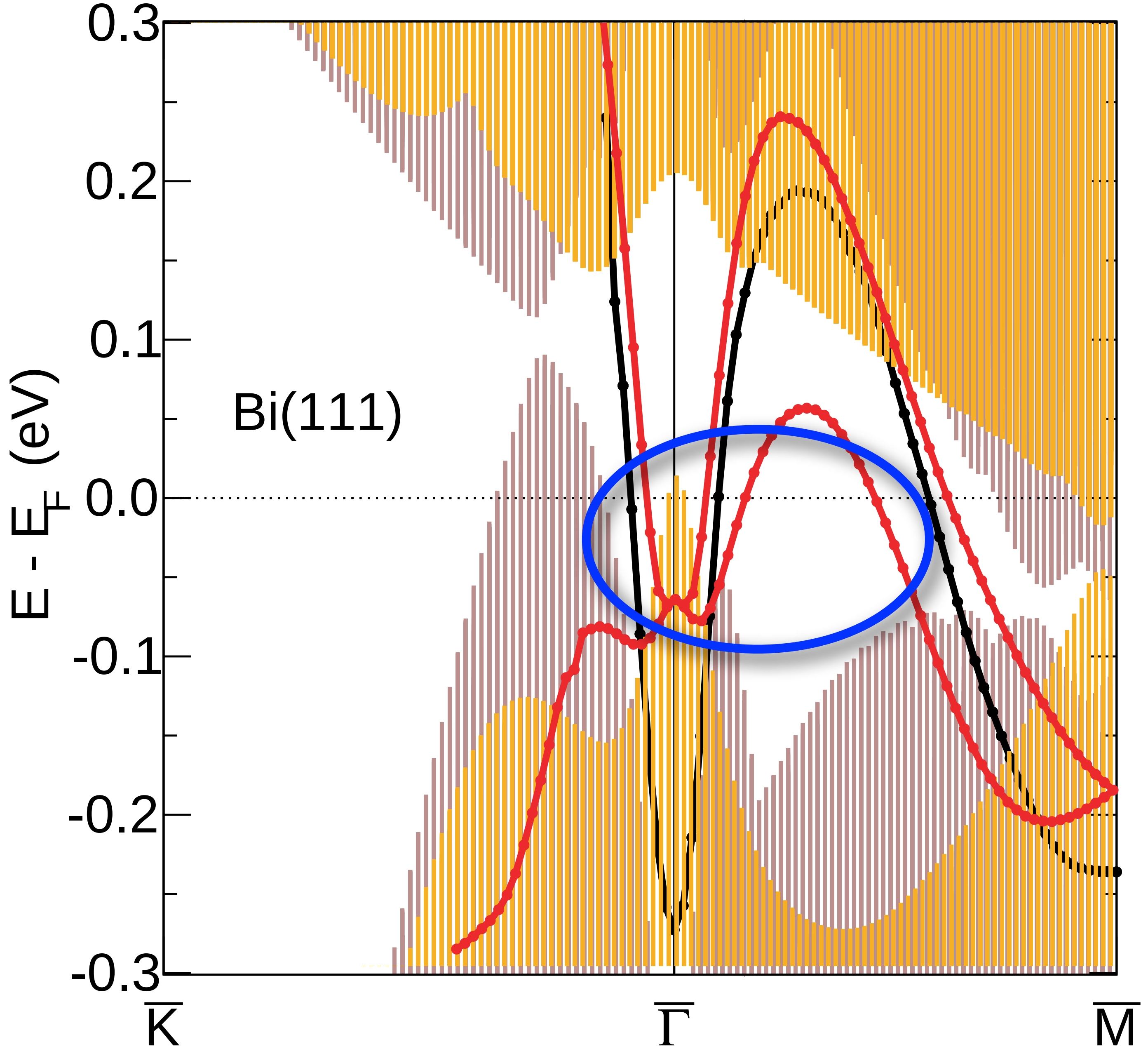
strong spin-orbit splitting on Bi surfaces



- profound change of dispersion and Fermi surface
- very good agreement with experiment

Yu. M. Koroteev, G. Bihlmayer, J. E. Gayone, E. V. Chulkov, S. Blügel, P. M. Echenique and Ph. Hofmann, Physical Review Letters **93**, 046403 (2004).

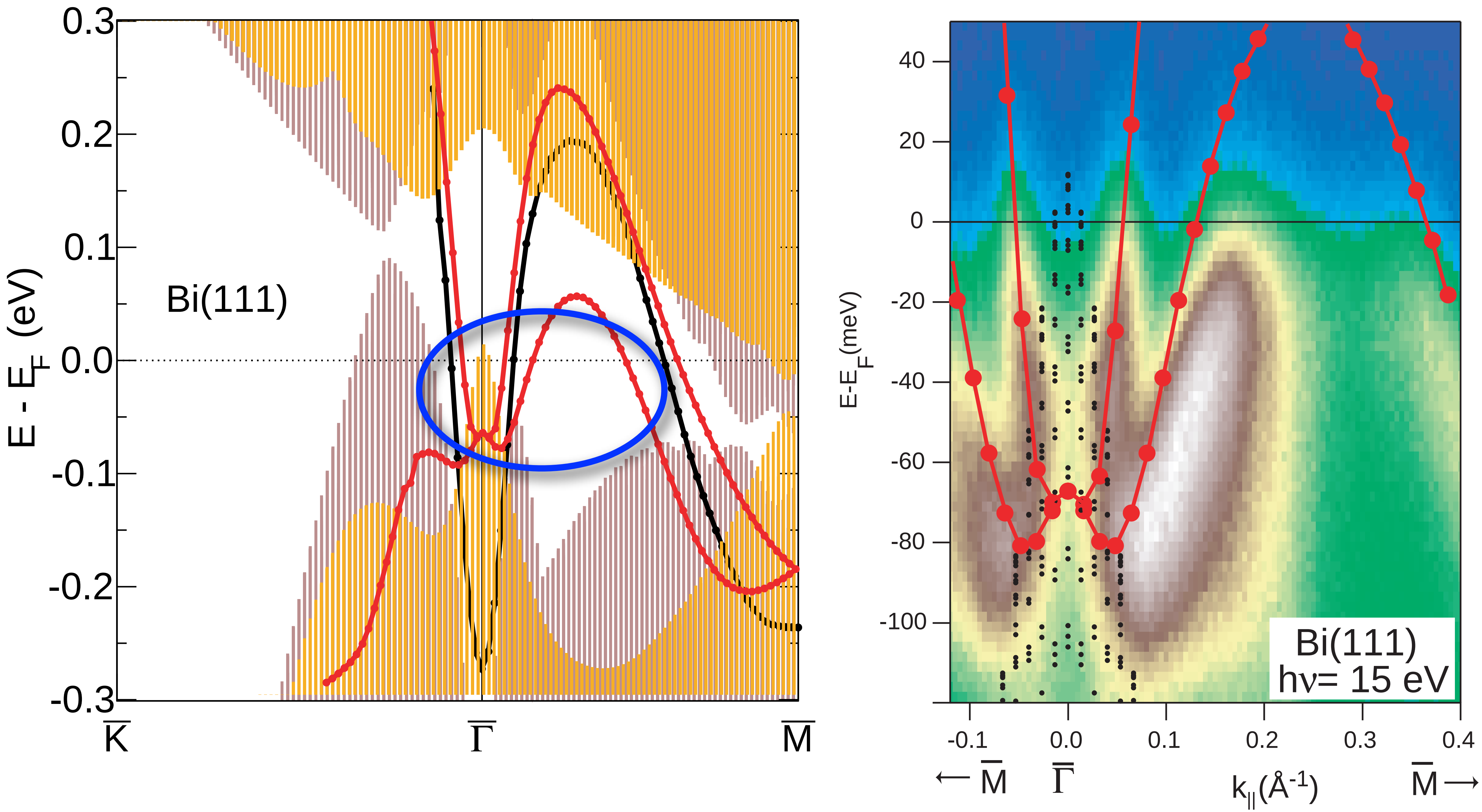
strong spin-orbit splitting on Bi surfaces



- profound change of dispersion and Fermi surface
- very good agreement with experiment

Yu. M. Koroteev, G. Bihlmayer, J. E. Gayone, E. V. Chulkov, S. Blügel, P. M. Echenique and Ph. Hofmann, Physical Review Letters **93**, 046403 (2004).

strong spin-orbit splitting on Bi surfaces

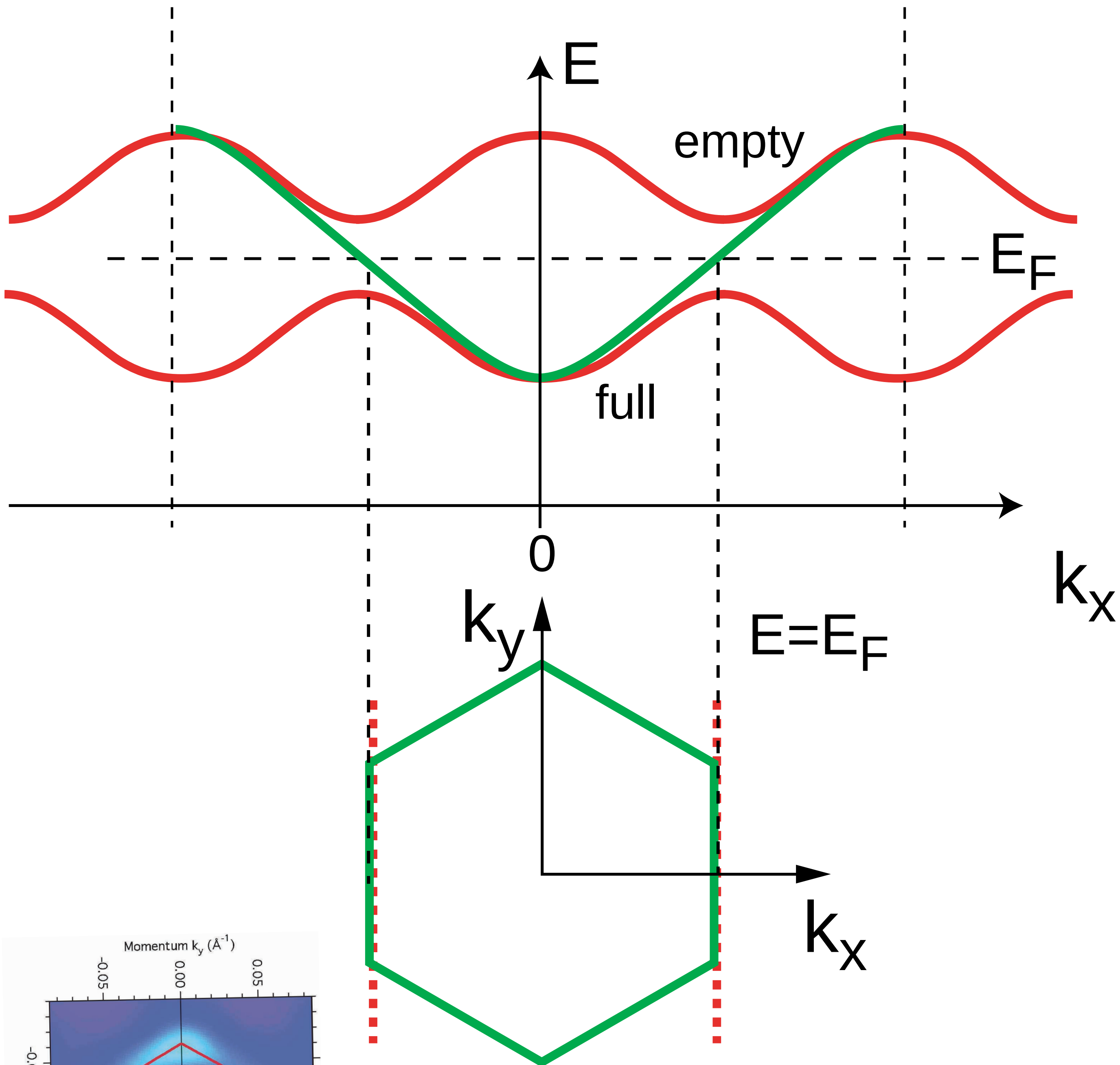


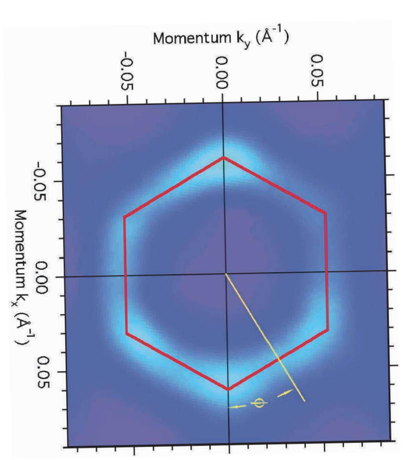
- profound change of dispersion and Fermi surface
- very good agreement with experiment

Yu. M. Koroteev, G. Bihlmayer, J. E. Gayone, E. V. Chulkov, S. Blügel, P. M. Echenique and Ph. Hofmann, Physical Review Letters **93**, 046403 (2004).

A charge density wave on Bi(111)?

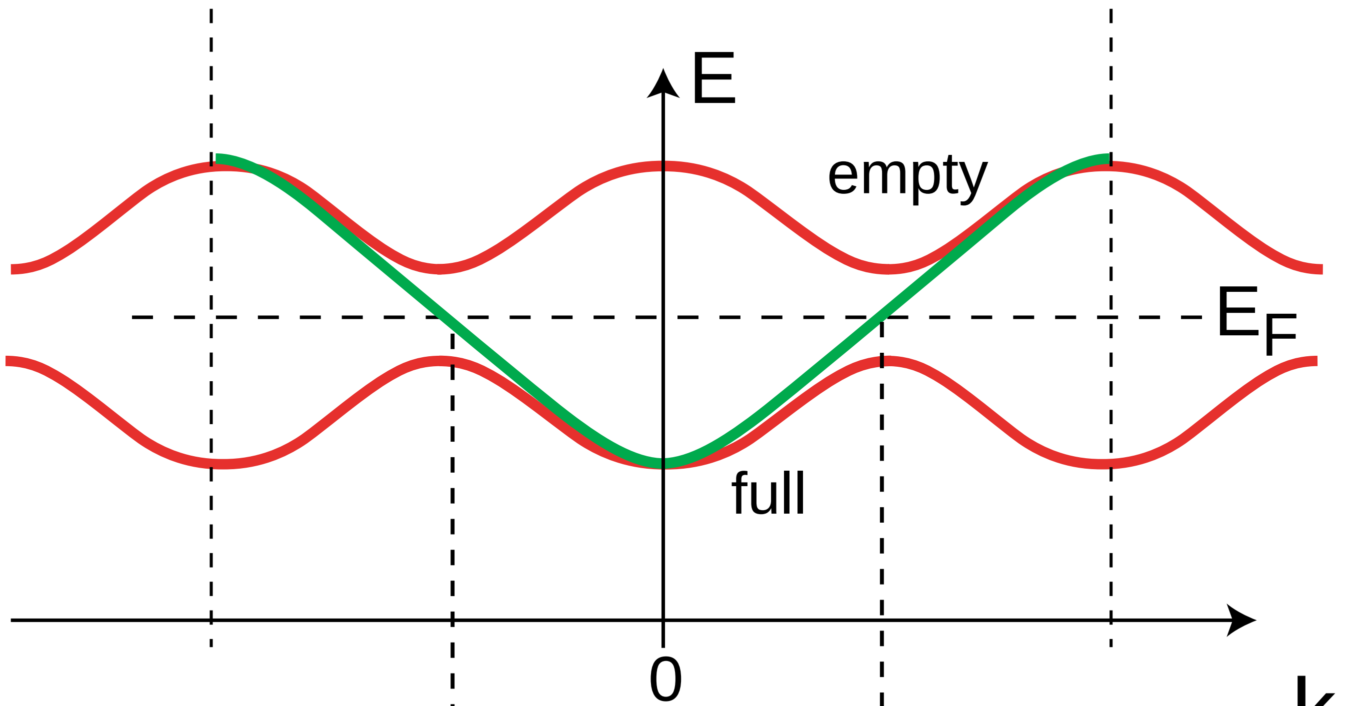
charge density wave on Bi(111)

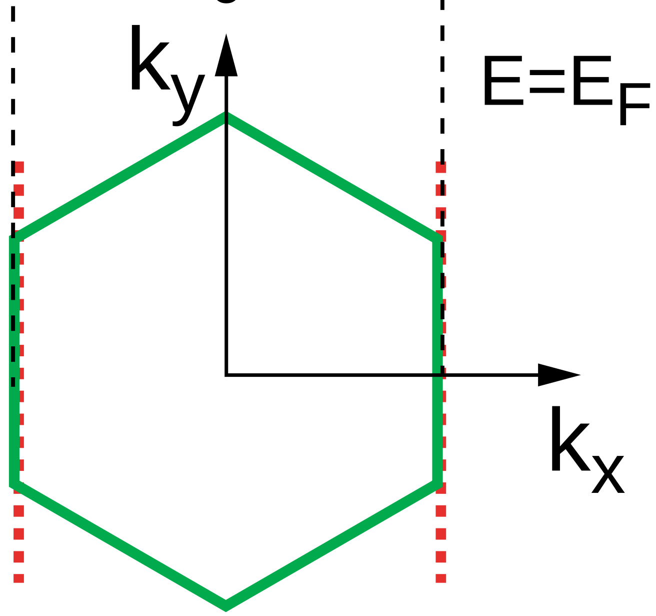


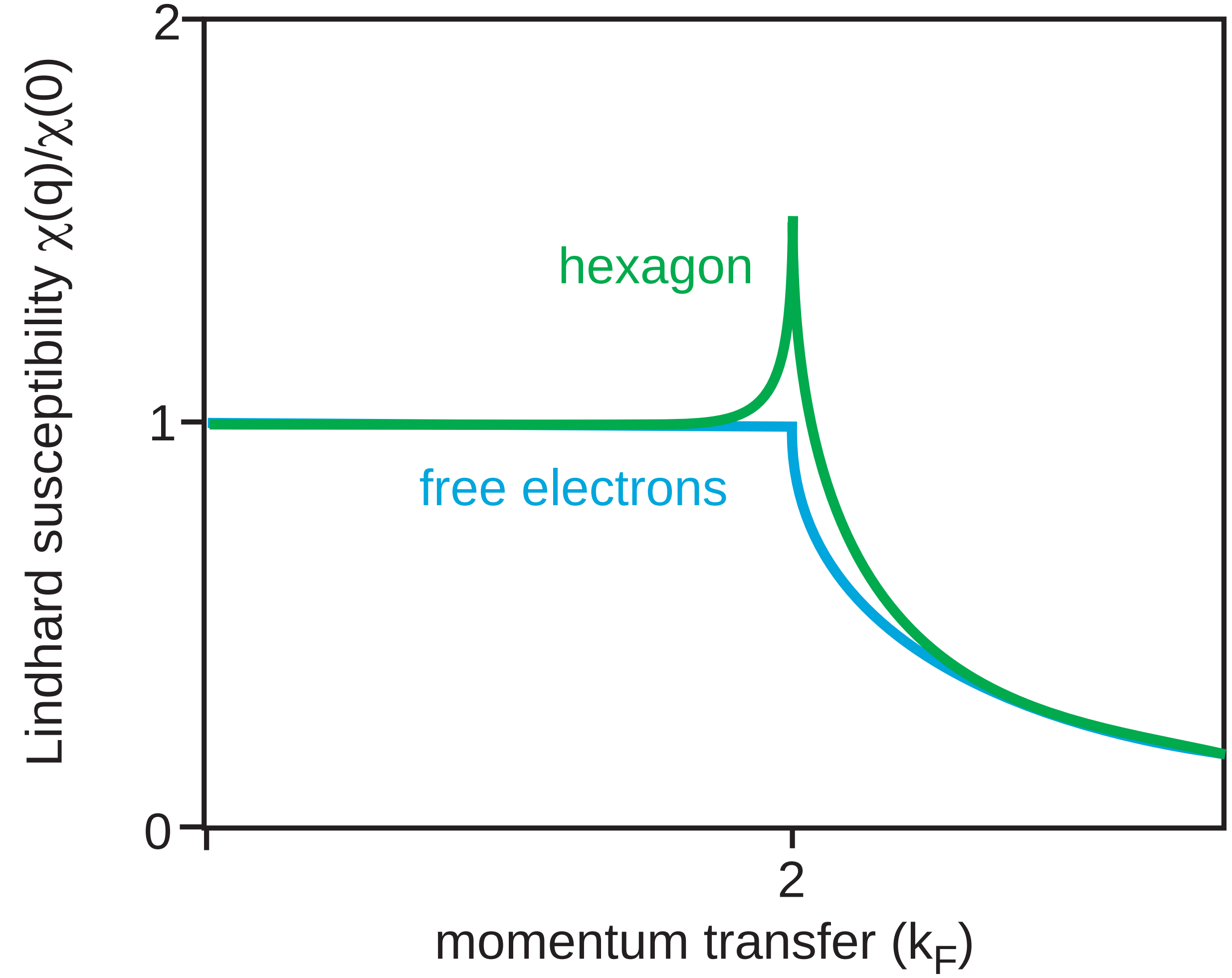


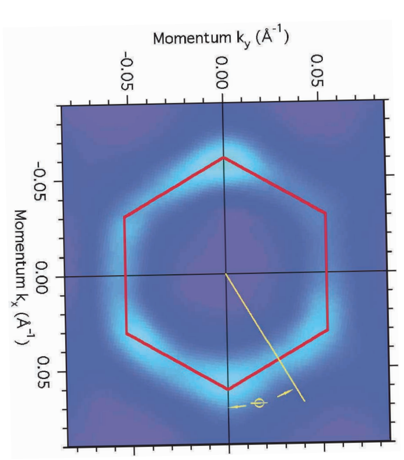
Ast and Höchst, PRL 90, 016403 (2003)

charge density wave on Bi(111)



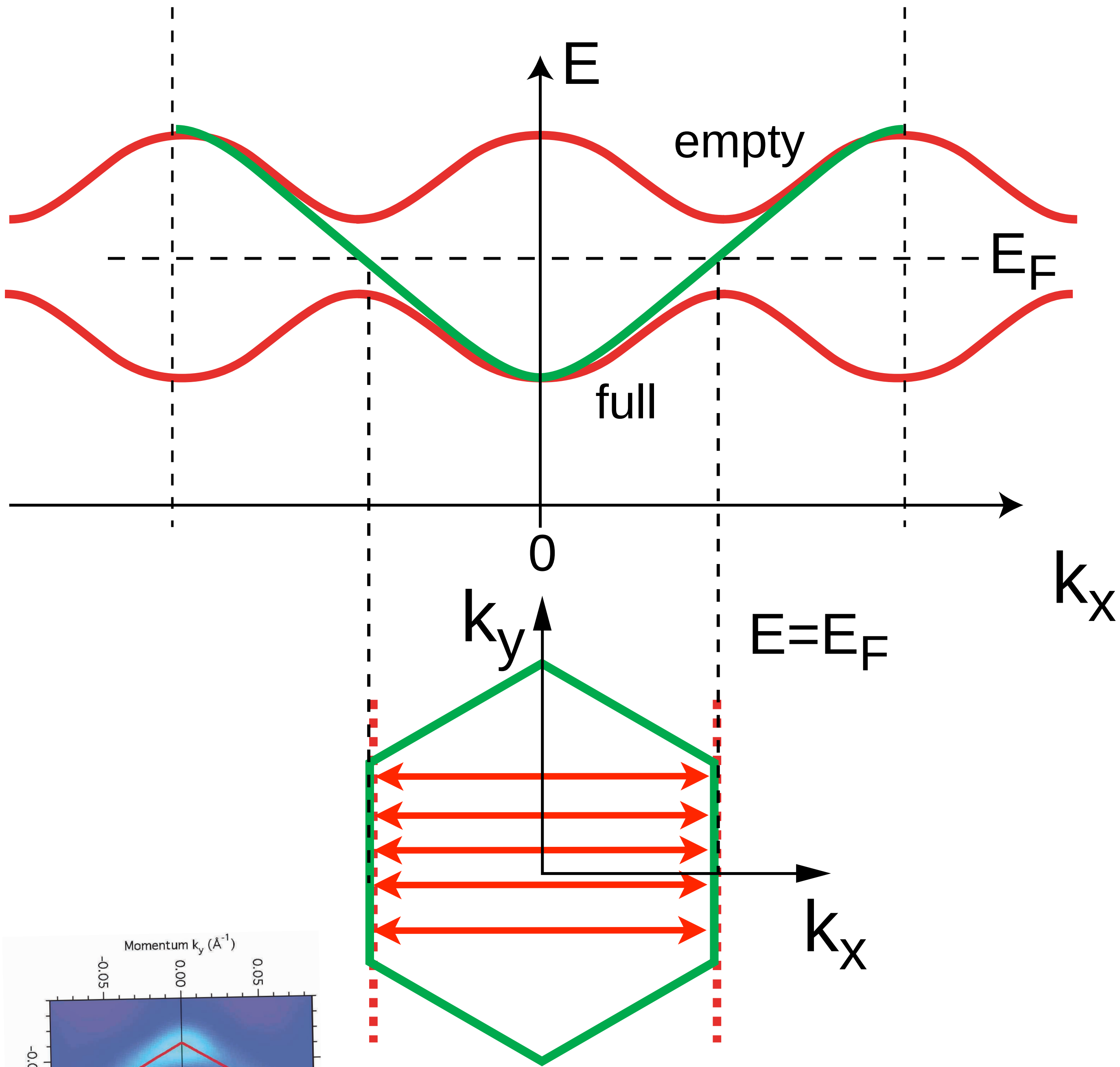


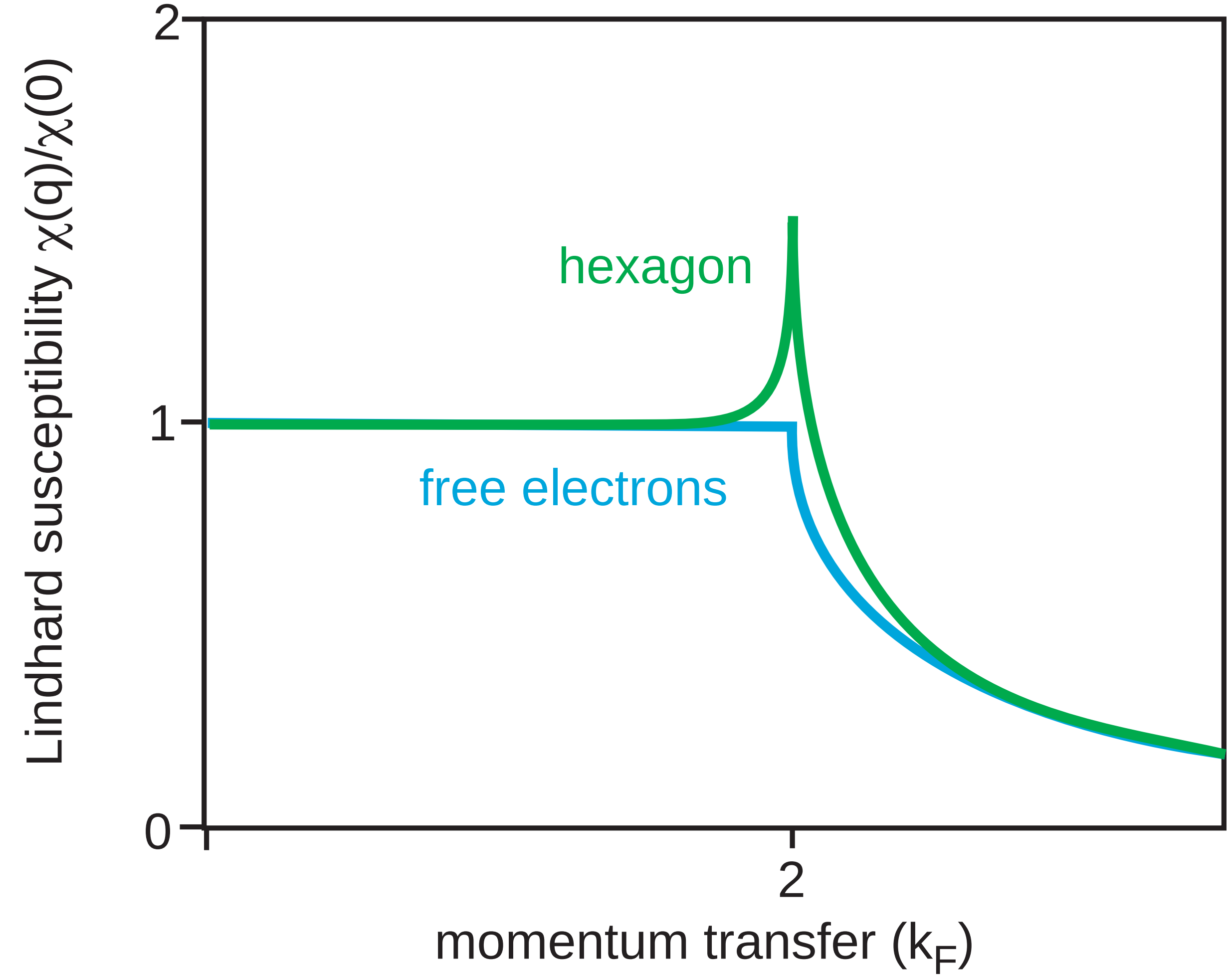


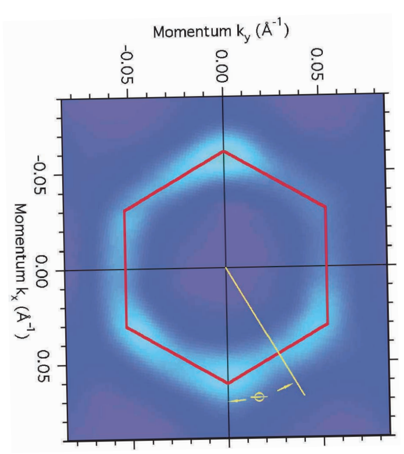


Ast and Höchst, PRL 90, 016403 (2003)

charge density wave on Bi(111)

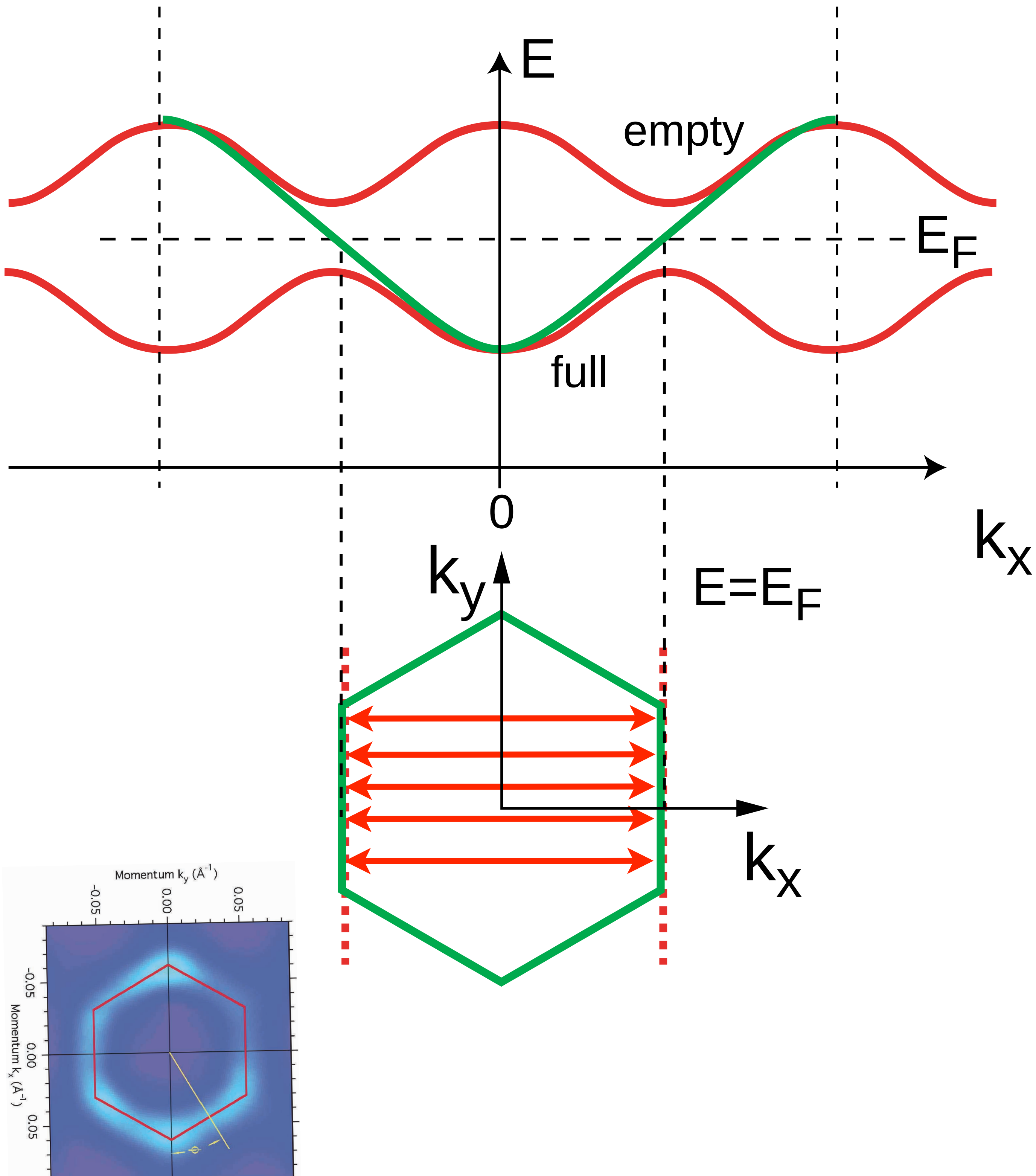




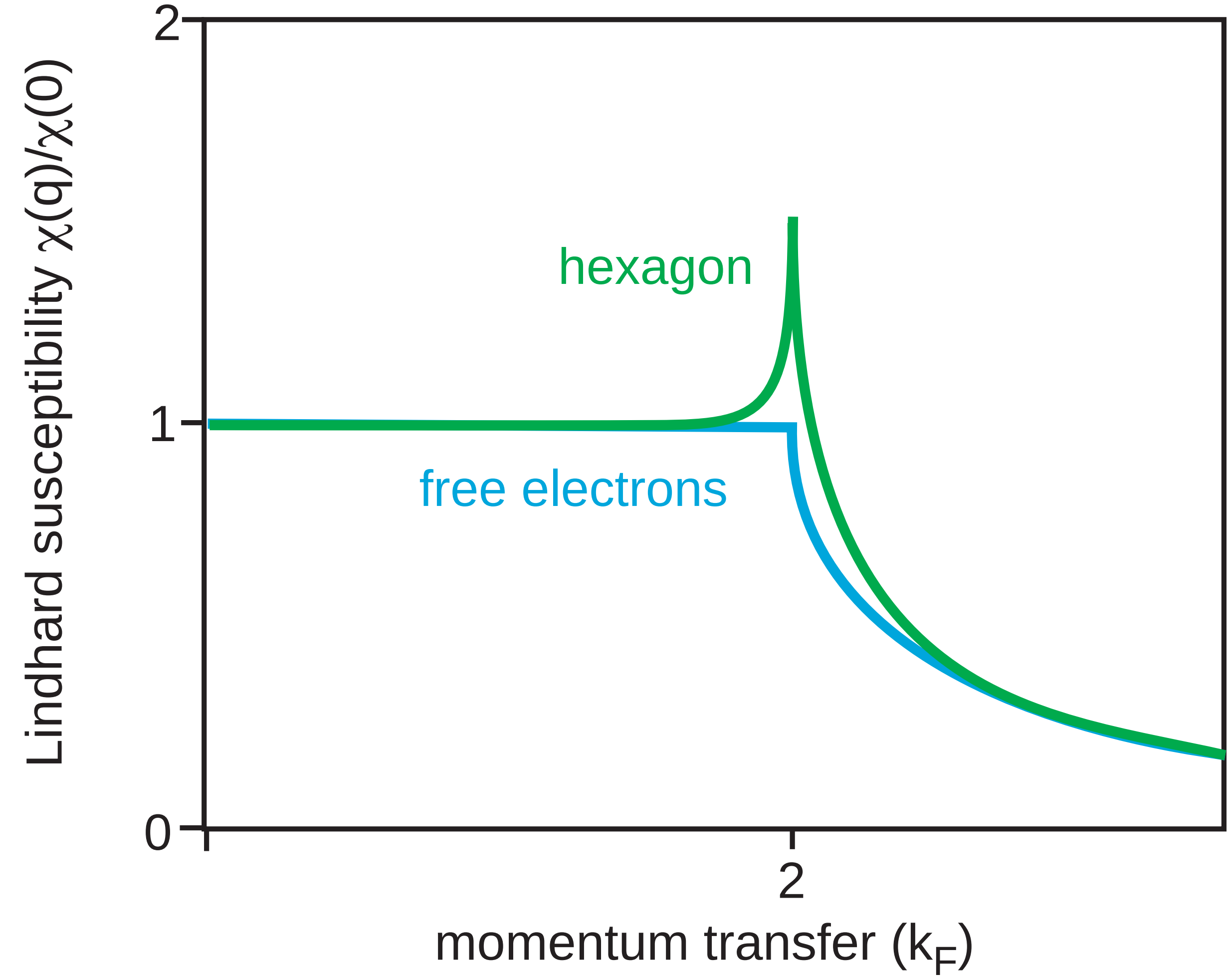


Ast and Höchst, PRL 90, 016403 (2003)

charge density wave on Bi(111)



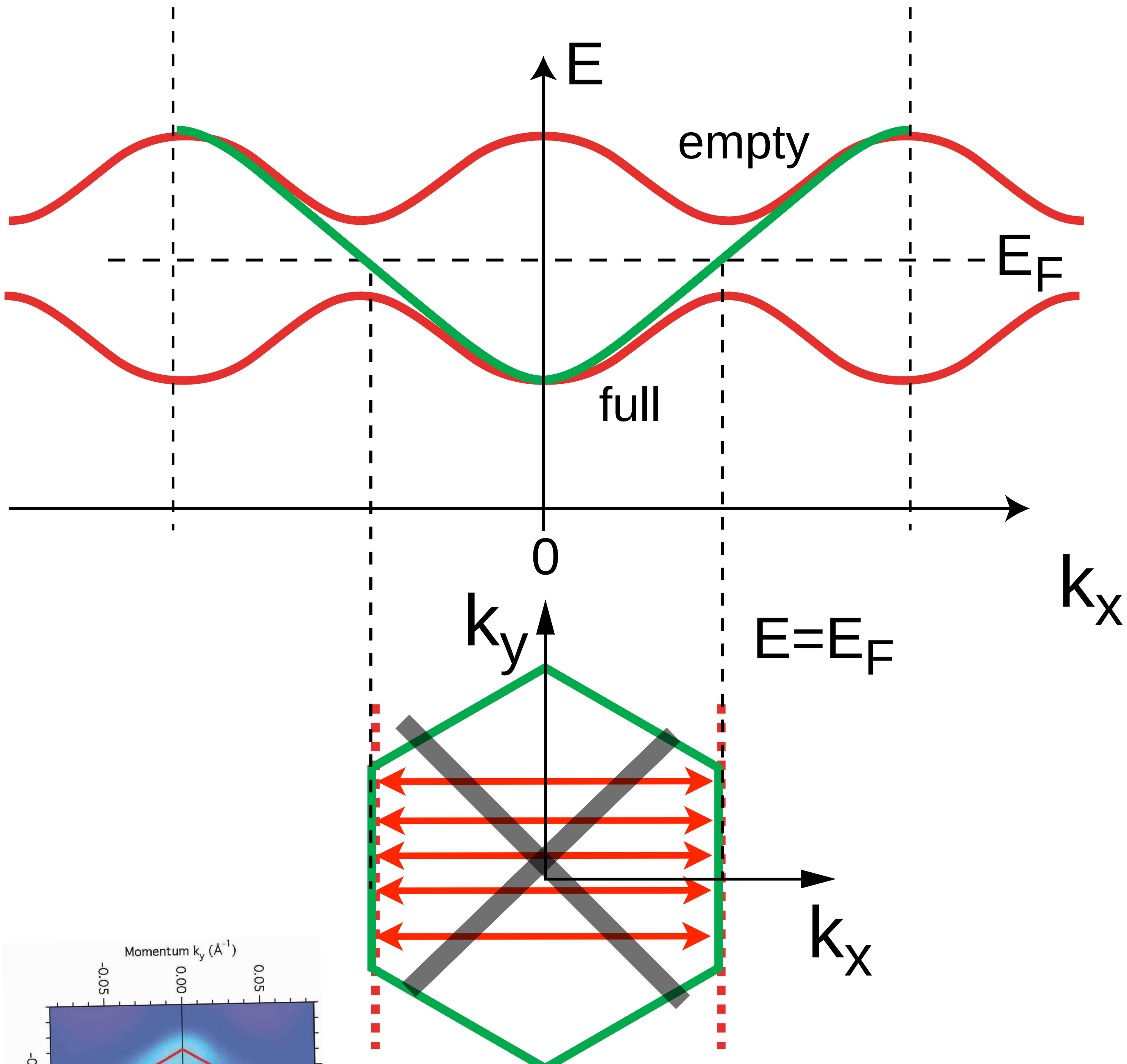
Ast and Höchst, PRL 90, 016403 (2003)

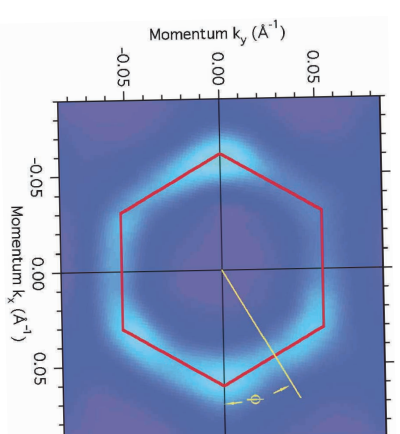


Lindhard susceptibility

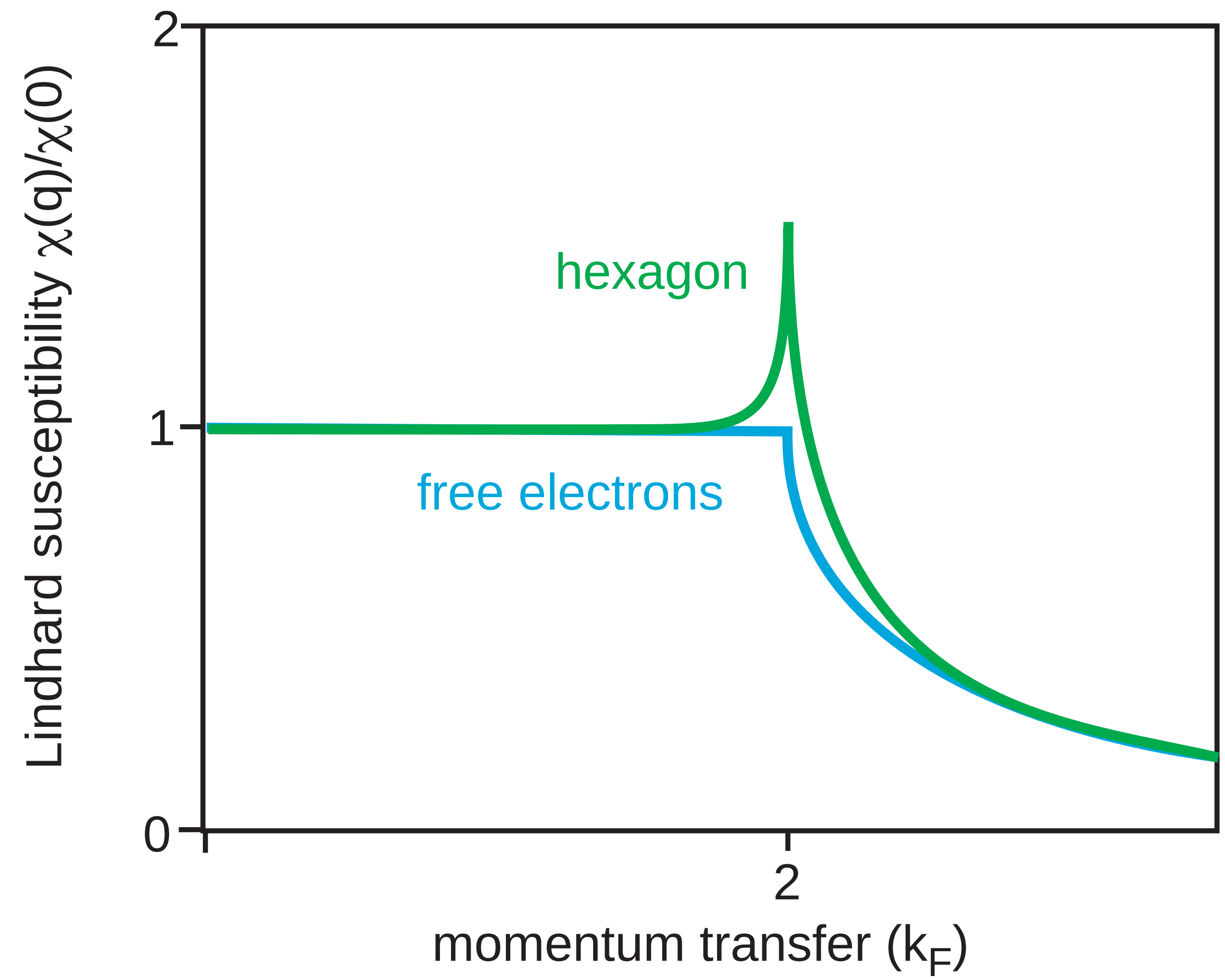
$$\chi(\vec{q}) = \int \frac{f(\vec{k}) - f(\vec{k}-\vec{q})d\vec{k}}{\epsilon(\vec{k}) - \epsilon(\vec{k}-\vec{q})(2\pi)^2}$$

charge density wave on Bi(111)





Ast and Höchst, PRL 90, 016403 (2003)

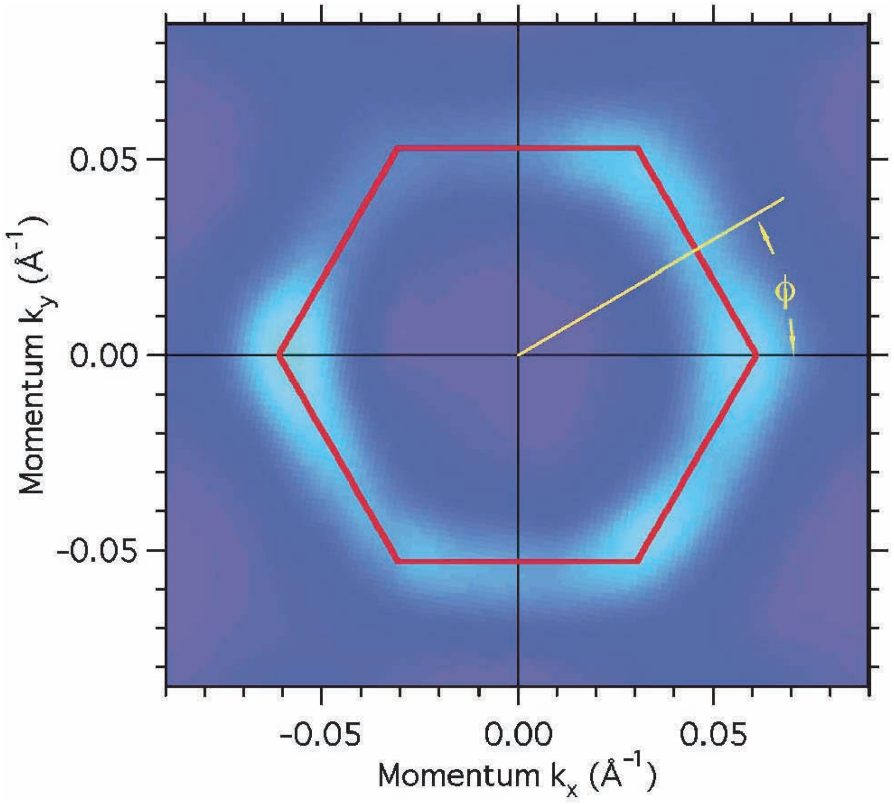


Lindhard susceptibility

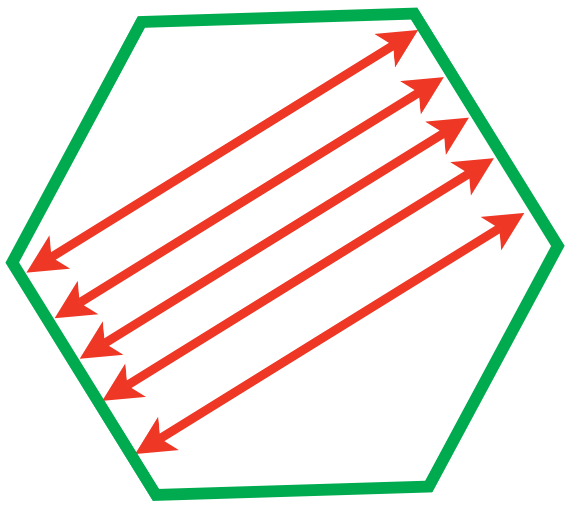
$$\chi(\vec{q}) = \int \frac{f(\vec{k}) - f(\vec{k}-\vec{q})d\vec{k}}{\epsilon(\vec{k}) - \epsilon(\vec{k}-\vec{q})(2\pi)^2}$$

Charge density wave on Bi(111)?

Fermi Surface
(photoemission intensity at E_F)

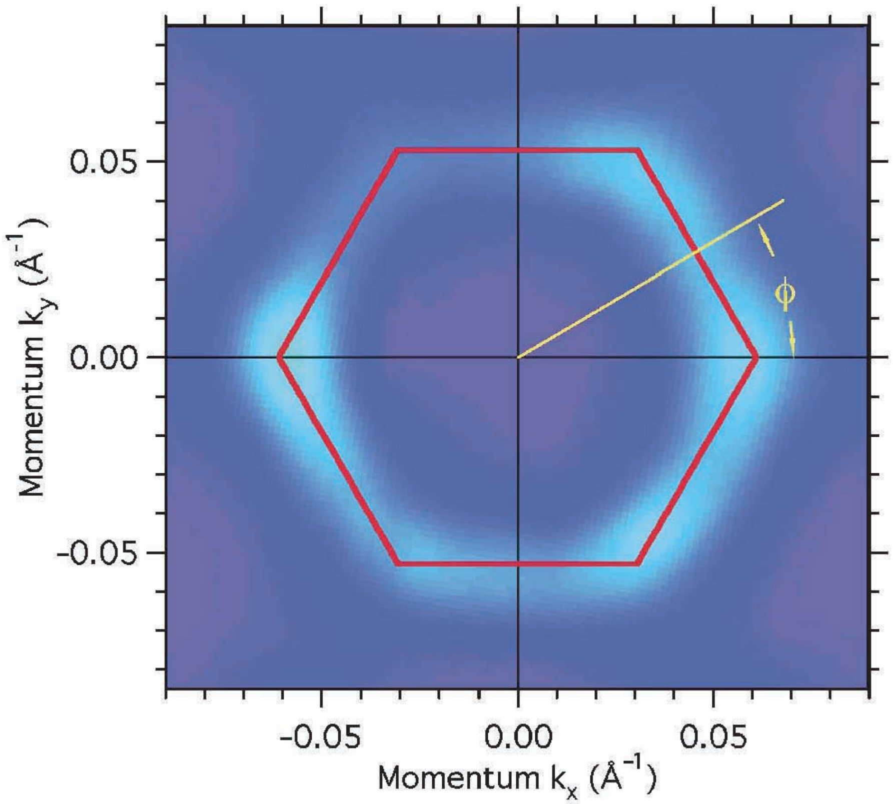


Ast and Höchst, PRL 90, 016403 (2003)

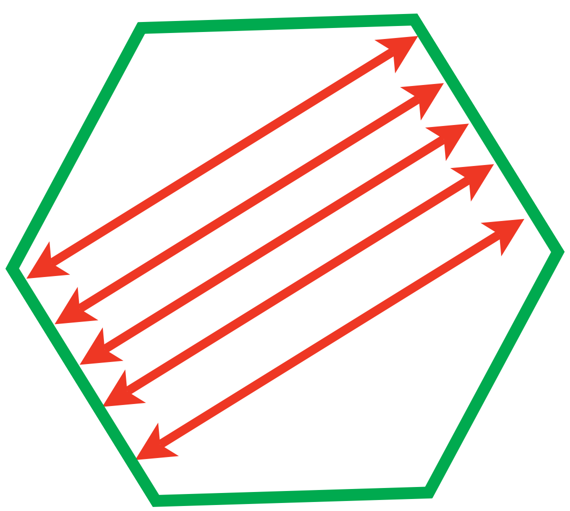


Charge density wave on Bi(111)?

Fermi Surface
(photoemission intensity at E_F)

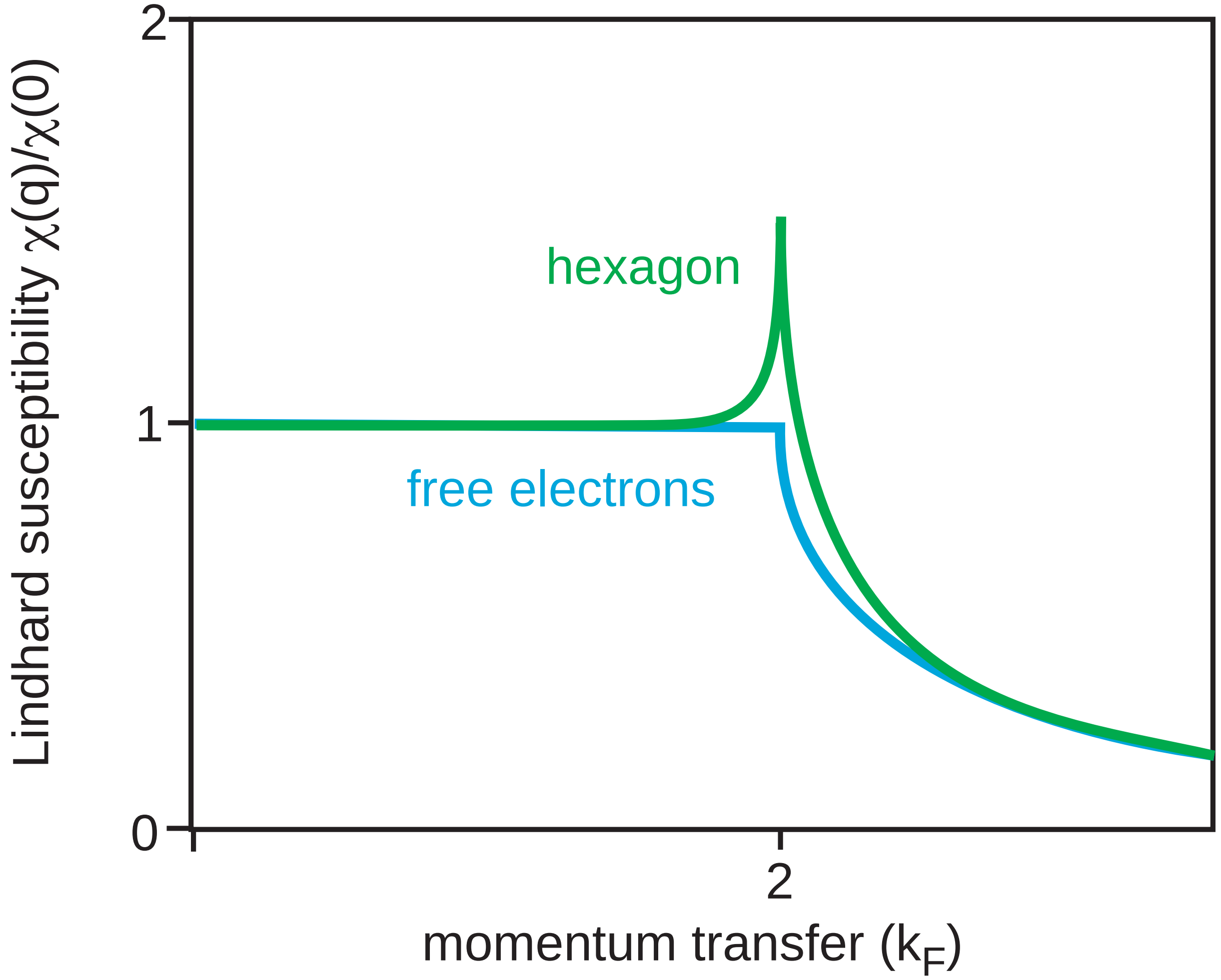


Ast and Höchst, PRL 90, 016403 (2003)



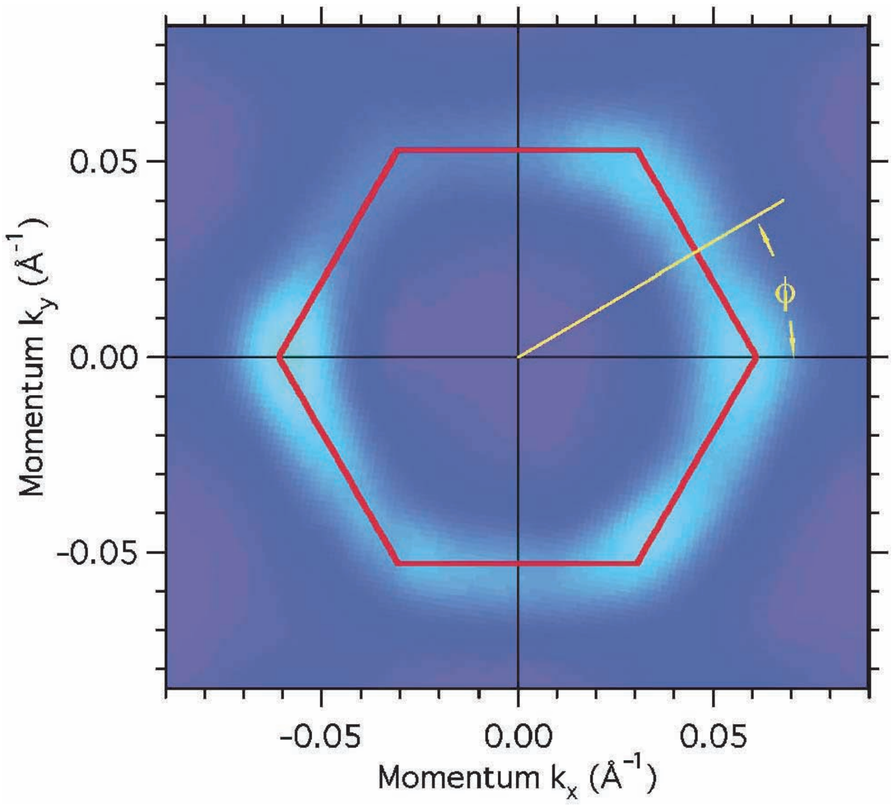
Lindhard susceptibility

$$\chi(\vec{q}) = \int \frac{f(\vec{k}) - f(\vec{k} - \vec{q})d\vec{k}}{\epsilon(\vec{k}) - \epsilon(\vec{k} - \vec{q})(2\pi)^2}$$

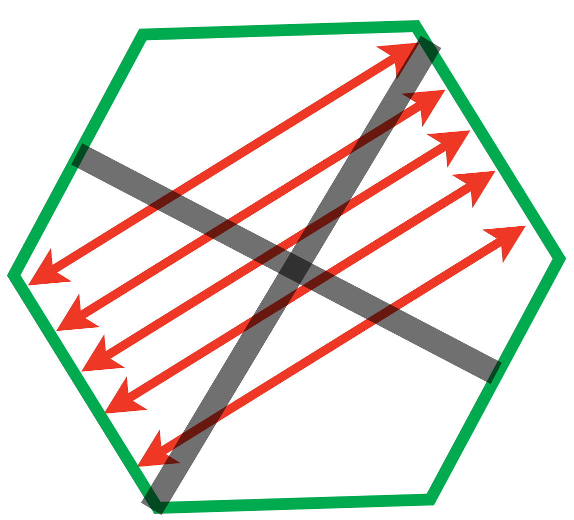


Charge density wave on Bi(111)?

Fermi Surface
(photoemission intensity at E_F)

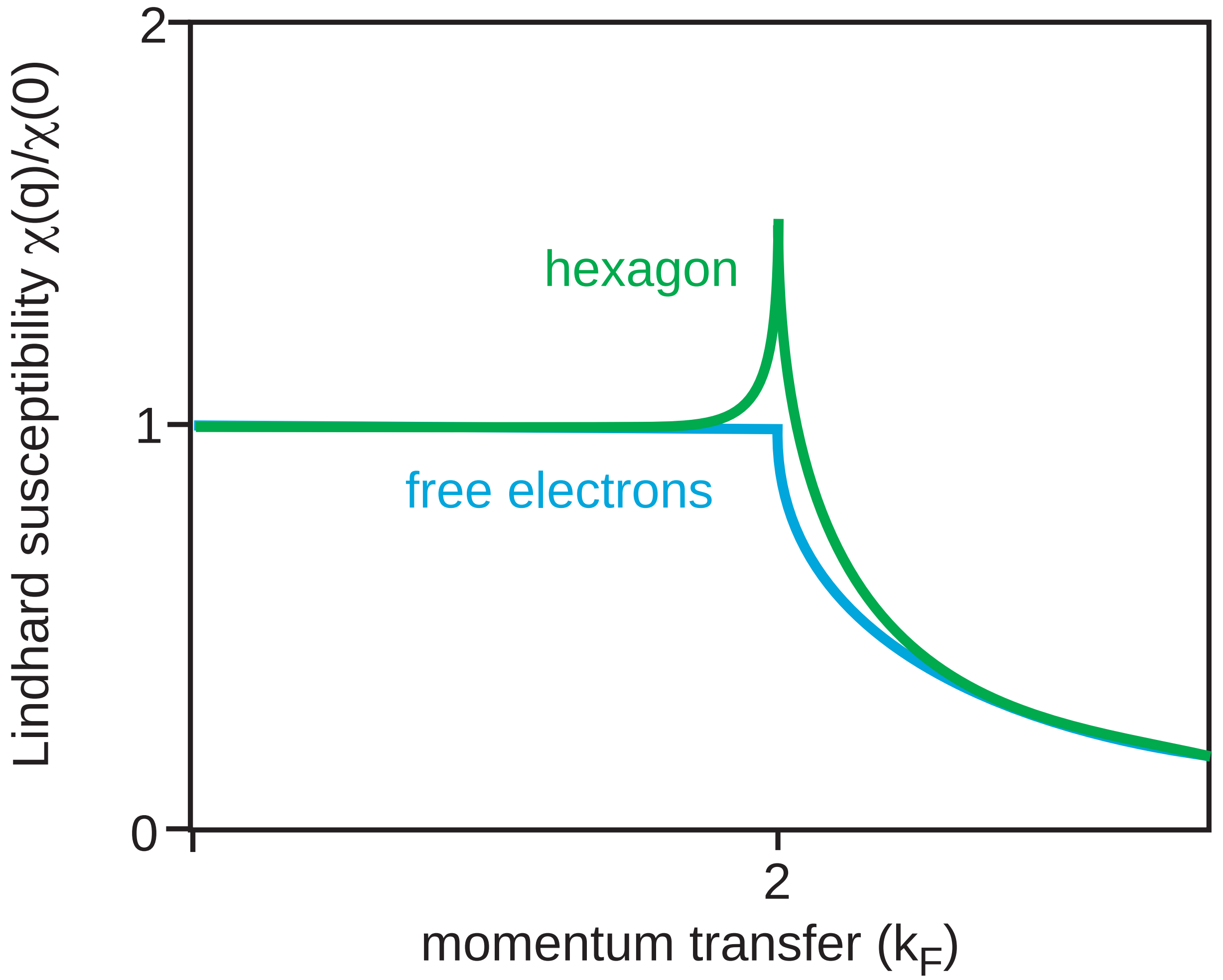


Ast and Höchst, PRL 90, 016403 (2003)



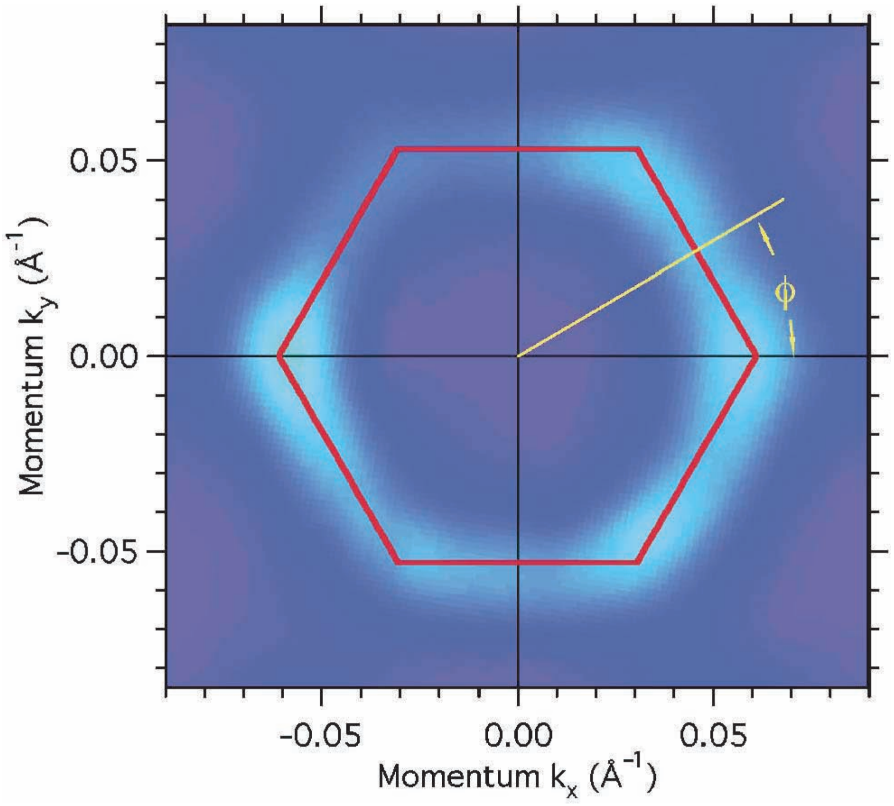
Lindhard susceptibility

$$\chi(\vec{q}) = \int \frac{f(\vec{k}) - f(\vec{k}-\vec{q})d\vec{k}}{\epsilon(\vec{k}) - \epsilon(\vec{k}-\vec{q})(2\pi)^2}$$



Charge density wave on Bi(111)?

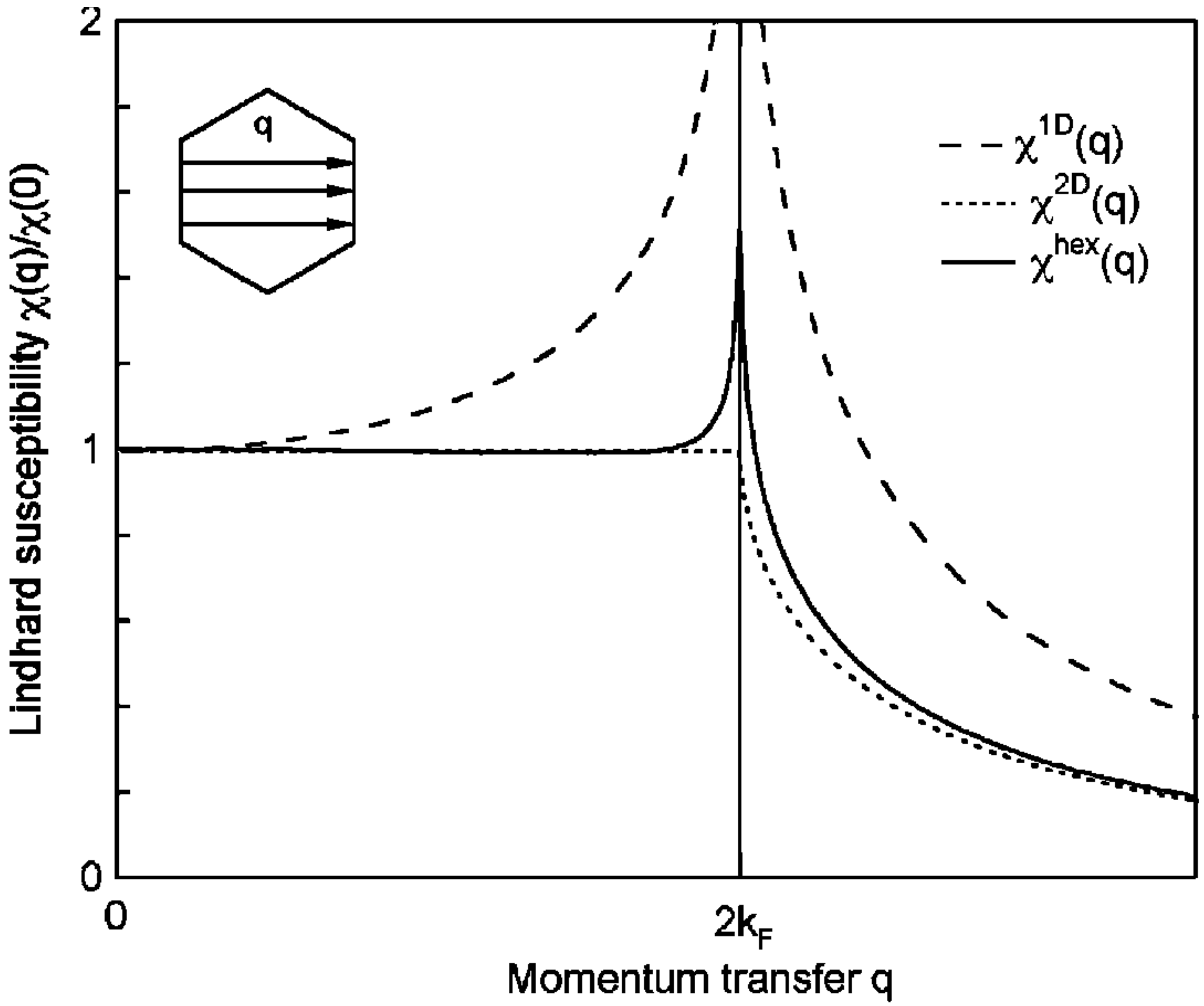
Fermi Surface
(photoemission intensity at E_F)

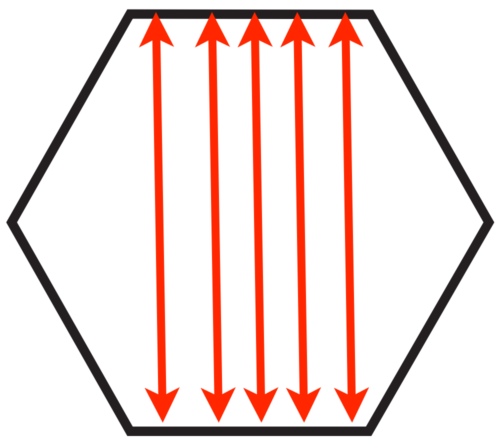


Ast and Höchst, PRL 90, 016403 (2003)

- A temperature-induced leading edge shift indicates a CDW formation caused by nesting.

There should not be a CDW



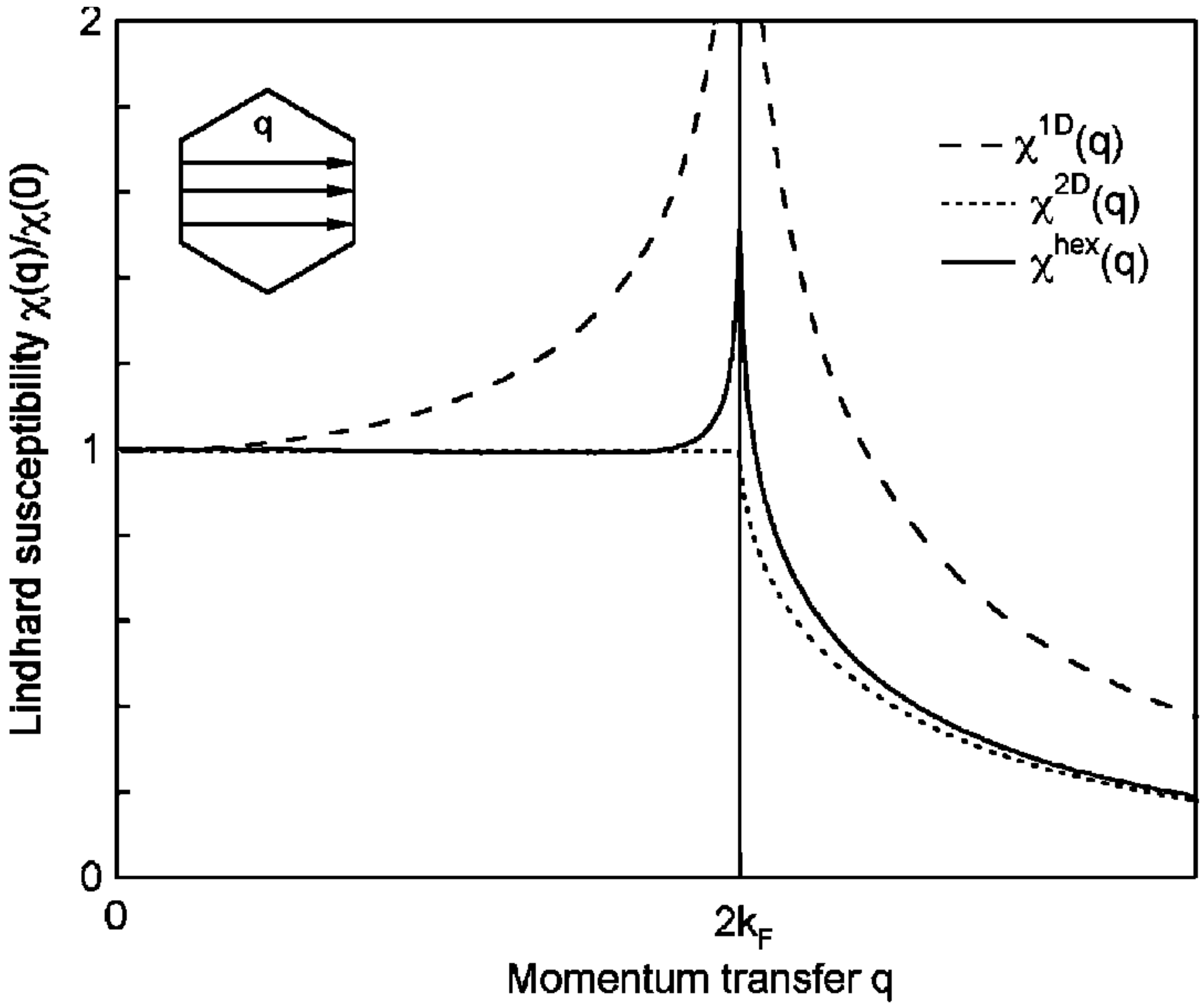


$$\chi(\vec{q}) = \int \frac{f(\vec{k}) - f(\vec{k}-\vec{q})d\vec{k}}{\epsilon(\vec{k}) - \epsilon(\vec{k}-\vec{q})(2\pi)^d}$$

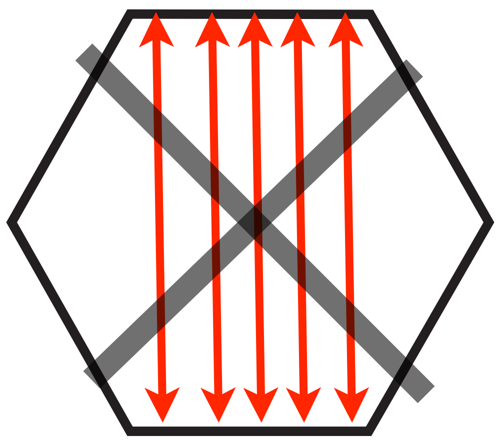
Ast and Höchst, PRL 90, 016403 (2003)

- for a spin-orbit spit Fermi surface, there should not be a singularity in the susceptibility.

There should not be a CDW



Ast and Höchst, PRL 90, 016403 (2003)

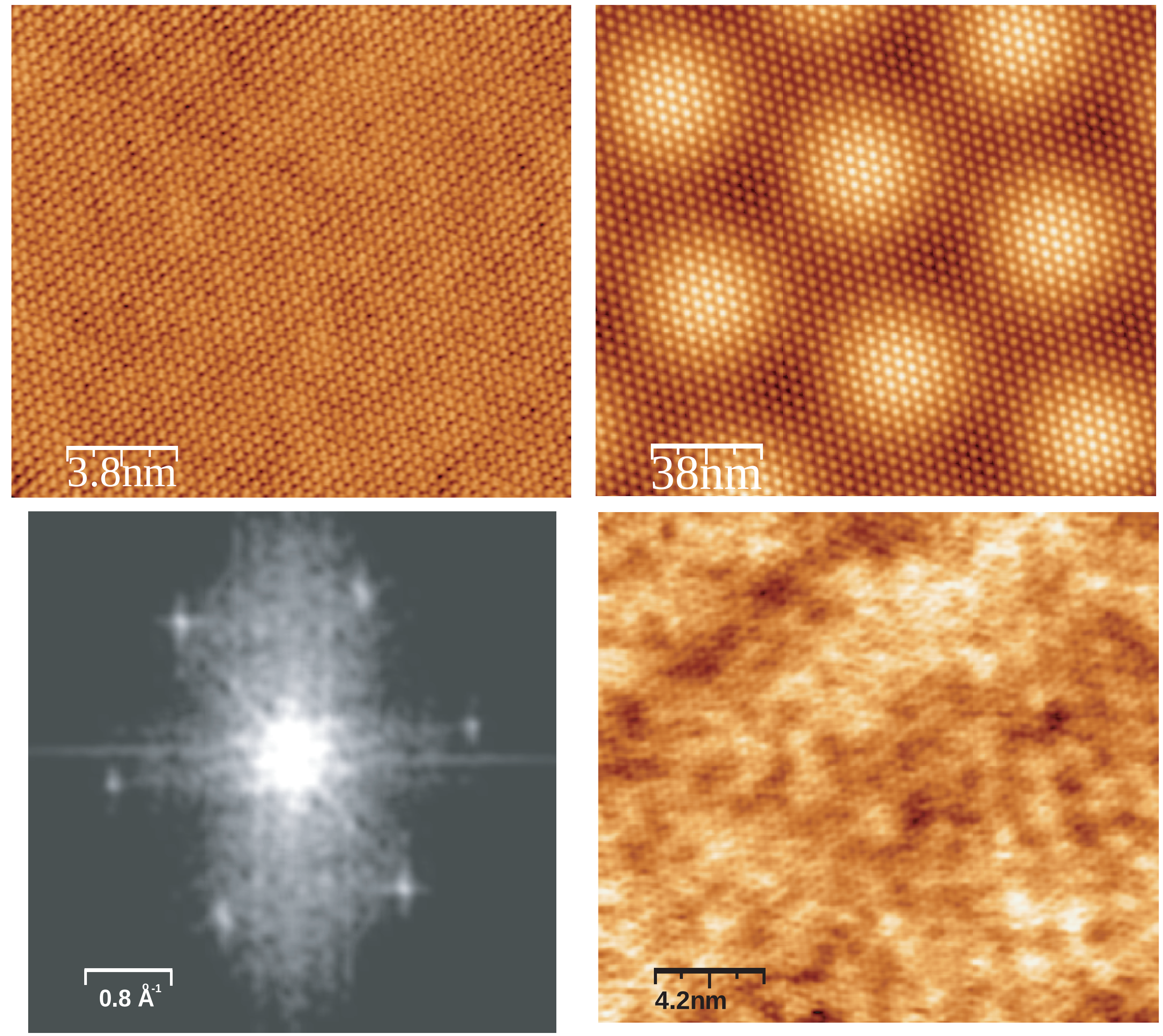


$$\chi(\vec{q}) = \int \frac{f(\vec{k}) - f(\vec{k} - \vec{q}) d\vec{k}}{\epsilon(\vec{k}) - \epsilon(\vec{k} - \vec{q})(2\pi)^d}$$

- for a spin-orbit spit Fermi surface, there should not be a singularity in the susceptibility.

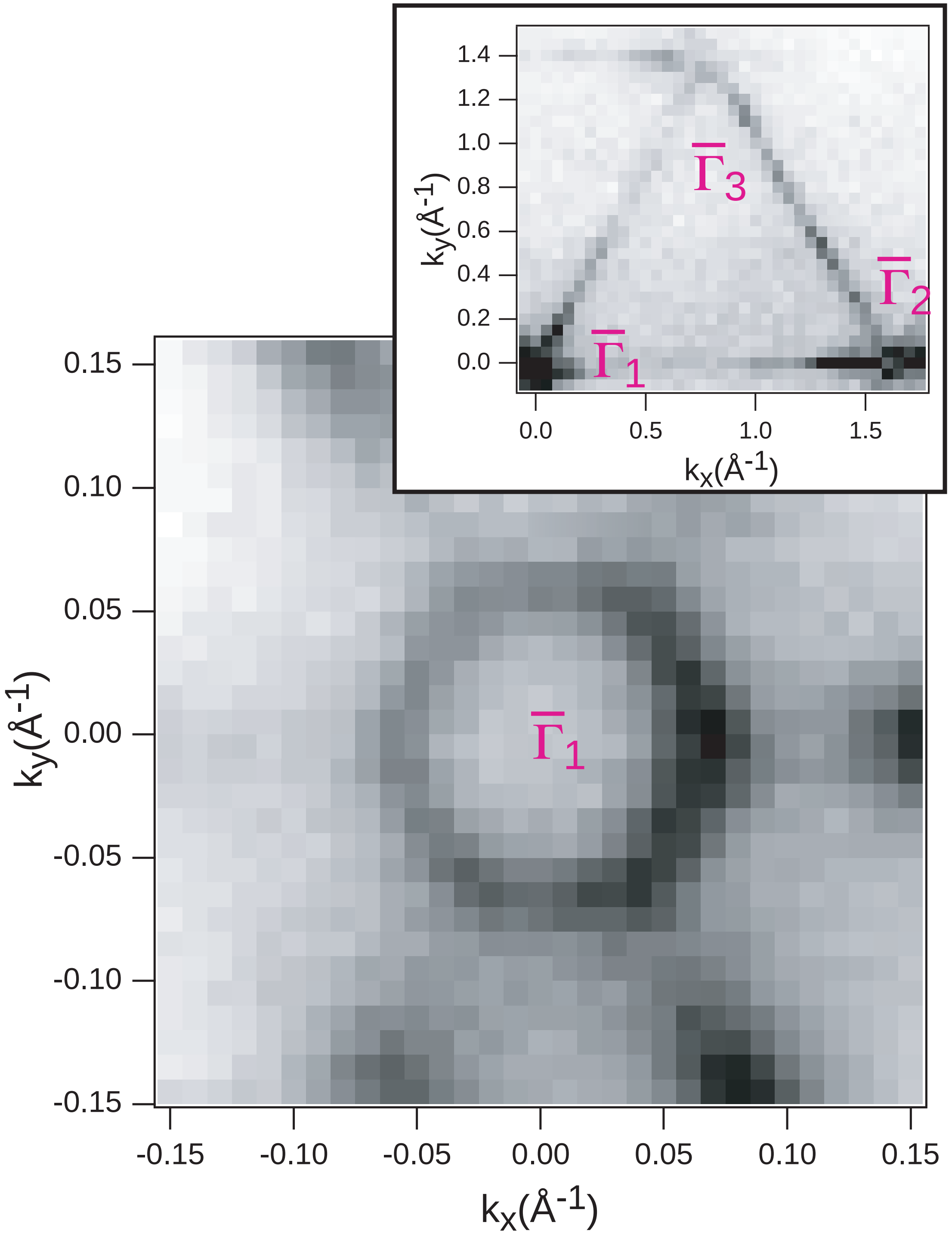
Is there a charge density wave on Bi(111)?

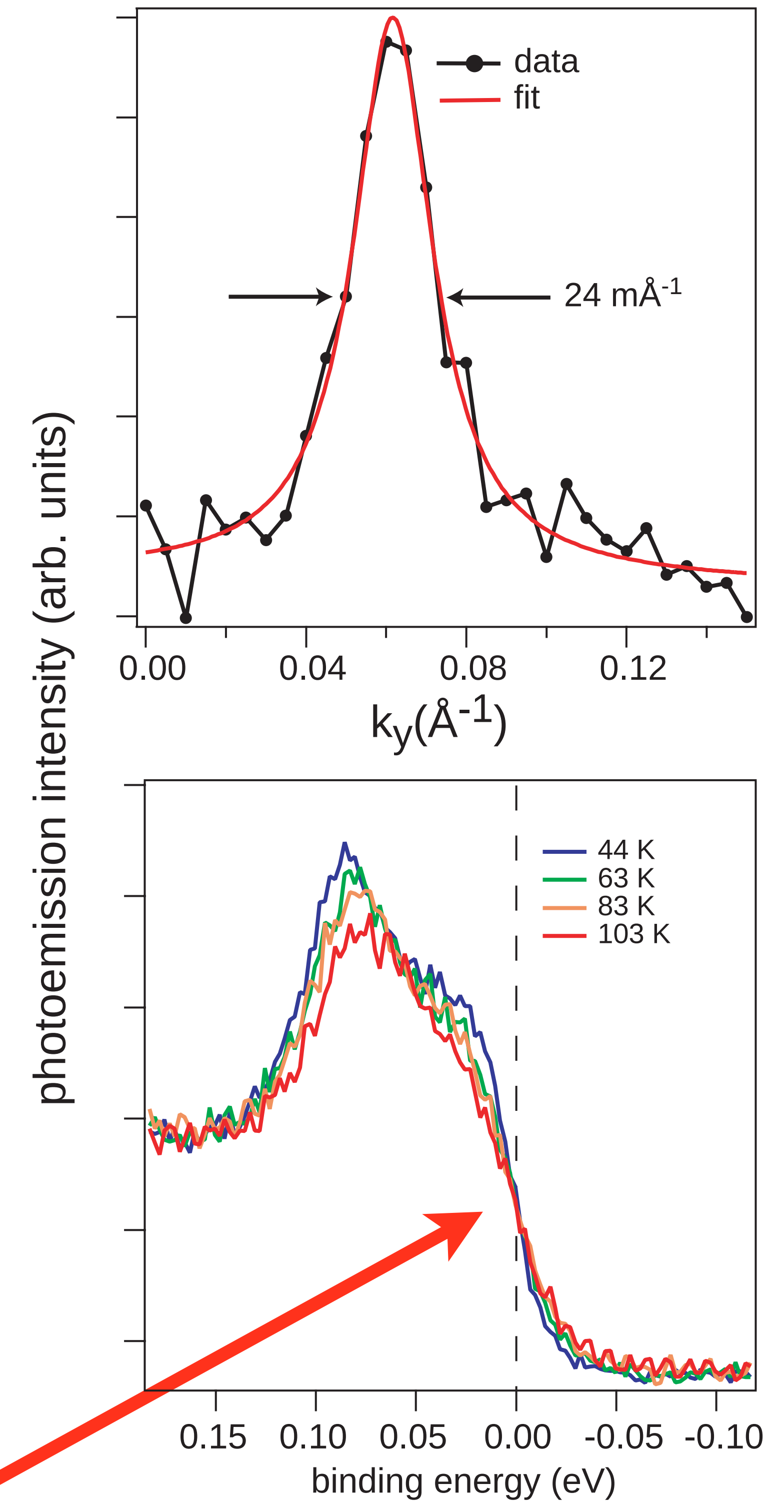
- STM does not show signs of a charge density wave.
- the observed structures are consistent with the picture of quasiparticle interference just developed.
- Transmission electron microscopy does not show a charge density wave either (not shown)



T. K. Kim, J. Wells, C. Kirkegaard, Z. Li, S. V. Hoffmann, J. E. Gayone, I. Fernandez-Torrente, P. Häberle, J. I. Pascual, K.T. Moore, A.J. Schwartz, H. He, J.C.H. Spence, K.H. Downing, S. Lazar, F.D. Tichelaar, S. V. Borisenko, M. Knupfer and Ph. Hofmann, Physical Review B **72**, 085440 (2005)

Is there a gap opening at low temperature?

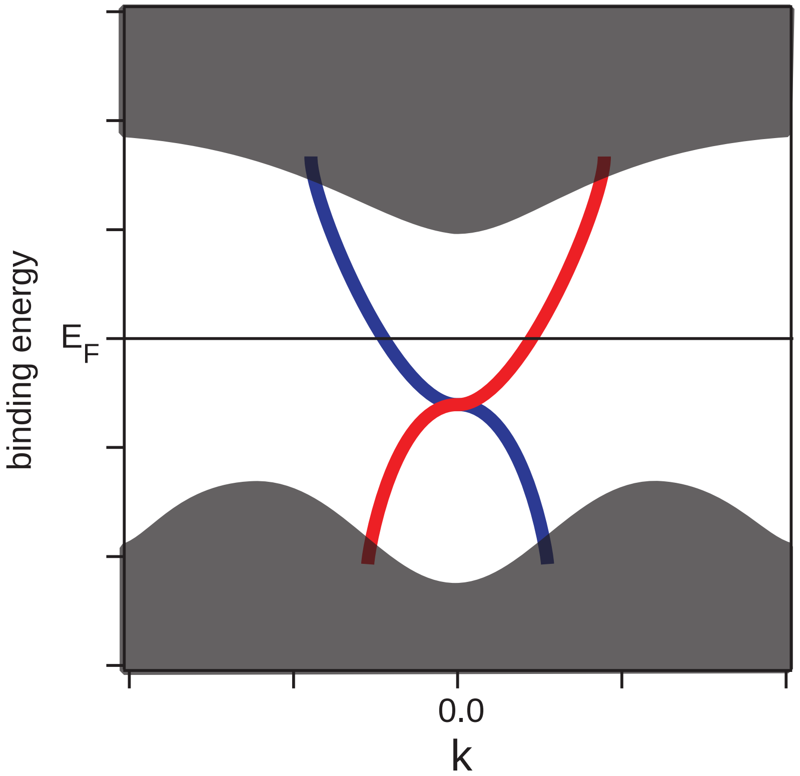


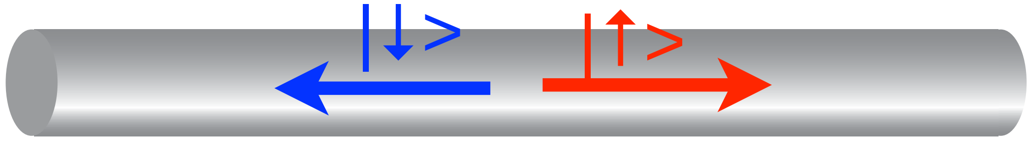


- no, there is not.

T. K. Kim, J. Wells, C. Kirkegaard, Z. Li, S. V. Hoffmann, J. E. Gayone, I. Fernandez-Torrente, P. Häberle, J. I. Pascual, K.T. Moore, A.J. Schwartz, H. He, J.C.H. Spence, K.H. Downing, S. Lazar, F.D. Tichelaar, S. V. Borisenko, M. Knupfer and Ph. Hofmann, Physical Review B **72**, 085440 (2005)

quantum spin Hall effect edge state





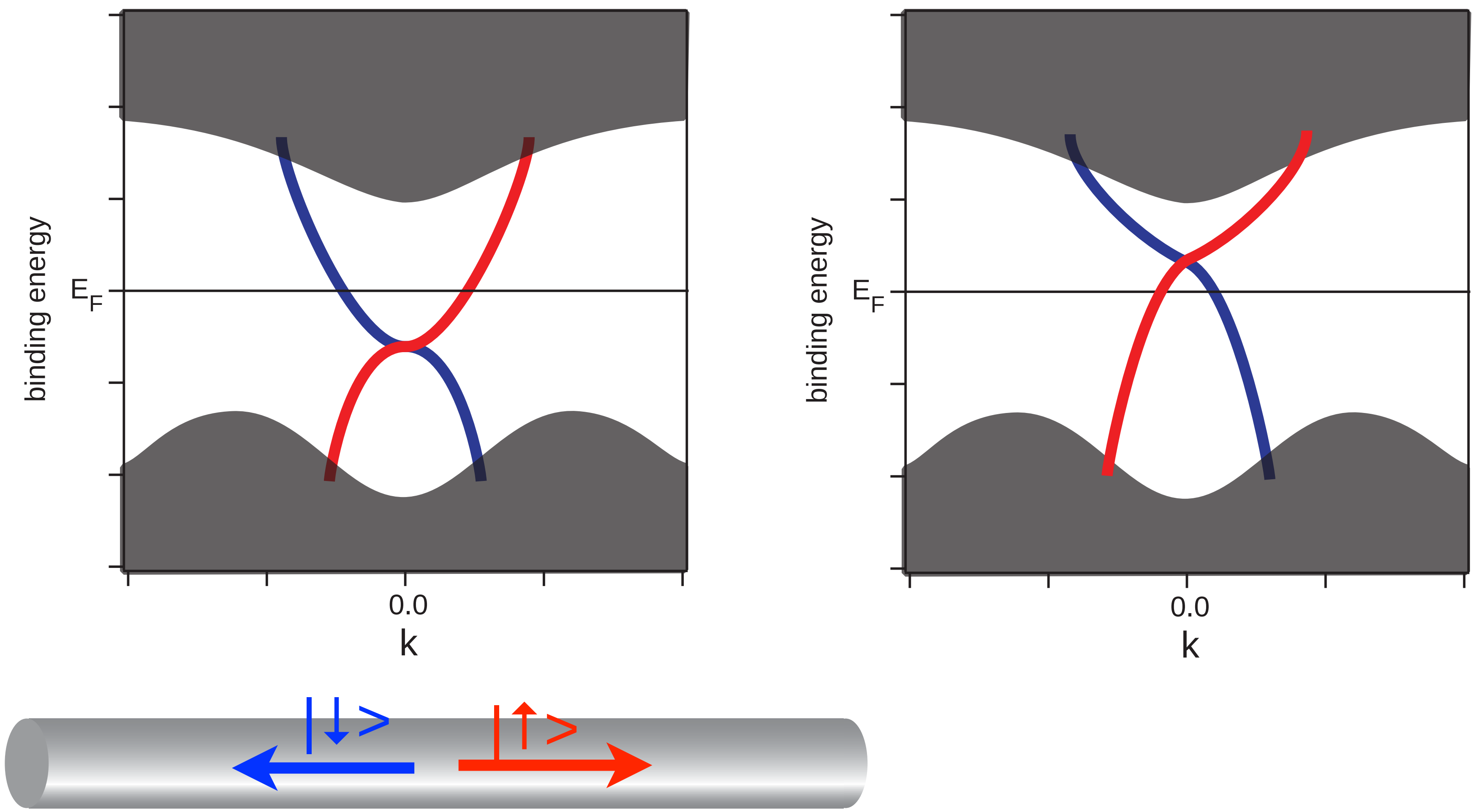
time-reversal symmetry:

$$\epsilon(\vec{k}, \uparrow) = \epsilon(-\vec{k}, \downarrow)$$

at k=0

$$\epsilon(\vec{k}_{\parallel} = 0, \uparrow) = \epsilon(-\vec{k}_{\parallel} = 0, \downarrow)$$

quantum spin Hall effect edge state



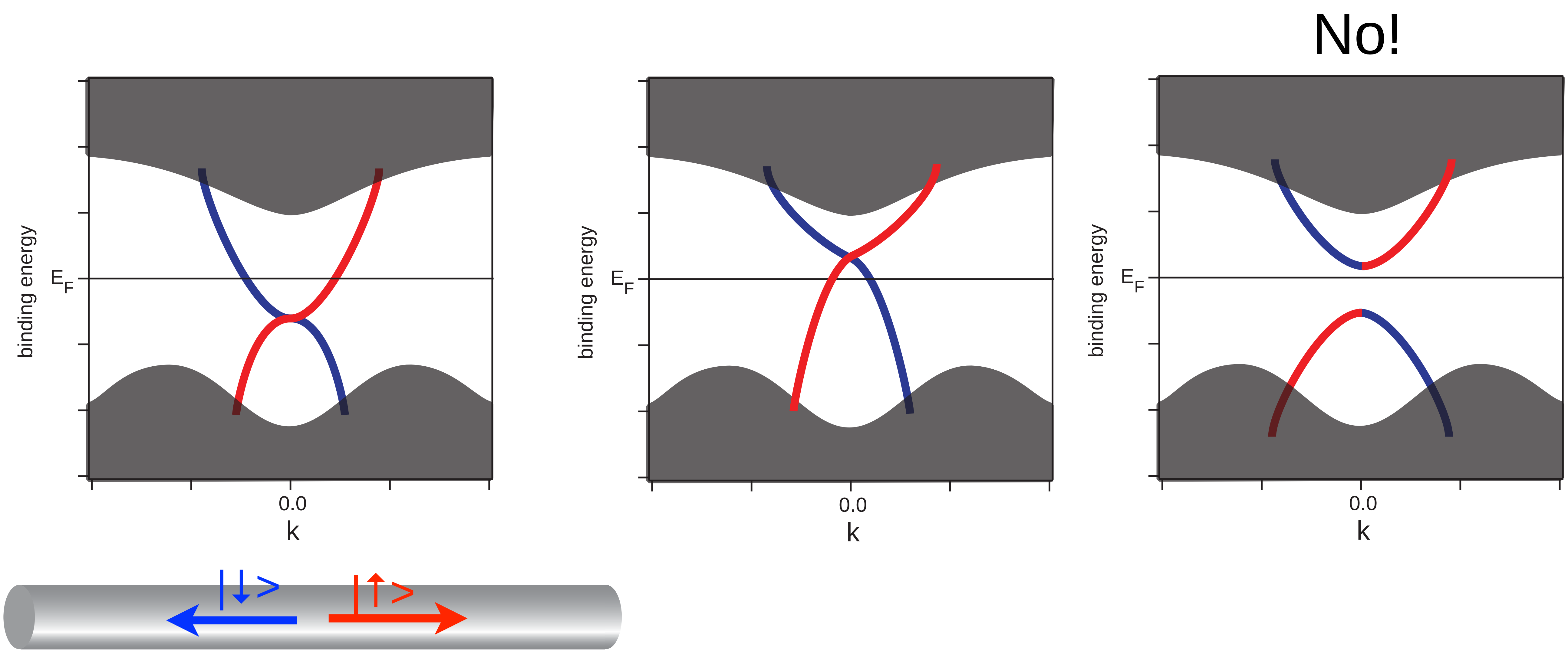
time-reversal symmetry:

$$\epsilon(\vec{k}, \uparrow) = \epsilon(-\vec{k}, \downarrow)$$

at k=0

$$\epsilon(\vec{k}_{\parallel} = 0, \uparrow) = \epsilon(-\vec{k}_{\parallel} = 0, \downarrow)$$

quantum spin Hall effect edge state



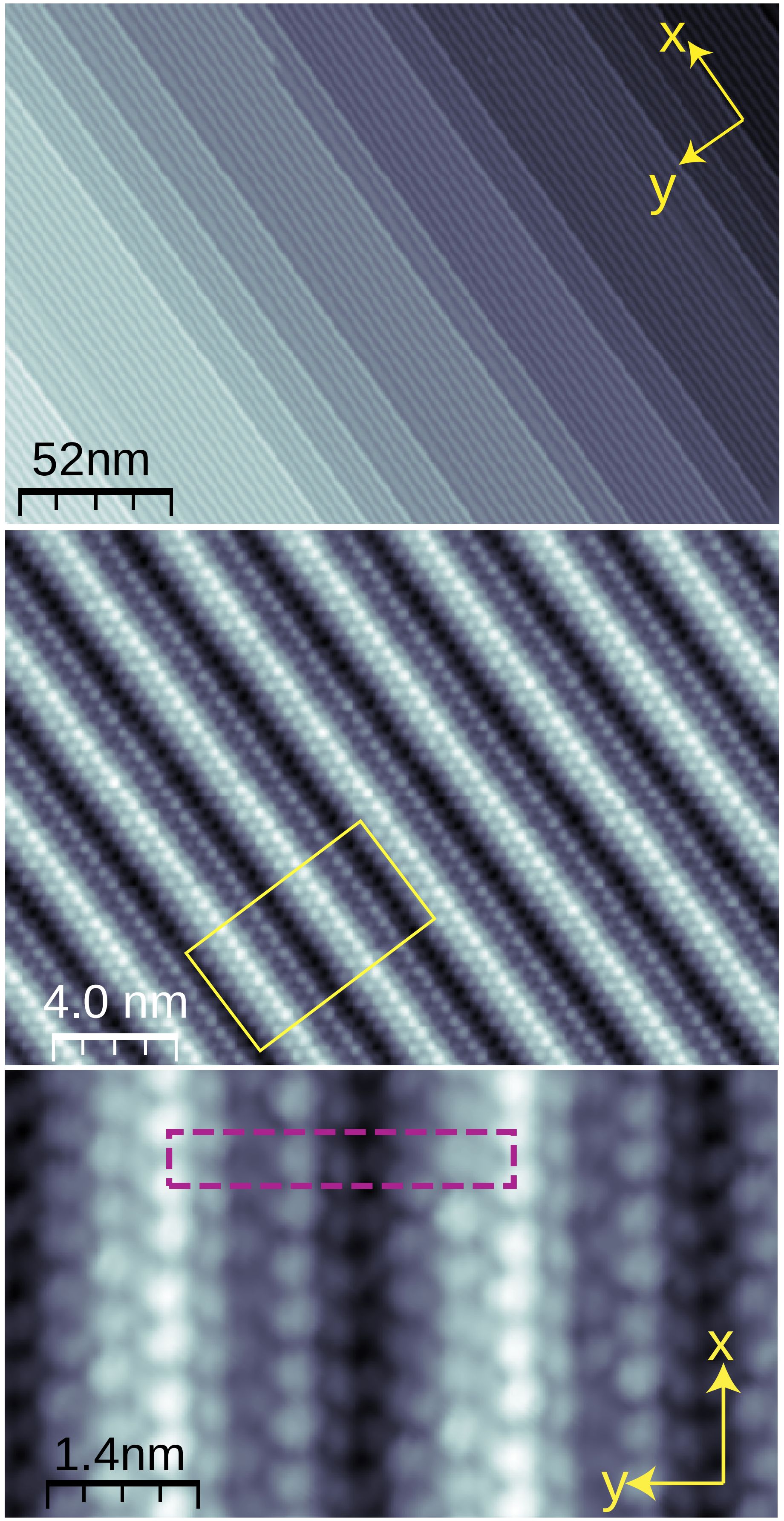
time-reversal symmetry:

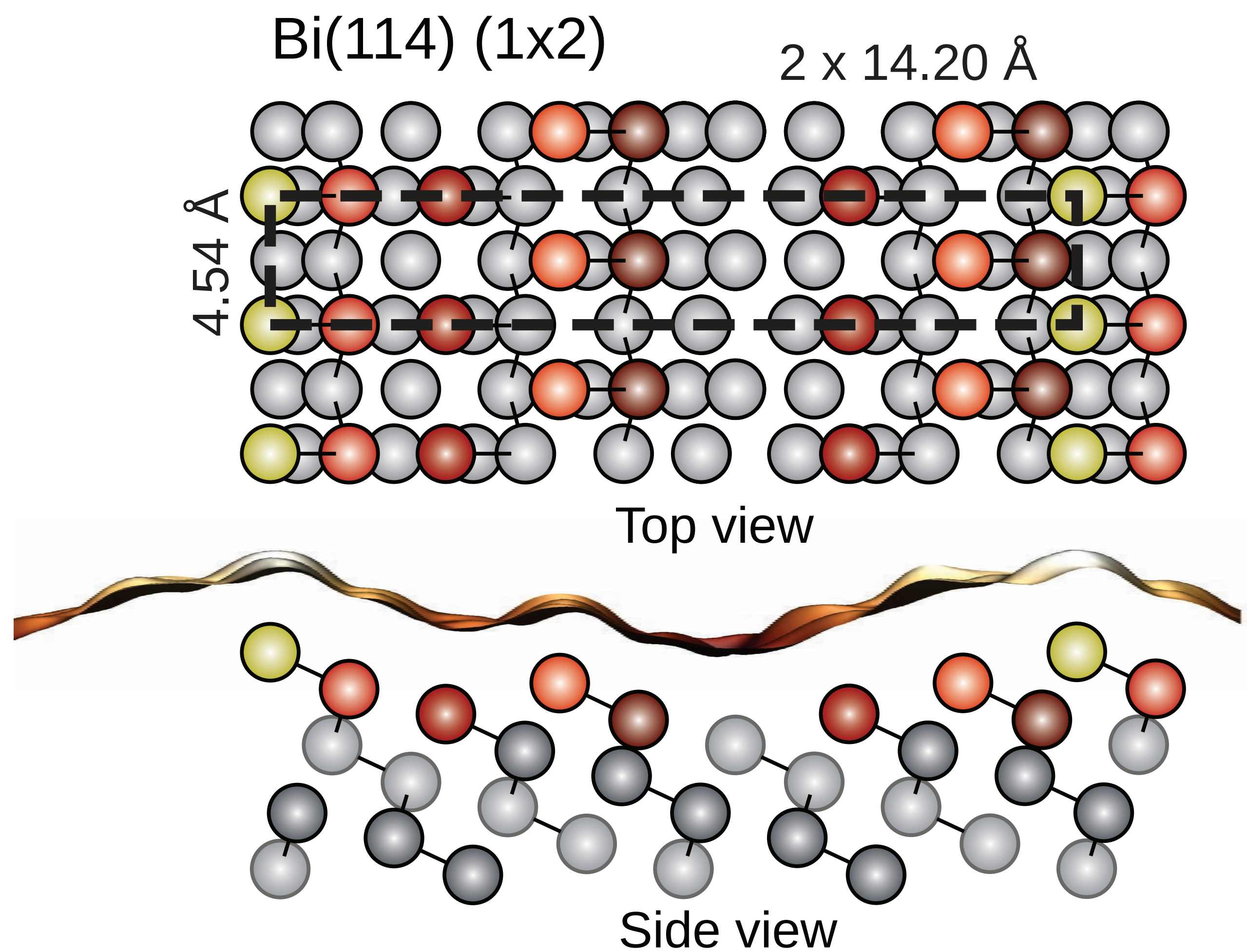
$$\epsilon(\vec{k}, \uparrow) = \epsilon(-\vec{k}, \downarrow)$$

at k=0

$$\epsilon(\vec{k}_{\parallel} = 0, \uparrow) = \epsilon(-\vec{k}_{\parallel} = 0, \downarrow)$$

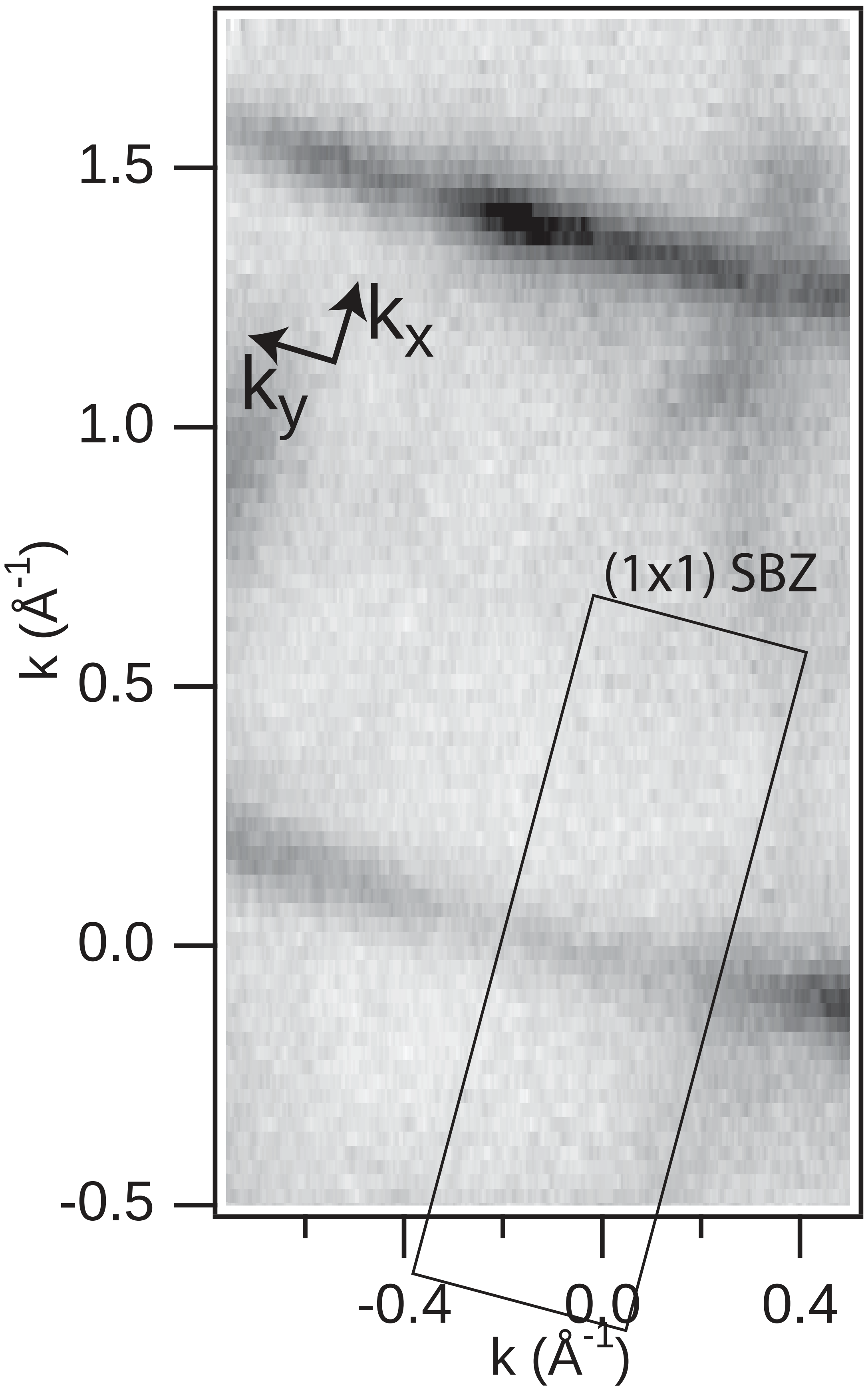
a highly one-dimensional surface: Bi(114)





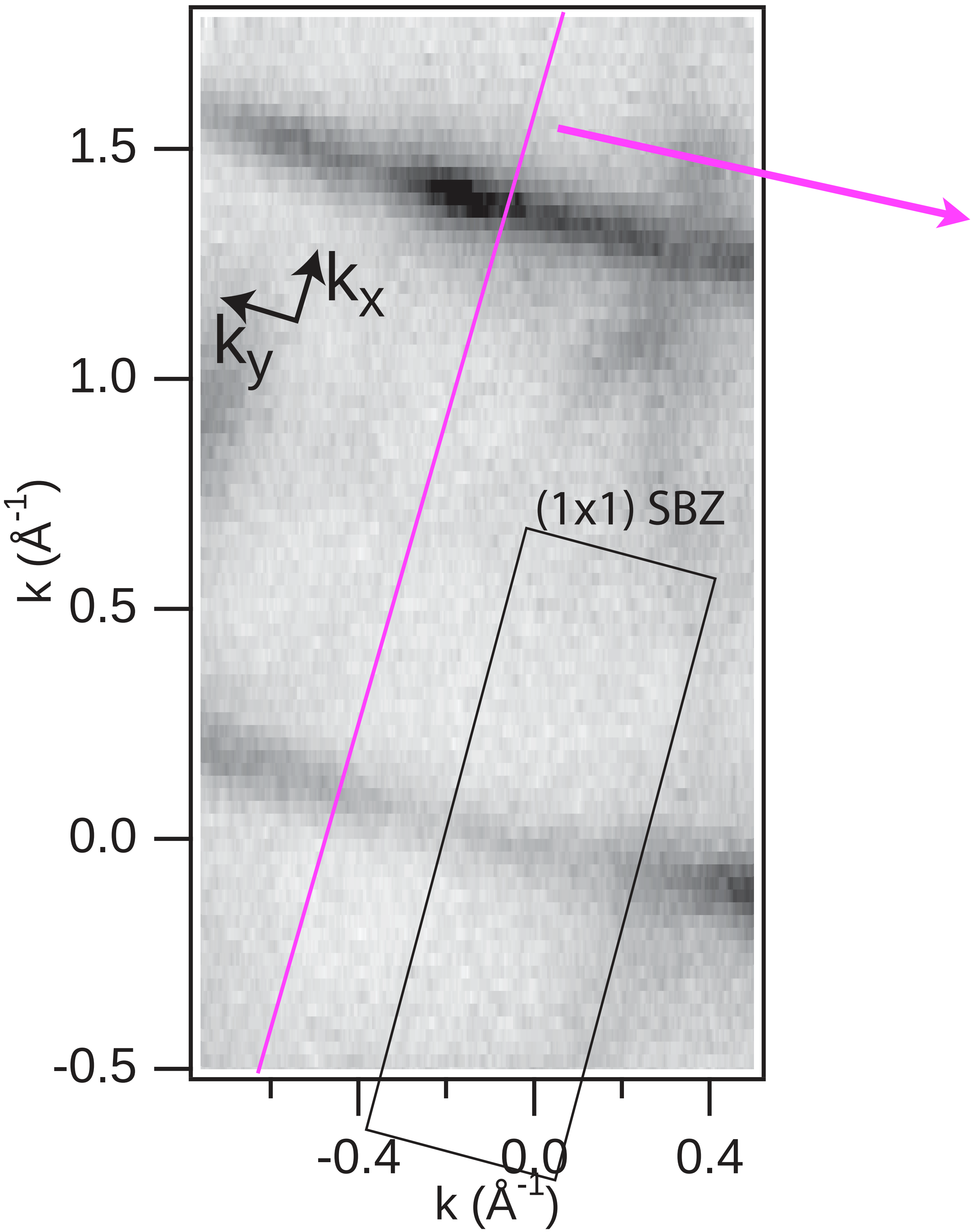
J. Wells et al., PRL **101**, 096802 (2009).

electronic structure of Bi(114)



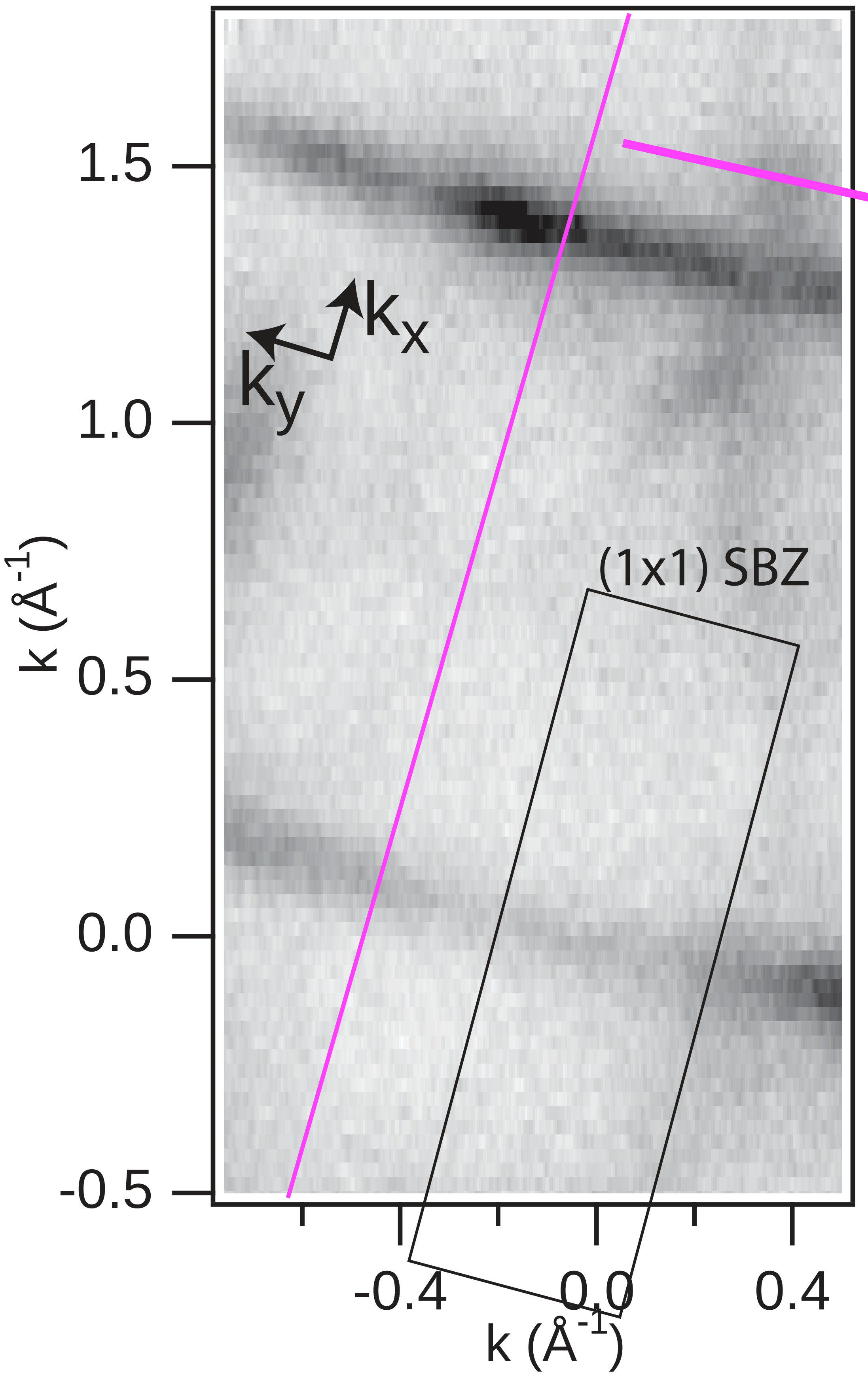
J. Wells et al., PRL **101**, 096802 (2009).

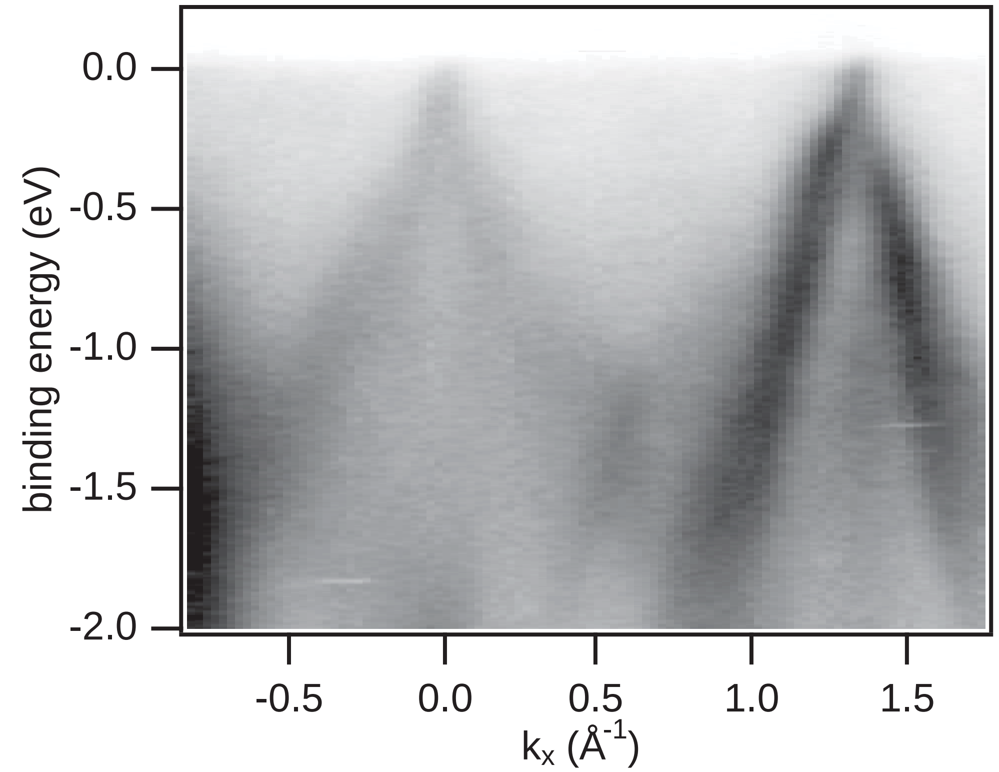
electronic structure of Bi(114)



J. Wells et al., PRL **101**, 096802 (2009).

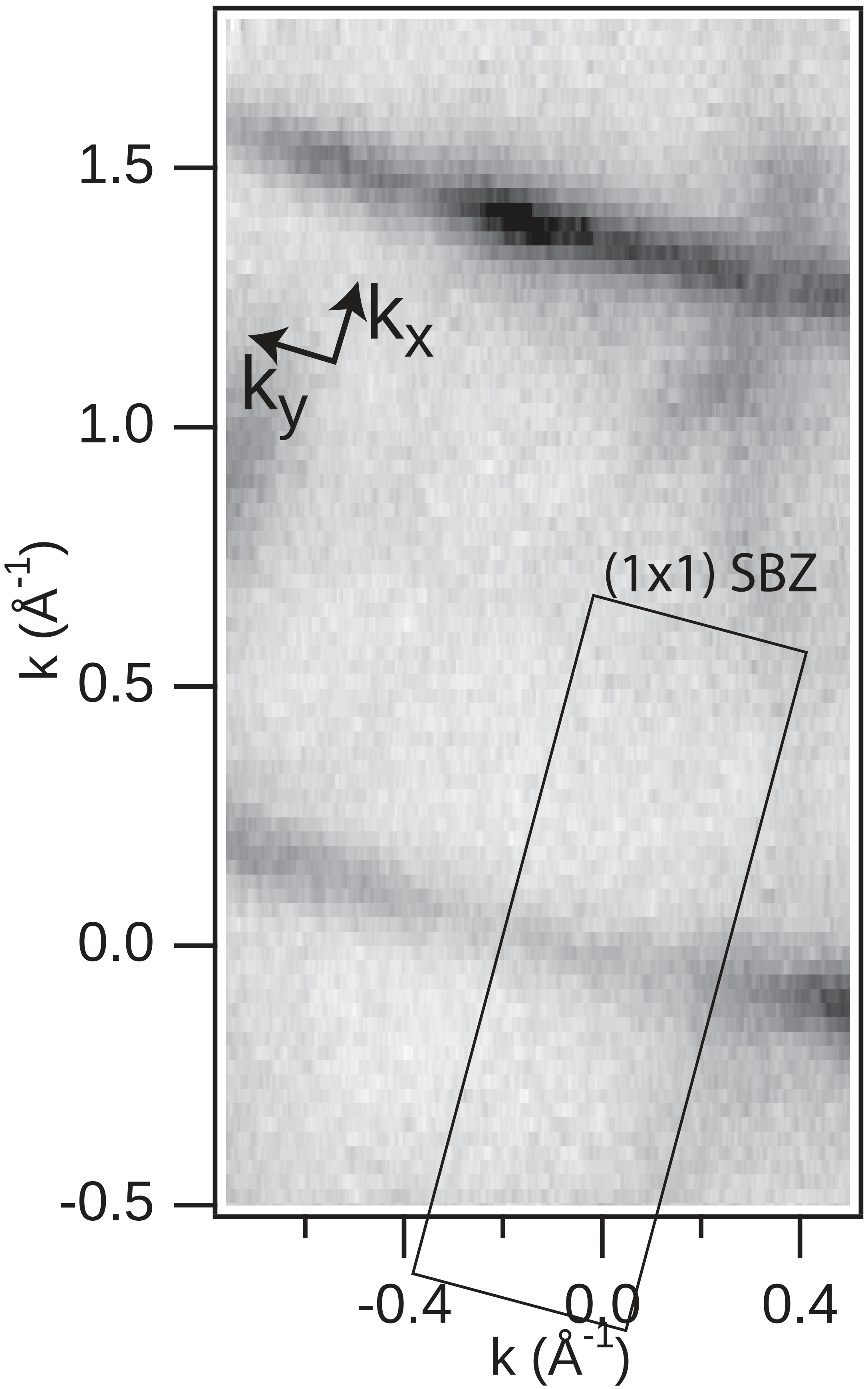
electronic structure of Bi(114)

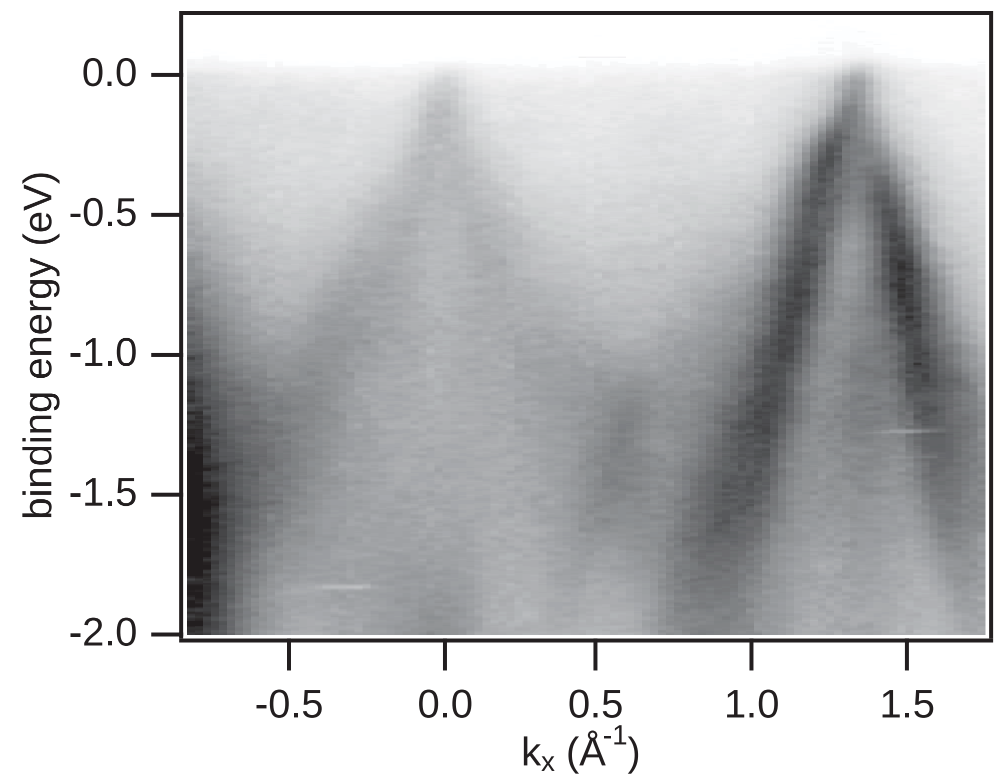




J. Wells et al., PRL **101**, 096802 (2009).

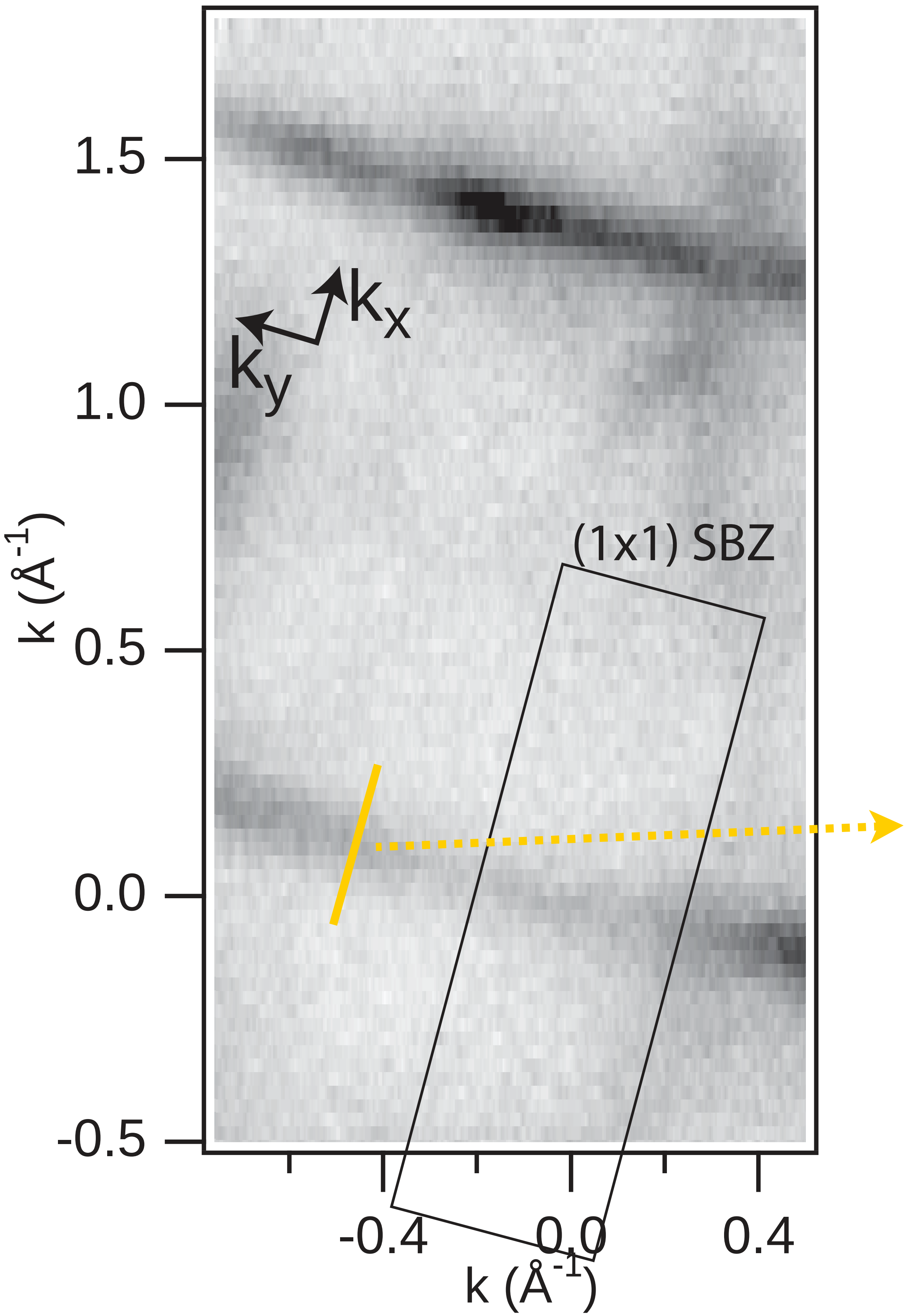
electronic structure of Bi(114)

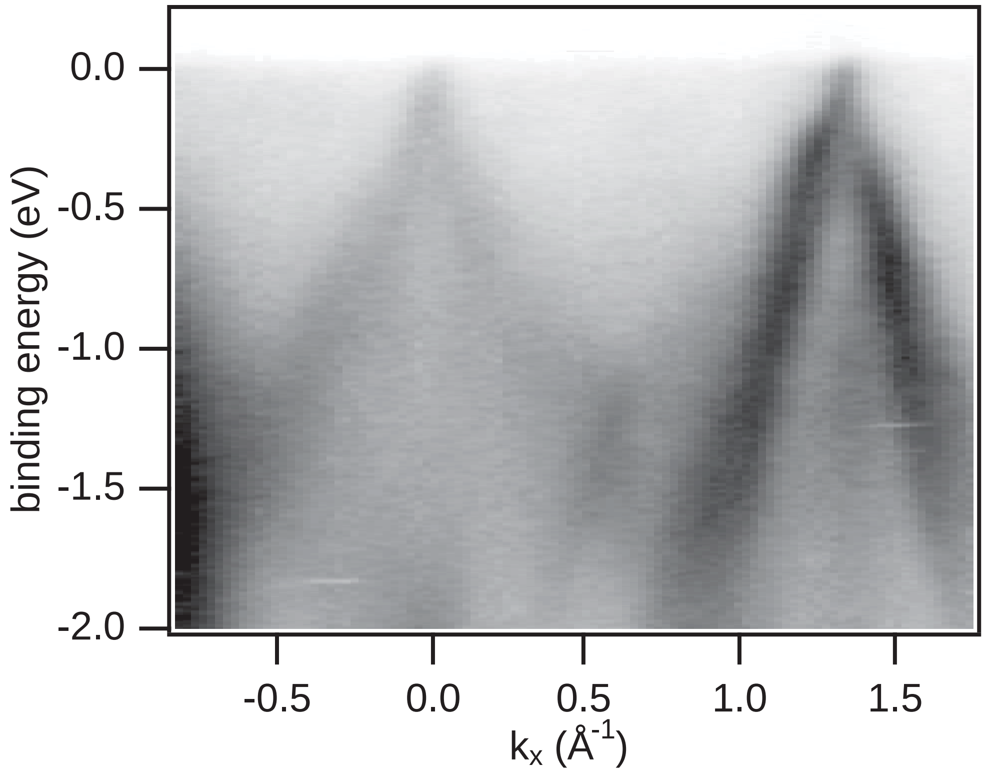




J. Wells et al., PRL **101**, 096802 (2009).

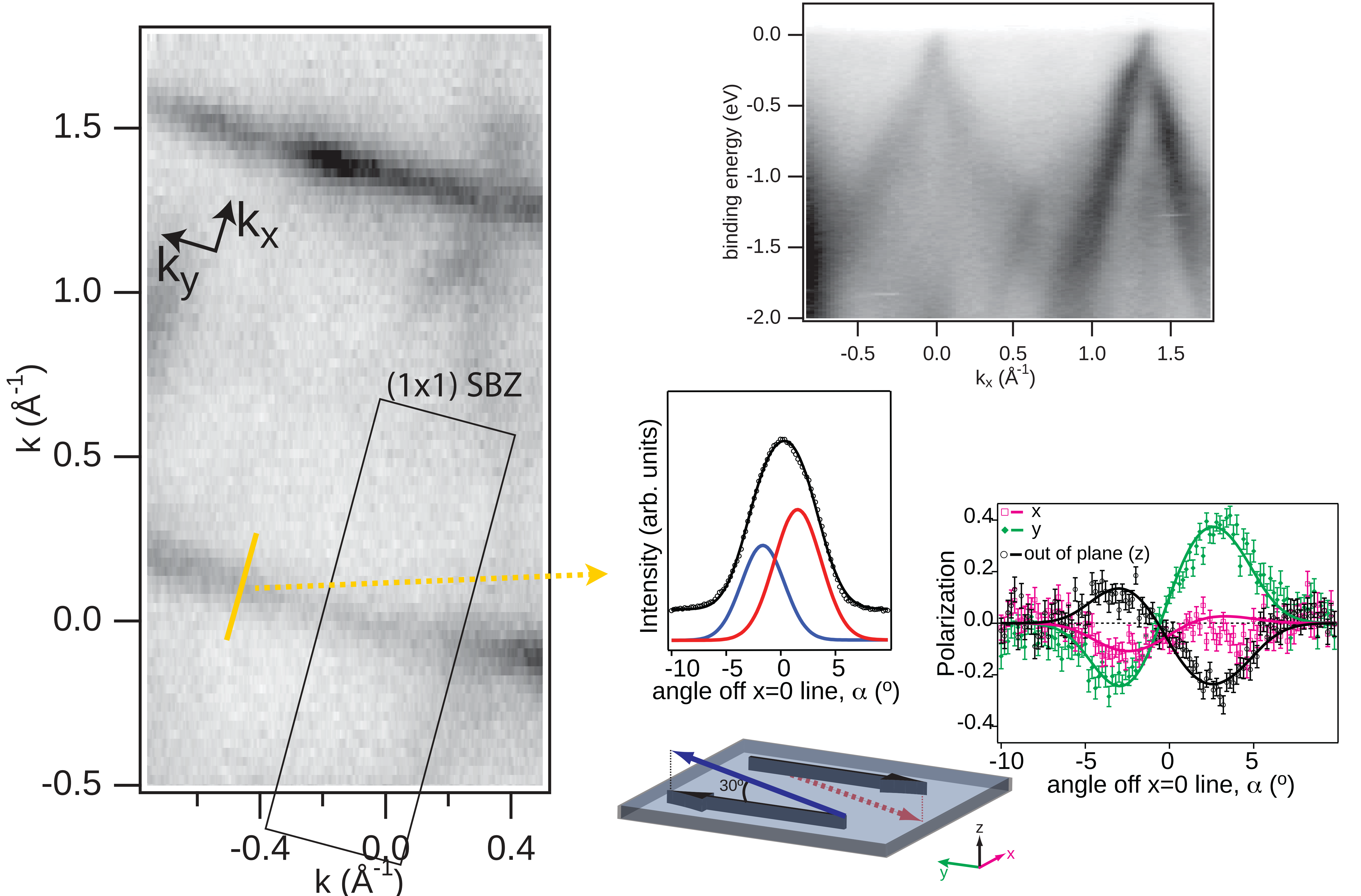
electronic structure of Bi(114)





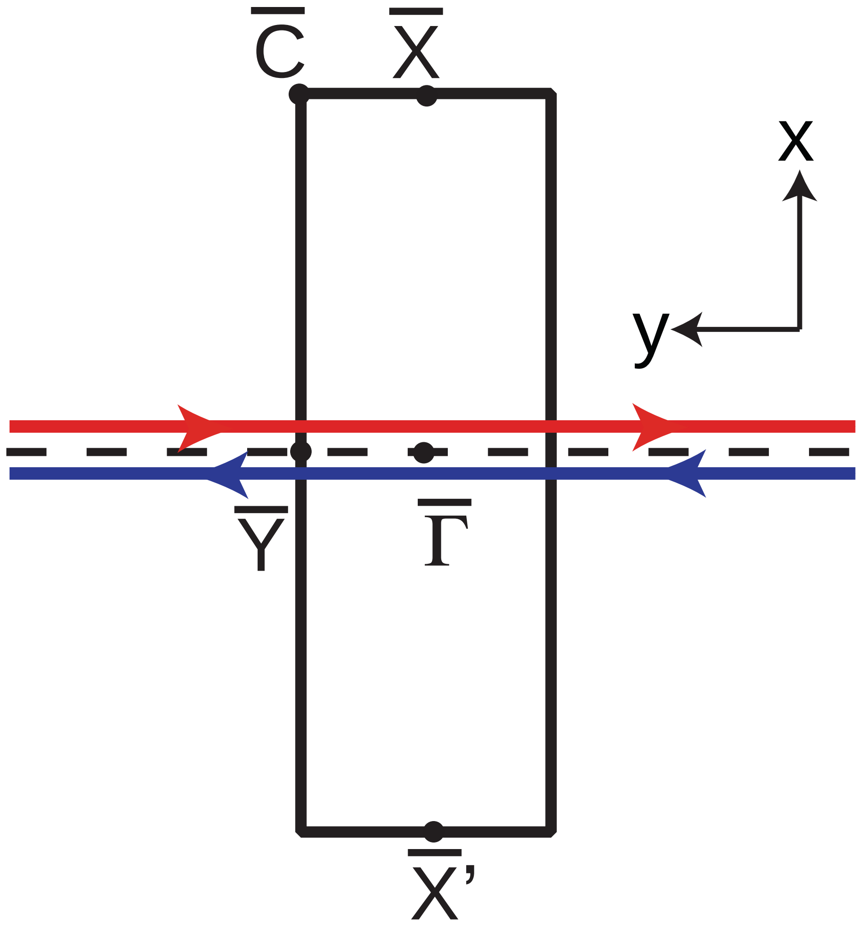
J. Wells et al., PRL **101**, 096802 (2009).

electronic structure of Bi(114)



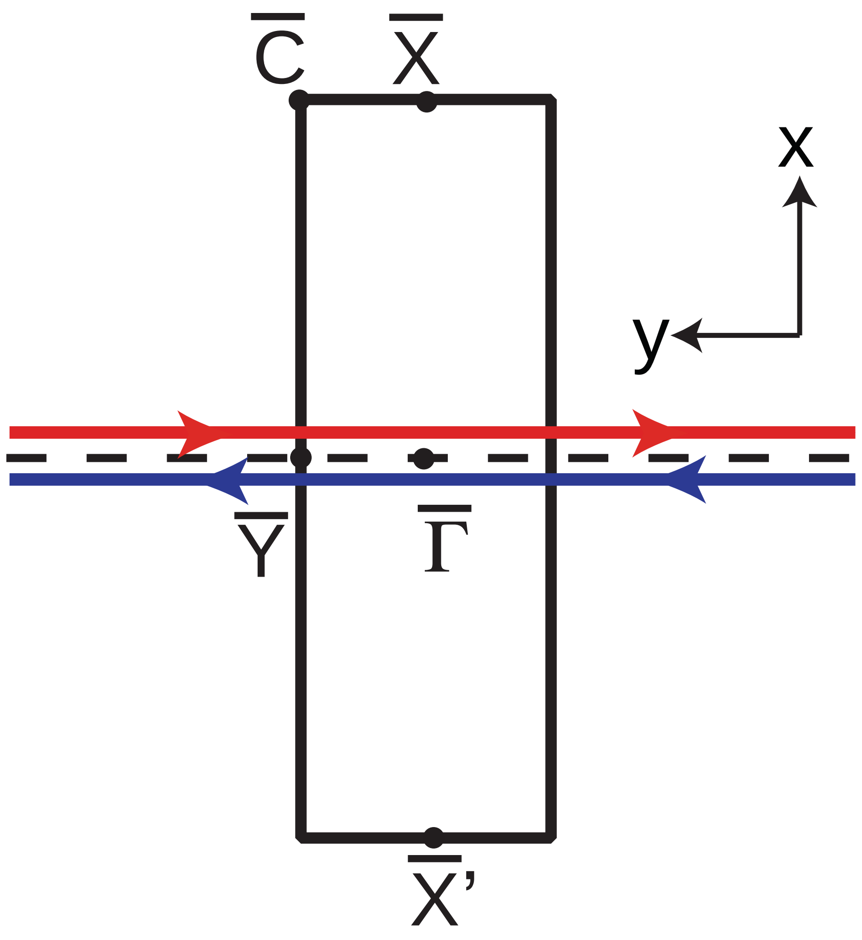
J. Wells et al., PRL **101**, 096802 (2009).

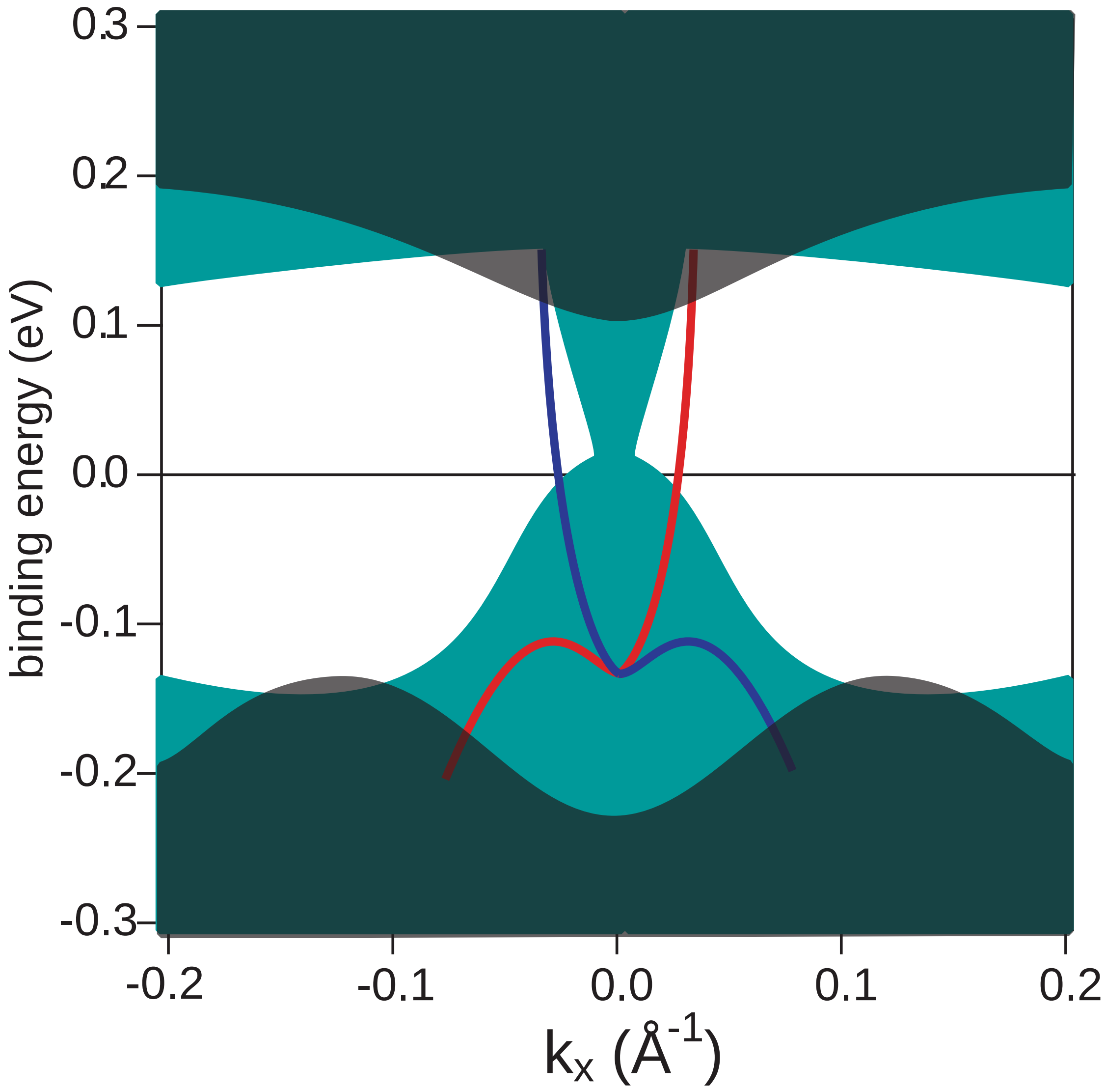
electronic structure of Bi(114) - simplified



J. Wells et al., PRL **101**, 096802 (2009).

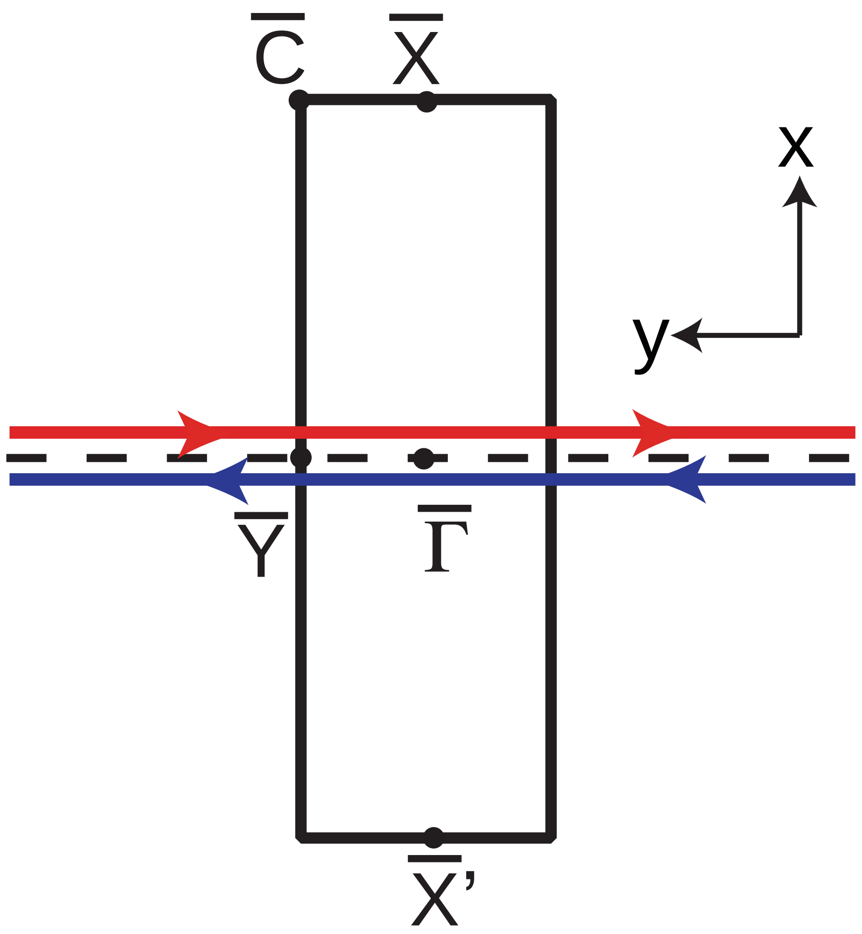
electronic structure of Bi(114) - simplified

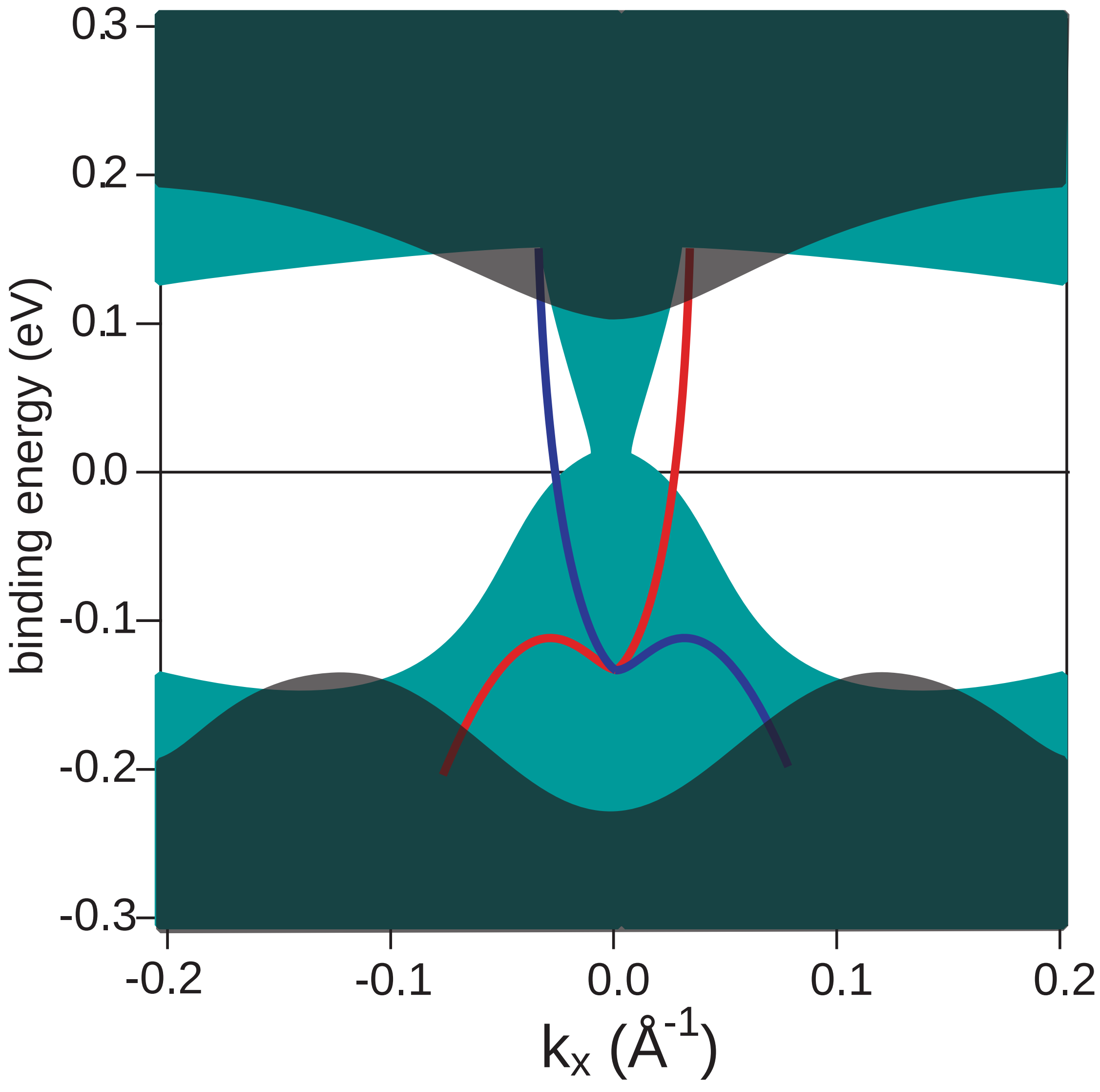


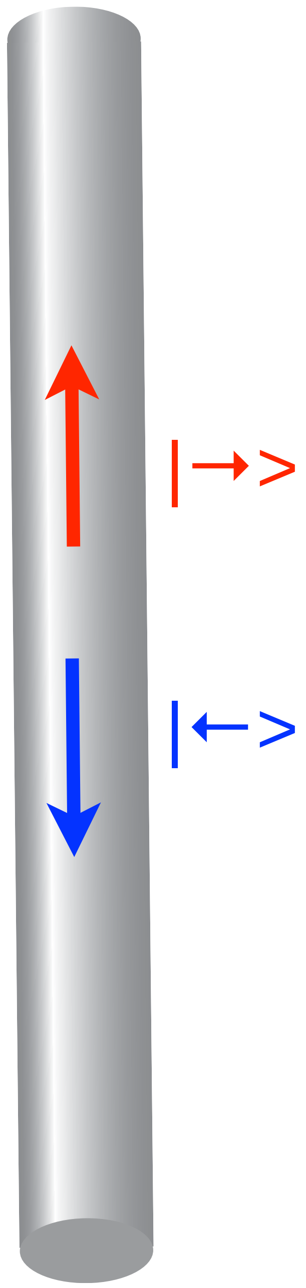


J. Wells et al., PRL **101**, 096802 (2009).

electronic structure of Bi(114) - simplified







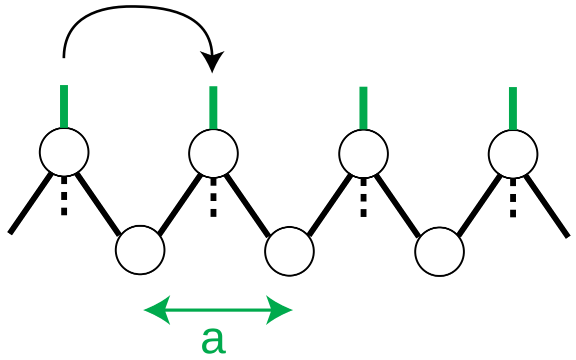
J. Wells et al., PRL **101**, 096802 (2009).

some conclusions

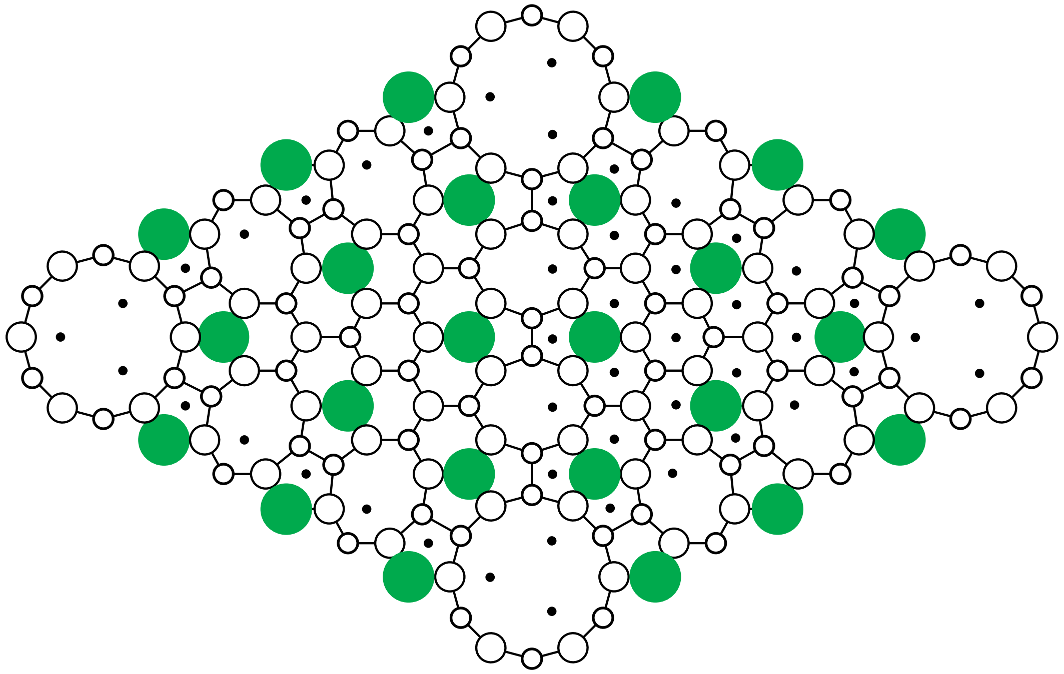
- The surfaces of Bi are good metals, even the (111) surface for which no bonds are broken.
- The reason is the symmetry-loss and the strong spin-orbit splitting.
- The peculiar spin structure leads to unusual standing electron waves and prevents charge density waves.
- In the one-dimensional case there is great similarity to the quantum spin Hall effect.

Ph. Hofmann, Surf. Sci. Rep. **81**, 191 (2006)

semiconductor surfaces:
2D metal -> Mott insulator

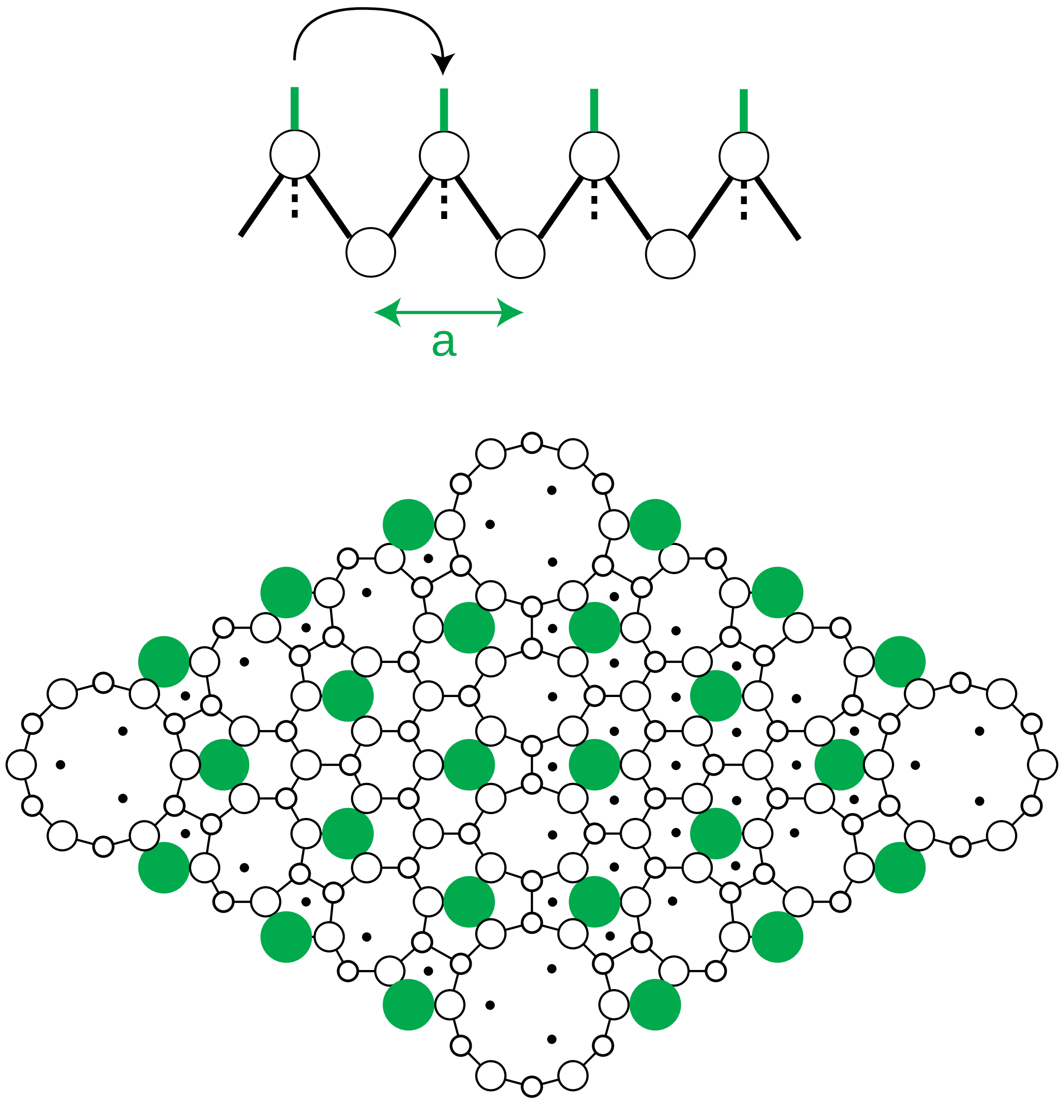


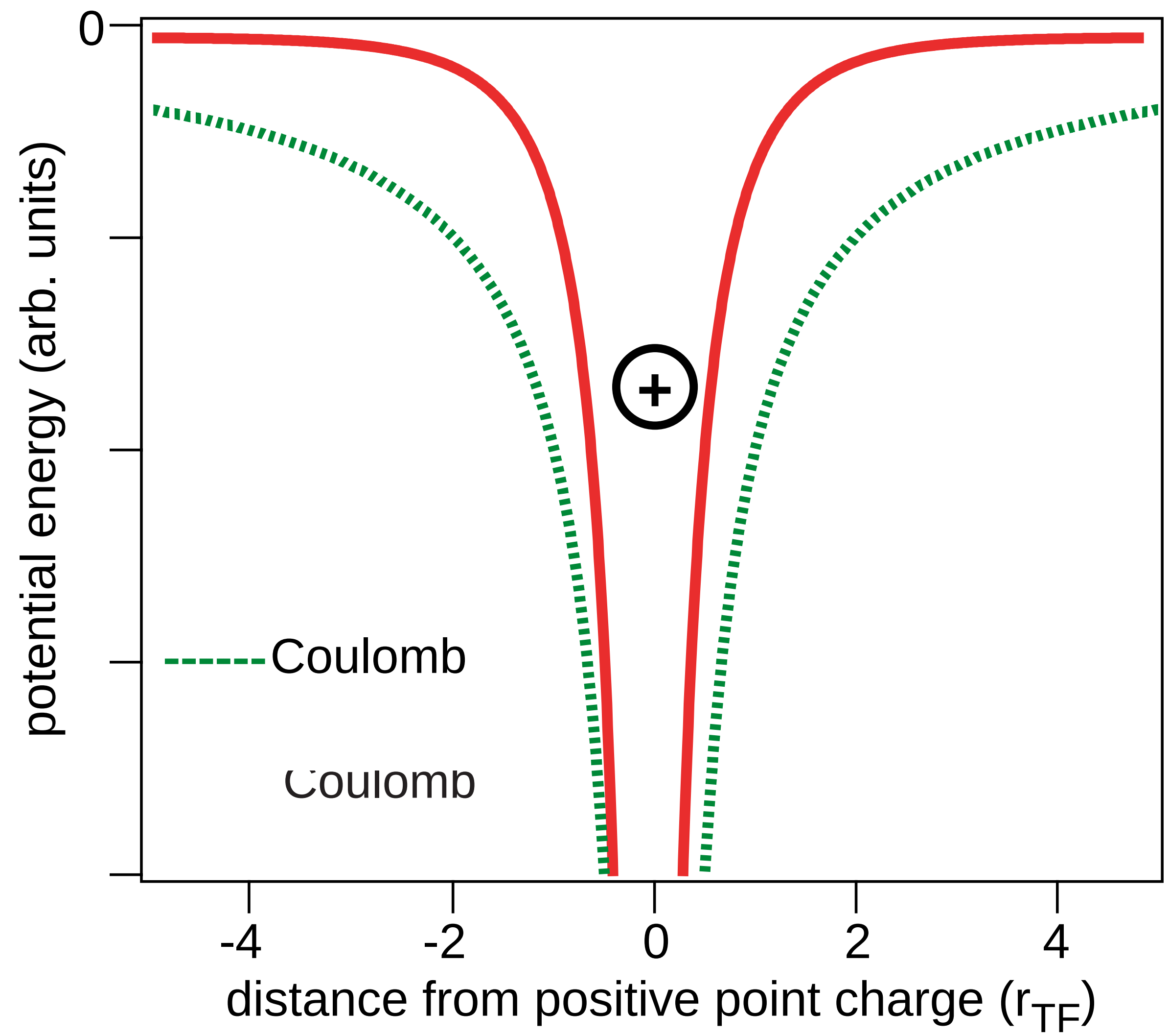
top view



semiconductor surfaces:
2D metal -> Mott insulator

top view

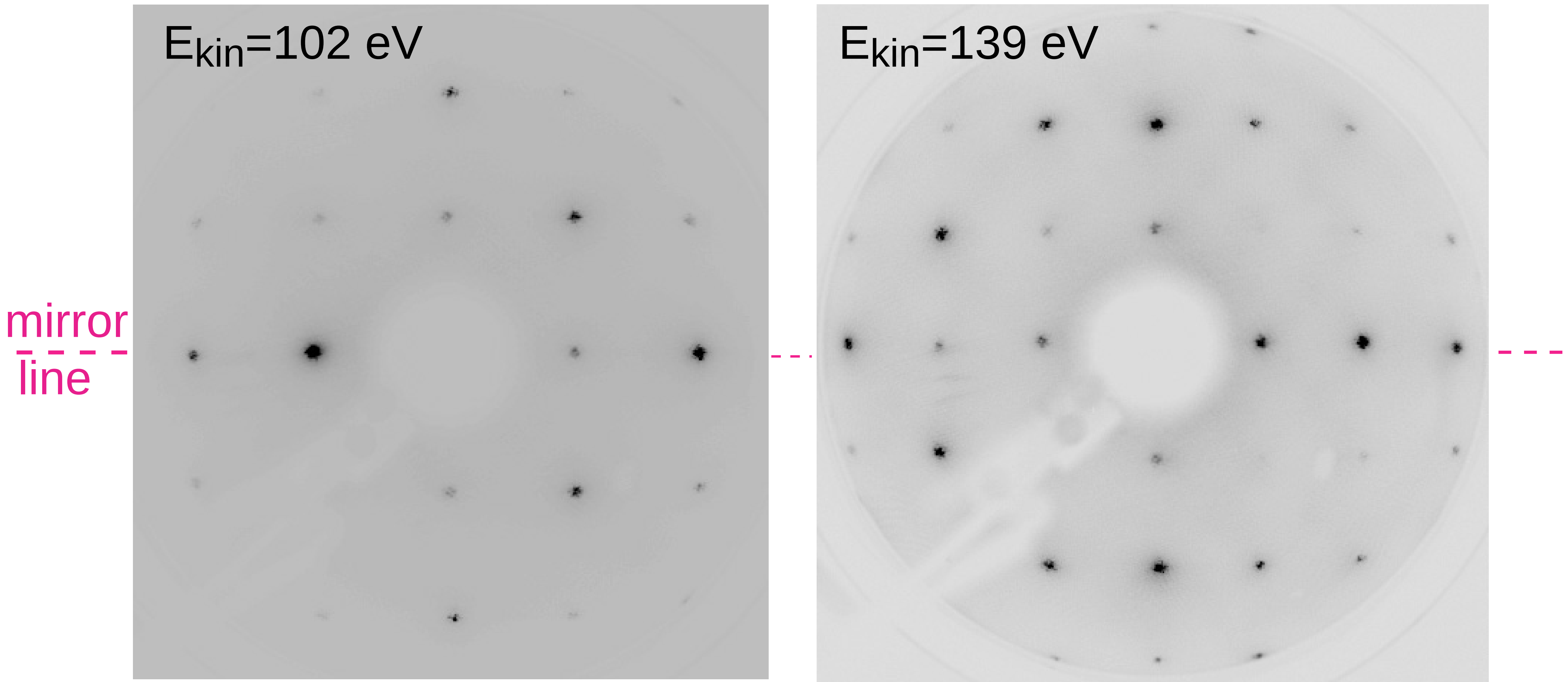




positive point charge in a metal

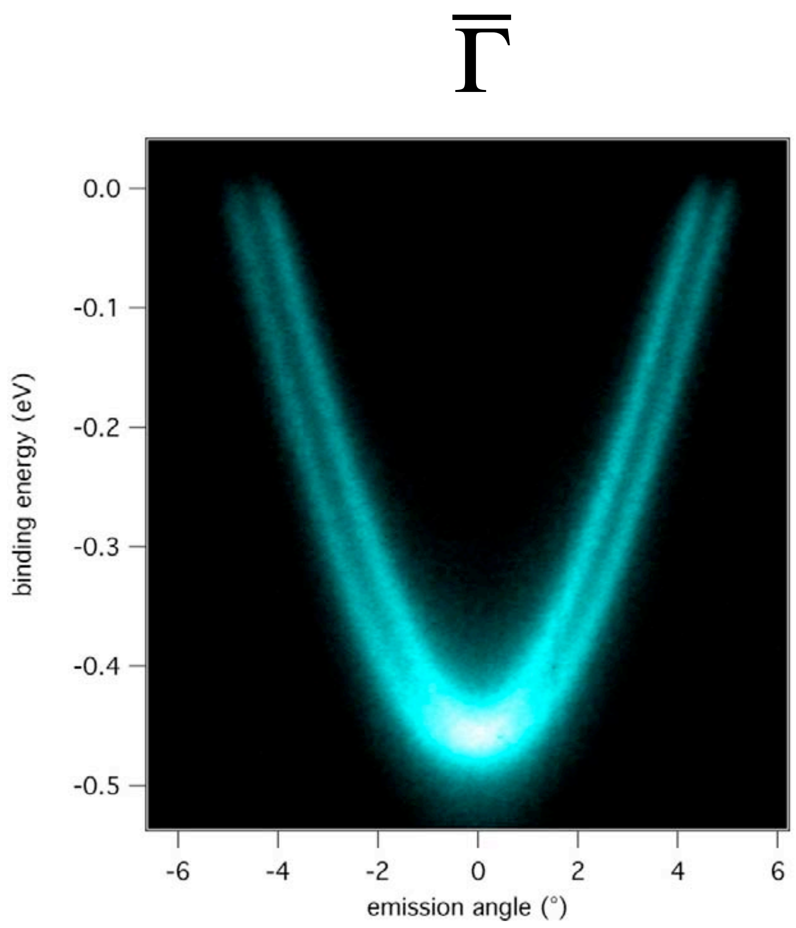
$$\phi(r) = \frac{1}{4\pi\epsilon_0}\frac{q}{r}e^{-r/r_{\mathrm{TF}}} \qquad r_{\mathrm{TF}} \propto n^{-\frac{1}{6}}$$

Bi(110): LEED pattern

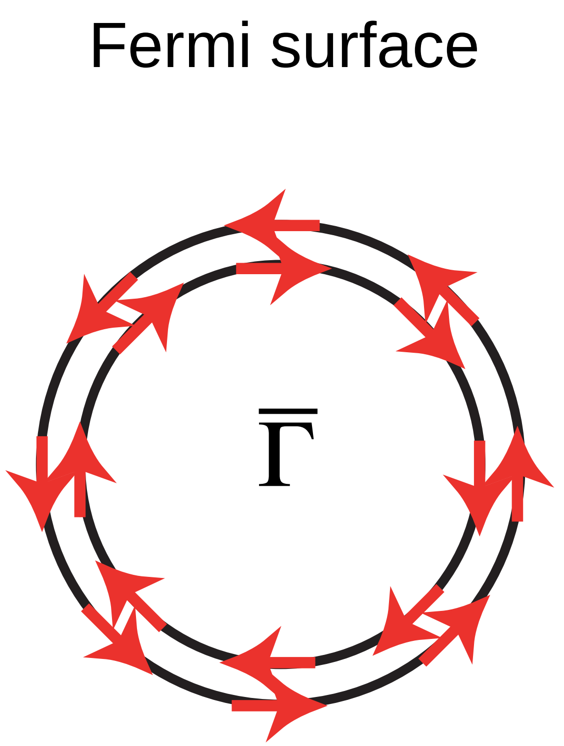


- The LEED pattern is (nearly) a square but there is only one mirror line.

Spin-orbit splitting of surface states



S. LaShell, B.A. McDougall and E. Jensen, PRL **77**, 3419 (1996)
(actual data from SGM-3 at ASTRID in Aarhus)



time reversal symmetry:

$$\epsilon(\vec{k},\uparrow) = \epsilon(-\vec{k},\downarrow)$$

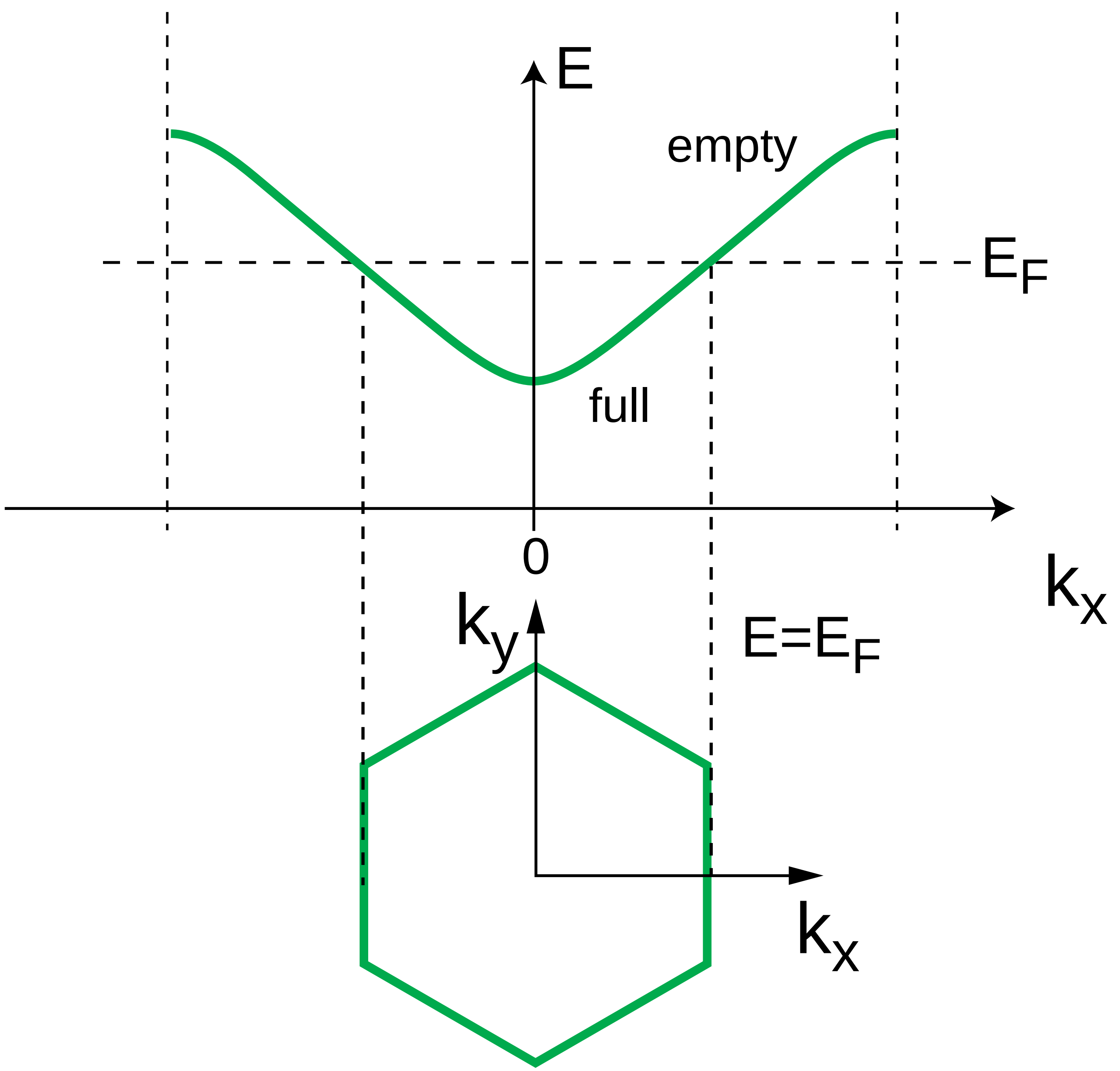
inversion symmetry:

$$\epsilon(\vec{k},\uparrow) = \epsilon(-\vec{k},\uparrow)$$

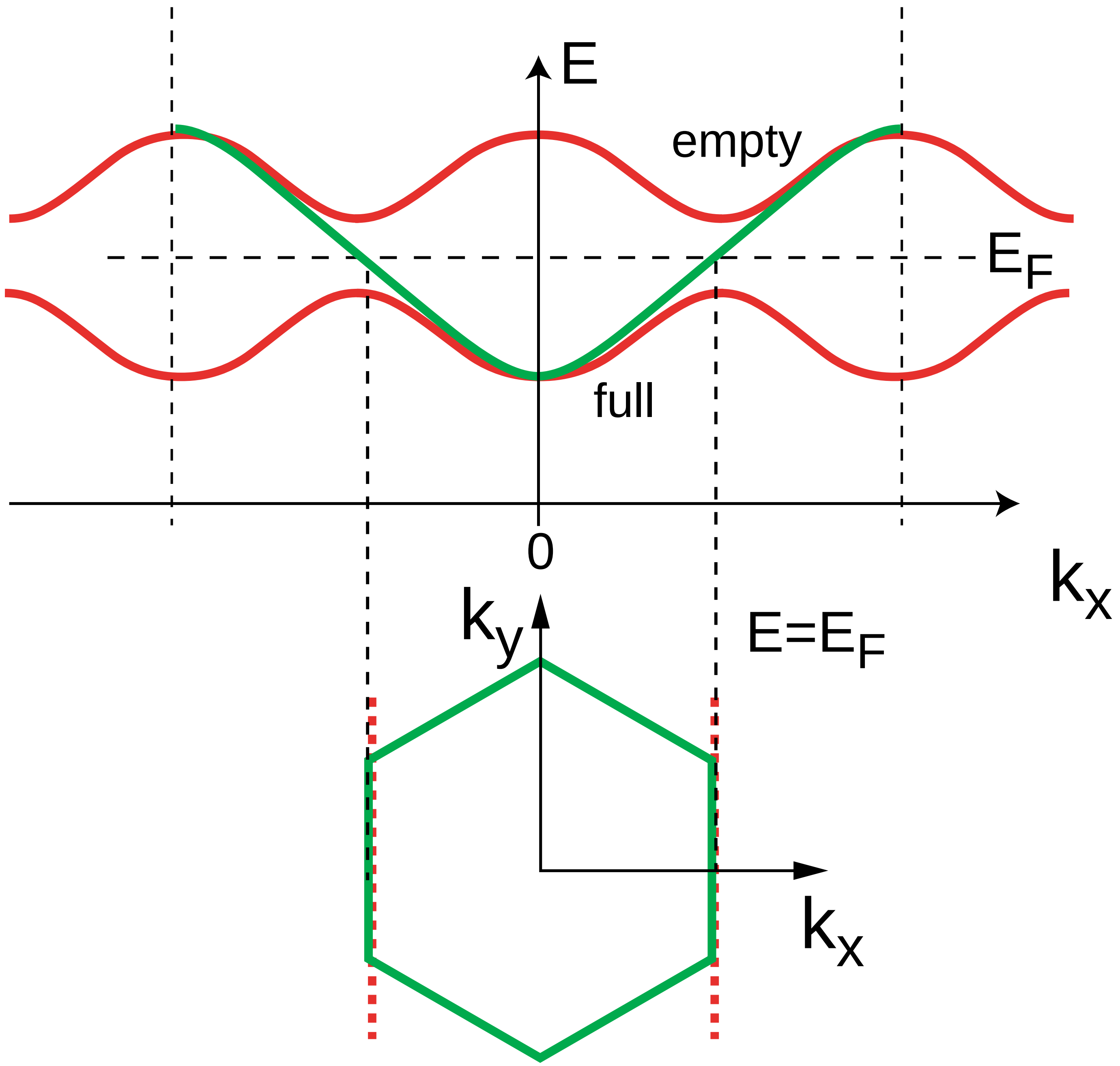
bulk: time reversal plus inversion symmetry: every state two fold degenerate (two spin directions)

surface: time reversal symmetry only: this degeneracy is lifted.

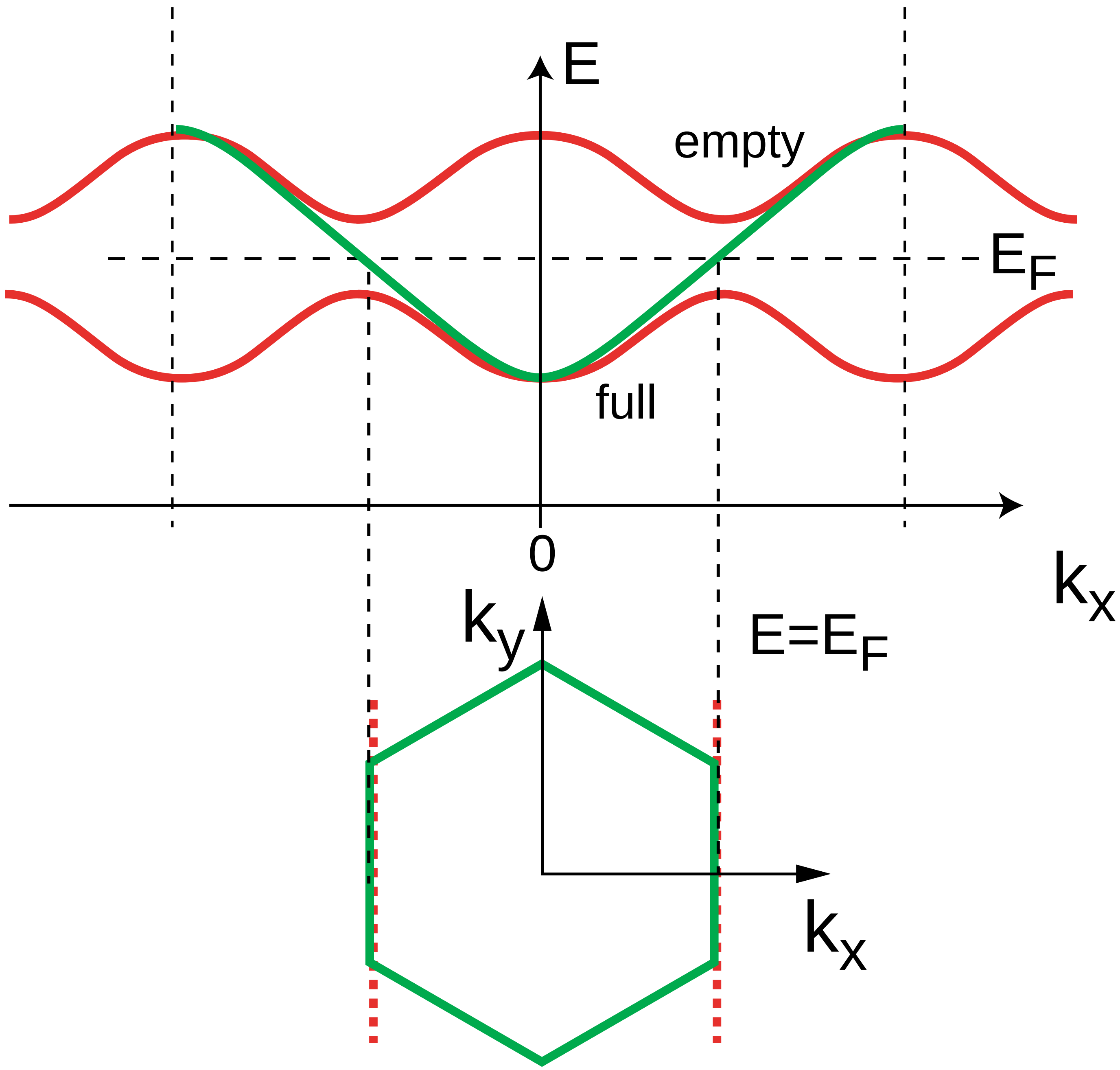
real 2D: Charge Density Waves



real 2D: Charge Density Waves

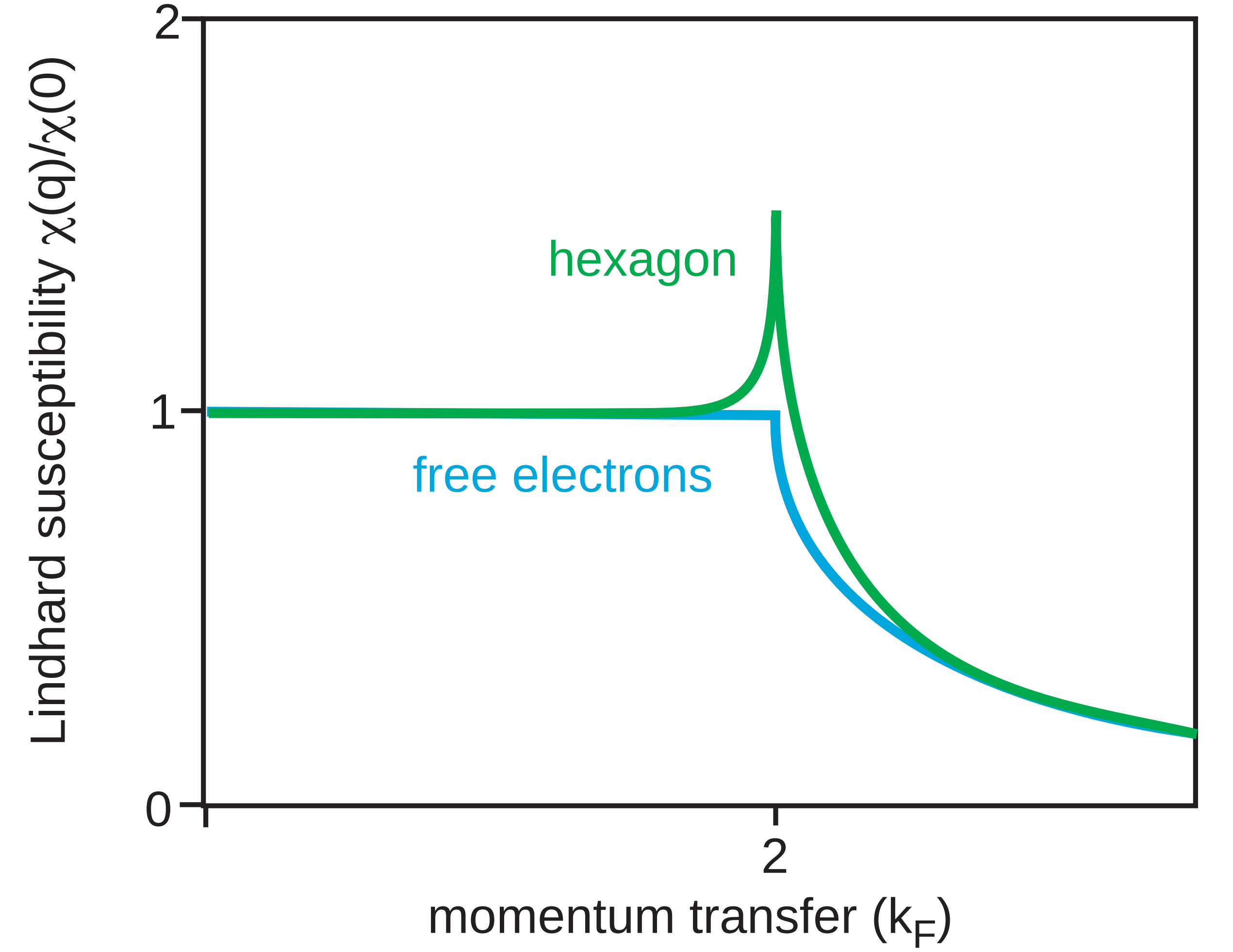


real 2D: Charge Density Waves

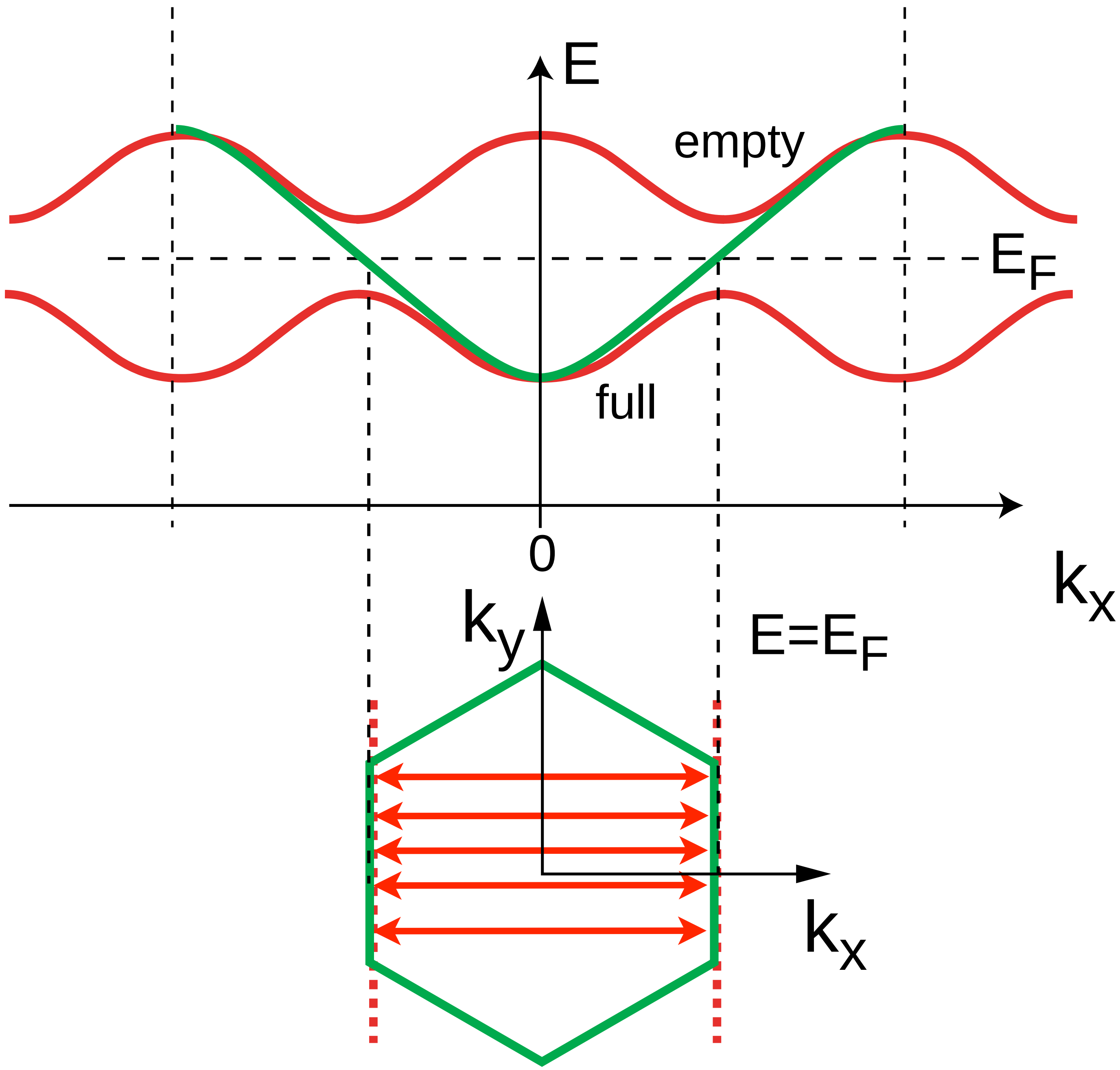


Lindhard susceptibility

$$\chi(\vec{q}) = \int \frac{f(\vec{k}) - f(\vec{k}-\vec{q})d\vec{k}}{\epsilon(\vec{k}) - \epsilon(\vec{k}-\vec{q})(2\pi)^2}$$



real 2D: Charge Density Waves



Lindhard susceptibility

$$\chi(\vec{q}) = \int \frac{f(\vec{k}) - f(\vec{k}-\vec{q})d\vec{k}}{\epsilon(\vec{k}) - \epsilon(\vec{k}-\vec{q})(2\pi)^2}$$