Eur. Phys. J. B **29**, 635–639 (2002)
DOI: 10.1140/epjb/e2002-00347-x

THE EUROPEAN PHYSICAL JOURNAL B

Resonant enhancement of charge transfer through surface states

R. Dick[a]

Department of Physics and Engineering Physics, University of Saskatchewan, 116 Science Place, Saskatoon,
SK S7N 5E2, Canada

Received 6 August 2002

Abstract. A model is proposed that treats electrons at surfaces as a combination of two-dimensional and three-dimensional degrees of freedom. This yields a simple formula for the surface state induced resonant enhancement of the transfer of electrons through a surface. The model also yields analytic approximations for the transition between two-dimensional and three-dimensional distance laws in the correlations between electrons in surface states.

PACS. 73.20.At Surface states, band structure, electron density of states – 73.40.-c Electronic transport in interface structures

1 Introduction

Surface states have been a subject of interest in condensed matter physics ever since the pioneering work of Tamm [1] and Shockley [2]. Using a finitely extended Kronig–Penney model, Tamm demonstrated the existence of surface localized states with damped probability amplitudes both towards the outer and the inner region of a material. In the simplest cases this can be understood as a consequence of the fact that their energy levels lie below the outside vacuum level and in a band gap of the bulk material. Shockley then demonstrated how the surface states emerge from atomic orbitals (see also [3] for first results on this in a weakly coupled electron approximation). Very useful introductions to the subject can be found in [4–6].

In recent years interest in the theory of surface states focused *e.g.* on investigations of their magnetic properties, exchange splitting, and spin polarization [7–9], and on calculations of different contributions to the width of surface states through their interactions with phonons and bulk and surface electrons, see *e.g.* [10] and references there. The subject of correlations between tightly bound surface electrons was addressed by Müller, Schiller and Nolting in a semi-infinite chain model [11], and this group also recently reported results on the appearance of surface states in low carrier density local-moment semiconducting films [12,13].

From an experimental point of view angle resolved photoemission spectroscopy has become a major analysis tool for the measurement of surface band structure and widths of surface states, see *e.g.* [4–6] and references there, and [14–27] for recent work, and after the invention of scanning tunneling microscopy, tunneling spectroscopy has become a second major experimental technique for the investigation of surface states [28–35]. Other techniques involve ballistic electron emission [36–39], time-resolved two-photon photoemission [22,40], and inverse photoemission [41]. Generically these methods reveal surface energy bands with effective electron masses in the range of bulk effective masses.

The purpose of the present paper is two-fold: First I would like to draw attention to the fact that translational excitations of non-occupied surface states along a surface or interface can yield a resonant enhancement of the energy-dependent penetration probability of electrons into semiconductors, where the resonance specifically depends on the momentum of the electron parallel to the surface. Furthermore, the possibility to observe genuine two-dimensional behavior in apparently two-dimensional systems is a pertinent subject of interest in condensed matter physics, and surface states are naturally considered a prime target in this endeavor: It should be possible to observe their intrinsically two-dimensional nature through two-dimensional distance laws in correlation functions of electrons in surface states. The model Hamiltonian introduced below to account for possible longitudinal excitations of surface states also makes a prediction on the transition between two-dimensional and three-dimensional distance laws in the correlations between electrons in surface states, but the result also indicates that actual observation of this behavior requires materials with much stronger curvature in the surface energy bands than in the bulk conduction band.

The model is introduced in Section 2, and the impact of the longitudinal modes on electron transmission probabilities is described in Section 3. The transition between two-dimensional and three-dimensional behavior of correlation functions in the quasi-free electron approximation of the model is described in Section 4.

---

[a] e-mail: `rainer@sask.usask.ca`

2 The model Hamiltonian

The wavefunction of surface electrons with an energy $\mathit{\Delta} E_S$ below the conduction band of a semiconductor is damped outside of the material with a penetration depth

$$d \approx 1.95\,\text{Å} \times \left(\frac{1\,\text{eV}}{\chi + \mathit{\Delta} E_S} \right)^{\frac{1}{2}},$$

where χ is the electron affinity of the semiconductor. Inside the material the surface state wavefunction drops oscillatory over a few atomic layers [4,6], because the energy levels of the surface states are located in the gap between the valence and conduction band and do not allow for a corresponding bulk mode.

However, surface electrons can move along the surface if they are not confined by defects, and this translational degree of freedom may imply some simple, yet interesting consequences.

In the simplest possible almost free electron approximation one might attempt to describe an electron in the presence of a surface by a standard single particle Hamiltonian, with the surface levels being taken into account through a localized (*e.g.* δ-function type) contribution to the potential U. Models for electrons in the presence of image states are often of this kind. The Hamiltonian of the corresponding non-relativistic quantum field ψ then has the same form as the first quantized expectation value:

$$H = \int \mathrm{d}^2\mathbf{x} \int \mathrm{d}z \left(\frac{\hbar^2}{2m} \left(\nabla\psi^+ \cdot \nabla\psi + \partial_z\psi^+ \cdot \partial_z\psi \right) \right.$$
$$\left. + \psi^+ U \psi \right).$$

Here and in the sequel all vectors are 2-dimensional vectors parallel to the planar surface, and z is the inward pointing coordinate orthogonal to the surface.

As it stands this is clearly an unsatisfactory model, no matter how sophisticated U is chosen, and at least one might try to take into account the different propagation properties in vacuum and in the bulk through a z-dependent inverse mass: $m^{-1} = m^{-1}(z) = m_0^{-1}\Theta(-z) + m_*^{-1}\Theta(z)$, where $\Theta(z)$ is the Heaviside function, m_0 is the free electron mass in vacuum, and m_* is an effective mass for propagation in the bulk below the surface. However, there are also the surface specific propagation modes with their own band structure and strict localization in transverse direction, and this motivates us to consider the following approximation for the Hamiltonian describing electron motion in the presence of a surface:

$$\begin{aligned} H = {} & \frac{\hbar^2}{2m_0} \int \mathrm{d}^2\mathbf{x} \int_{z<0} \mathrm{d}z \left(\nabla\psi^+ \cdot \nabla\psi + \partial_z\psi^+ \cdot \partial_z\psi \right) \\ & + \frac{\hbar^2}{2m_*} \int \mathrm{d}^2\mathbf{x} \int_{z>0} \mathrm{d}z \left(\nabla\psi^+ \cdot \nabla\psi + \partial_z\psi^+ \cdot \partial_z\psi \right) \\ & + \int \mathrm{d}^2\mathbf{x} \int \mathrm{d}z\, \psi^+ U \psi + \frac{\hbar^2}{2\mu} \int \mathrm{d}^2\mathbf{x}\, \nabla\psi^+ \cdot \nabla\psi \Big|_{z=0}, \end{aligned} \quad (1)$$

which corresponds to an effective mass description of electron motion both on and off the surface. The novel feature of the Hamiltonian (1) is the inclusion of a two-dimensional kinetic term to account for electronic motion corresponding to the surface state energy bands.

The surface mass parameter μ has the dimension of a mass per length and could be converted into an estimate of an actual surface electron mass through $m_S^* \approx \mu L$, where L is a measure for the transverse extension of the surface state wavefunction.

It is trivial, but useful for the later reasoning, to write down the Lagrangian related to (1):

$$\begin{aligned} L = {} & \frac{\mathrm{i}\hbar}{2} \int \mathrm{d}^2\mathbf{x} \int \mathrm{d}z \left(\psi^+ \dot{\psi} - \dot{\psi}^+ \psi \right) \\ & - \frac{\hbar^2}{2m_0} \int \mathrm{d}^2\mathbf{x} \int_{z<0} \mathrm{d}z \left(\nabla\psi^+ \cdot \nabla\psi + \partial_z\psi^+ \cdot \partial_z\psi \right) \\ & - \frac{\hbar^2}{2m_*} \int \mathrm{d}^2\mathbf{x} \int_{z>0} \mathrm{d}z \left(\nabla\psi^+ \cdot \nabla\psi + \partial_z\psi^+ \cdot \partial_z\psi \right) \\ & - \int \mathrm{d}^2\mathbf{x} \int \mathrm{d}z \psi^+ U \psi - \frac{\hbar^2}{2\mu} \int \mathrm{d}^2\mathbf{x} \nabla\psi^+ \cdot \nabla\psi \Big|_{z=0}. \end{aligned} \quad (2)$$

This loosely resembles the concept of dimensionally hybrid action principles, which recently attracted a lot of interest in cosmology and particle physics, see [42] for a review. Besides the fact that the present model is non-relativistic and interpolates between two and three dimensions rather than four-dimensional and five-dimensional Minkowski spaces, the main difference between our current model and the particle physics models concerns the fact that here we are not led to a superposition of action principles, but of Hamiltonians from different dimensions. There is no need and no rationale in the present setting to include a two-dimensional time derivative term in (2).

The single particle Schrödinger equation corresponding to (2) is

$$\begin{aligned} \mathrm{i}\hbar\dot{\psi} = {} & U\psi - \frac{\hbar^2}{2\mu}\delta(z)\mathit{\Delta}\psi - \frac{1}{2}\left(\frac{\hbar^2}{m_*} - \frac{\hbar^2}{m_0} \right) \delta(z)\partial_z\psi \\ & - \frac{1}{2}\left(\frac{\hbar^2}{m_0}\Theta(-z) + \frac{\hbar^2}{m_*}\Theta(z) \right) \left(\mathit{\Delta}\psi + \partial_z^2\psi \right). \end{aligned} \quad (3)$$

3 Resonant enhancement of electron transmission through surfaces

The momentum of an electron is denoted by $(\mathbf{p}, p_\perp) = (\hbar\mathbf{k}, \hbar k_\perp)$, where $\mathbf{p}$ is the momentum parallel to the planar surface.

An interesting implication of the presence of the two-dimensional kinetic term in (1, 3) is a dependence of electron transmission rates through the surface on the longitudinal momentum $\mathbf{p}$ of the incident electron, which can be understood as the consequence of a resonance condition between the incident electrons and surface states. To elucidate this we use a simple potential approximation $U = U(z)$ for the surface with

$$U(z) = -w\delta(z) - \chi\theta(z). \quad (4)$$

Here the vacuum level is chosen to be 0 and χ is the electron affinity of the bulk material. w is a measure of the electron affinity of the surface states:

$$w \simeq (\chi + \mathit{\Delta} E_S) L,$$

where $\mathit{\Delta} E_S$ is the energy gap between the surface states and the conduction band ($\mathit{\Delta} E_S < 0$ for surface states which overlap with the conduction band).

Equation (3) with the potential (4) yields for the electron transmission probability through the surface

$$T = \frac{k_\perp k'_\perp}{m_0 m_*} \left[\left(\frac{\mathbf{k}^2}{2\mu} - \frac{w}{\hbar^2} \right)^2 + \frac{1}{4} \left(\frac{k_\perp}{m_0} + \frac{k'_\perp}{m_*} \right)^2 \right]^{-1}, \quad (5)$$

where $\hbar k_\perp$ is the transverse momentum of the electron outside of the material and $\hbar k'_\perp$ is the transverse momentum inside the material. They are related to each other and the longitudinal momentum $\hbar \mathbf{k}$ through

$$\frac{\hbar^2 k'^2_\perp}{m_*} = 2\chi + \frac{\hbar^2 k^2_\perp}{m_0} + \hbar^2 \mathbf{k}^2 \left(\frac{1}{m_0} - \frac{1}{m_*} \right) \cdot \quad (6)$$

The surface states lead to an enhancement of the surface transmission probability for low longitudinal momentum $\hbar |\mathbf{k}| < 2\sqrt{\mu w}$, while they suppress transmission at higher longitudinal momentum. The resonance at

$$\hbar^2 \mathbf{k}^2 = 2\mu w \simeq 2 m^*_S (\chi + \mathit{\Delta} E_S)$$

would appear as a Breit–Wigner shaped dip in the reflection rate $R = 1 - T$ of electrons incident on the surface, if the effective mass m_* is close to m_0 (otherwise the dependence of $k'_\perp$ on $\mathbf{k}$ would distort the Breit–Wigner shape). This might provide a way to test applicability of the dimensionally hybrid Hamiltonian (1) for a simple modeling of the impact of surface states on charge transfer through surfaces.

Expansion of (5) around $|\mathbf{k}| \simeq \sqrt{2\mu w}/\hbar$ shows that in terms of intrinsic material properties the width of the resonance depends on the quality factor

$$w/\mu \propto (\chi + \mathit{\Delta} E_S)/m^*_S c^2.$$

4 The transition between two and three dimensions

If a system were truly two-dimensional the free two-point correlation functions in it were given by logarithmic functions or appropriate derivatives of it. It is also well known that the logarithmic infrared divergence of two-dimensional potentials forces a strictly two-dimensional Coulomb gas to be electrically neutral.

However, the actual observation of the transition between two-dimensional and three-dimensional distance laws for correlations in approximately two-dimensional systems like thin films seems a very elusive problem.

Here I would like to point out that the model Hamiltonian (1) allows for the derivation of an equilibrium correlation function $\langle \psi(\mathbf{x}) \psi^+(\mathbf{x}') \rangle$ of surface electrons which can be given in closed form and interpolates between the two-dimensional logarithmic potential and the three-dimensional $1/r$ law.

Since the surface states are localized near the surface we may assume that the contribution from the potential in (1) for these states effectively reduces to a two-dimensional potential term $\int \mathrm{d}^2\mathbf{x}\, \psi^+ u \psi|_{z=0}$:

$$\begin{aligned} H = {} & \frac{\hbar^2}{2m_0} \int \mathrm{d}^2\mathbf{x} \int_{z<0} \mathrm{d}z \left(\nabla\psi^+ \cdot \nabla\psi + \partial_z \psi^+ \cdot \partial_z \psi \right) \\ & + \frac{\hbar^2}{2m_*} \int \mathrm{d}^2\mathbf{x} \int_{z>0} \mathrm{d}z \left(\nabla\psi^+ \cdot \nabla\psi + \partial_z \psi^+ \cdot \partial_z \psi \right) \\ & + \int \mathrm{d}^2\mathbf{x} \left(\frac{\hbar^2}{2\mu} \nabla\psi^+ \cdot \nabla\psi + \psi^+ u \psi \right) \bigg|_{z=0} . \end{aligned} \quad (7)$$

The generating functional for correlation functions on the surface is[1]

$$\begin{aligned} Z[j, j^+] = {} & \int \mathrm{d}\psi \mathrm{d}\psi^+ \exp\bigl(-\beta H[\psi, \psi^+] \bigr) \\ & \times \exp\Bigl(- \int \mathrm{d}^2\mathbf{x} \left[\psi^+(\mathbf{x}, 0) j(\mathbf{x}) + j^+(\mathbf{x}) \psi(\mathbf{x}, 0) \right] \Bigr) \\ = {} & \exp\Bigl(-\beta \int \mathrm{d}^2\mathbf{x}\, \frac{\delta}{\delta j(\mathbf{x})} u(\mathbf{x}) \frac{\delta}{\delta j^+(\mathbf{x})} \Bigr) Z_0[j, j^+], \end{aligned} \quad (8)$$

where the potential term has been split off in the usual way. The calculation of Z_0 is a little trickier than usual due to the change in mass and δ-function contributions from the surface:

With the "free" Hamiltonian

$$H_0 = H - \int \mathrm{d}^2\mathbf{x}\, \psi^+(\mathbf{x}, 0) u(\mathbf{x}) \psi(\mathbf{x}, 0)$$

and the convention for convolutions

$$(G \circ j)(\mathbf{x}, z) = \int \mathrm{d}^2\mathbf{x}'\, G(\mathbf{x} - \mathbf{x}', z) j(\mathbf{x}')$$

one finds

$$\begin{aligned} & \beta H_0[\psi, \psi^+] + \int \mathrm{d}^2\mathbf{x} \left[\psi^+(\mathbf{x}, 0) j(\mathbf{x}) + j^+(\mathbf{x}) \psi(\mathbf{x}, 0) \right] = \\ & -\frac{\hbar^2 \beta}{2} \int \mathrm{d}^2\mathbf{x} \int \mathrm{d}z \left(\psi^+ + \frac{2\overline{m}}{\hbar^2 \beta} j^+ \circ G \right) \\ & \times \left[\left(\frac{1}{m_0} \mathit{\Theta}(-z) + \frac{1}{m_*} \mathit{\Theta}(z) \right) \left(\mathit{\Delta} + \partial_z^2 \right) + \frac{1}{\mu} \delta(z) \mathit{\Delta} \right. \\ & \left. + \left(\frac{1}{m_*} - \frac{1}{m_0} \right) \delta(z) \partial_z \right] \left(\psi + \frac{2\overline{m}}{\hbar^2 \beta} G \circ j \right) \\ & - \frac{2\overline{m}}{\hbar^2 \beta} j^+ \circ G \circ j \bigg|_{z=0} , \end{aligned} \quad (9)$$

---

[1] As usual $\delta/\delta j$ acts from the right if ψ is fermionic.

where

$$\overline{m}=\frac{2m_0m_*}{m_0+m_*}$$

and the Green's function is defined through

$$\begin{aligned}&\left(\frac{\overline{m}}{m_0}\Theta(-z)+\frac{\overline{m}}{m_*}\Theta(z)\right)\left(\Delta+\partial_z^2\right)G(\mathbf{x},z)\\&+\frac{\overline{m}}{\mu}\delta(z)\Delta G(\mathbf{x},0)+\left(\frac{\overline{m}}{m_*}-\frac{\overline{m}}{m_0}\right)\delta(z)\partial_z G(\mathbf{x},z)\\&=-\delta(\mathbf{x})\delta(z).\end{aligned}\tag{10}$$

This yields

$$\begin{aligned}&Z_0[j,j^+]\propto\exp\left(\frac{2\overline{m}}{\hbar^2\beta}j^+\circ G\circ j\bigg|_{z=0}\right)=\\&\exp\left(\frac{2\overline{m}}{\hbar^2\beta}\int\mathrm{d}^2\mathbf{x}\int\mathrm{d}^2\mathbf{x}'\,j^+(\mathbf{x})G(\mathbf{x}-\mathbf{x}',0)j(\mathbf{x}')\right).\end{aligned}\tag{11}$$

Equation (10) can be solved with a Fourier *ansatz*

$$G(\mathbf{x},z)=\frac{1}{(2\pi)^3}\int\mathrm{d}^2\mathbf{k}\int\mathrm{d}k_\perp\,G(\mathbf{k},k_\perp)\exp[\mathrm{i}(\mathbf{k}\cdot\mathbf{x}+k_\perp z)].\tag{12}$$

Insertion yields with

$$\int_0^{\pm\infty}\mathrm{d}z\,\exp(\mathrm{i}k'_\perp z)=\mathrm{i}\mathcal{P}\frac{1}{k'_\perp}\pm\pi\delta(k'_\perp)$$

the equation

$$\begin{aligned}&\frac{\overline{m}}{2\pi}\mathcal{P}\int\mathrm{d}k'_\perp\left[\frac{k^2}{\mu}+\mathrm{i}\left(\frac{1}{m_0}-\frac{1}{m_*}\right)\left(k'_\perp-\frac{1}{k'_\perp}\right)\right]G(\mathbf{k},k'_\perp)\\&+\left(k^2+k_\perp^2\right)G(\mathbf{k},k_\perp)=1.\end{aligned}\tag{13}$$

This determines the $k_\perp$-dependence of the propagator

$$G(\mathbf{k},k_\perp)=\frac{f(k)}{k^2+k_\perp^2},\tag{14}$$

and with

$$\frac{1}{\pi}\int_{-\infty}^{\infty}\mathrm{d}k'_\perp\,\frac{1}{k^2+k'^2_\perp}=\frac{1}{k}$$

we find the Green's function

$$G(\mathbf{k},k_\perp)=\frac{1}{(1+k\ell)(k^2+k_\perp^2)},\tag{15}$$

where the length scale ℓ is defined through

$$\ell=\frac{\overline{m}}{2\mu}\cdot$$

In the transverse coordinate (15) reads

$$G(\mathbf{k},z)=\frac{1}{2k(1+\ell k)}\exp(-k|z|).\tag{16}$$

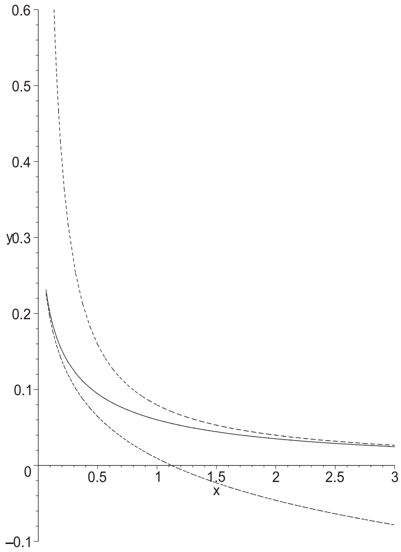

Fig. 1. The solid line is the Green's function (18) of the surface electrons as a function of $x=r/\ell$, in units of ℓ^{-1}. The upper dashed line is the three-dimensional $1/4\pi r$ distance law, and the lower dashed line is the two-dimensional logarithmic Green's function.

The resulting solution in configuration space is[2]

$$\begin{aligned}G(\mathbf{x},z)&=\frac{1}{8\pi^2}\int_0^\infty\mathrm{d}k\int_0^{2\pi}\mathrm{d}\varphi\,\frac{\exp[k(\mathrm{i}r\cos\varphi-|z|)]}{1+k\ell}\\&=\frac{1}{4\pi}\int_0^\infty\mathrm{d}k\,\frac{\exp(-k|z|)}{1+k\ell}J_0(kr).\end{aligned}\tag{17}$$

The perturbation series (8, 11) requires the Green's function on the surface, which can be expressed as a linear combination of a Struve function and a Bessel function of the second kind:

$$G(\mathbf{x})=G(\mathbf{x},z)\Big|_{z=0}=\frac{1}{8\ell}\left[\mathbf{H}_0\left(\frac{r}{\ell}\right)-Y_0\left(\frac{r}{\ell}\right)\right]\cdot\tag{18}$$

This interpolates between two-dimensional and three-dimensional distance laws

$$\begin{aligned}r\ll\ell:\quad G(\mathbf{x})&=\frac{1}{4\pi\ell}\left[-\gamma-\ln\left(\frac{r}{2\ell}\right)+\frac{r}{\ell}+\mathcal{O}\left(\frac{r^2}{\ell^2}\right)\right],\\r\gg\ell:\quad G(\mathbf{x})&=\frac{1}{4\pi r}\left[1-\frac{\ell^2}{r^2}+\mathcal{O}\left(\frac{\ell^4}{r^4}\right)\right]\cdot\end{aligned}$$

$G(\mathbf{x})$ along with the limiting cases is plotted in Figure 1.

5 Conclusion

The Hamiltonian (1) provides a simple model for electrons which can propagate both in the bulk and through surface modes. It predicts a resonant enhancement of charge

---

[2] I follow the conventions of [43] for Bessel and Struve functions.

transfer through a surface if the kinetic energy in the motion parallel to the surface matches the energy level of a surface state.

It also allows for an analytic calculation of the correlation function

$$\langle\psi(\mathbf{x})\psi^{+}(\mathbf{x}')\rangle\big|_{U=0} = \frac{2\overline{m}}{\hbar^2\beta}G(\mathbf{x}-\mathbf{x}')$$

between quasi-free surface electrons, which explicitly interpolates between the usual distance laws for free electrons in two and in three dimensions. However, the transition scale

$$\ell = \frac{m_0 m_*}{(m_0+m_*)\mu} \simeq \frac{m_0 m_*}{(m_0+m_*)m_S^*}L$$

will usually be of the order of the transverse extension of the surface state wavefunctions. Experimental verification of the two-dimensional short-distance behavior of surface electron correlations as predicted in (18) thus will require materials with $m_S^* \ll m_*$ to ensure $\ell \gg L$.

This work was supported in part by NSERC of Canada.

References

1. I. Tamm, Phys. Z. Sow. **1**, 733 (1932)
2. W. Shockley, Phys. Rev. **56**, 317 (1939)
3. A.W. Maue, Z. Phys. **94**, 717 (1935)
4. S.G. Davison, M. Stęślicka, *Basic Theory of Surface States* (Clarendon Press, Oxford 1992)
5. H. Lüth, *Solid Surfaces, Interfaces and Thin Films*, 4th edn. (Springer-Verlag, Berlin 2001)
6. W. Mönch, *Semiconductor Surfaces and Interfaces*, 3rd edn. (Springer-Verlag, Berlin 2001)
7. W. Nolting, T. Dambeck, G. Borstel, Z. Phys. B **94**, 409 (1994)
8. R. Schiller, W. Müller, W. Nolting, Eur. Phys. J. B **2**, 249 (1998)
9. R. Schiller, W. Müller, W. Nolting, J. Phys. Cond. Matt. **11**, 9589 (1999)
10. A. Eiguren, B. Hellsing, F. Reinert, G. Nicolay, E.V. Chulkov, V.M. Silkin, S. Hüfner, P.M. Echenique, Phys. Rev. Lett. **88**, 066805 (2002)
11. W. Müller, R. Schiller, W. Nolting, Eur. Phys. J. B **16**, 705 (2000)
12. R. Schiller, W. Nolting, Phys. Rev. Lett. **86**, 3847 (2001)
13. R. Schiller, W. Müller, W. Nolting, Phys. Rev. B **64**, 134409 (2001)
14. B.A. McDougall, T. Balasubramanian, E. Jensen, Phys. Rev. B **51**, 13891 (1995)
15. R. Panagio, R. Matzdorf, G. Meister, A. Goldmann, Surf. Sci. **336**, 113 (1995)
16. S. LaShell, B.A. McDougall, E. Jensen, Phys. Rev. Lett. **77**, 3419 (1996)
17. F. Theilmann, R. Matzdorf, G. Meister, A. Goldmann, Phys. Rev. B **56**, 3632 (1997)
18. A. Goldmann, R. Matzdorf, F. Theilmann, Surf. Sci. **414**, L932 (1998)
19. M. Hengsberger, R. Fresard, D. Purdie, P. Segovia, Y. Baer, Phys. Rev. B **60**, 10796 (1999)
20. S. Lashell, E. Jensen, T. Balasubramanian, Phys. Rev. B **61**, 2371 (2000)
21. P. Straube, F. Pforte, T. Michalke, K. Berge, A. Gerlach, A. Goldmann, Phys. Rev. B **61**, 14027 (2000)
22. Th. Fauster, Ch. Reuss, I.L. Shumay, M. Weinelt, F. Theilmann, A. Goldmann, Phys. Rev. B **61**, 16168 (2000)
23. F. Baumberger, T. Greber, J. Osterwalder, Phys. Rev. B **62**, 15431 (2000); Phys. Rev. B **64**, 195411 (2001)
24. F. Reinert, G. Nicolay, S. Schmidt, D. Ehm, S. Hüfner, Phys. Rev. B **63**, 115415 (2001)
25. G. Nicolay, F. Reinert, S. Hüfner, P. Blaha, Phys. Rev. B **65**, 033407 (2001)
26. C. Schüssler-Langehaine, H. Ott, A.Yu. Grigoriev, A. Möller, R. Meier, Z. Hu, C. Mazumdar, G. Kaindl, E. Weschke, Phys. Rev. B **65**, 214410 (2002)
27. J.N. Crain, K.N. Altmann, Ch. Bromberger, F.J. Himpsel, `cond-mat/0205005`
28. R.J. Hamers, R.M. Tromp, J.E. Demuth, Phys. Rev. Lett. **56**, 1972 (1986)
29. M.F. Crommie, C.P. Lutz, D.M. Eigler, Science **262**, 218 (1993); Nature **363**, 524 (1993)
30. E.J. Heller, M.F. Crommie, C.P. Lutz, D.M. Eigler, Nature **369**, 464 (1994)
31. J. Li, W.-D. Schneider, R. Berndt, O.R. Bryant, S. Crampin, Phys. Rev. Lett. **81**, 4464 (1998)
32. L. Bürgi, O. Jeandupeux, H. Brune, K. Kern, Phys. Rev. Lett. **82**, 4516 (1999)
33. J.E. Ortega, S. Speller, A.R. Bachmann, A. Mascaraque, E.G. Michel, A. Narmann, A. Mugarza, A. Rubio, F.J. Himpsel, Phys. Rev. Lett. **84**, 6110 (2000)
34. J.J. Pascual, Z. Song, J.J. Jackiw, K. Horn, H.-P. Rust, Phys. Rev. B **63**, 241103 (2001)
35. A. Bauer, A. Mühlig, D. Wegner, G. Kaindl, Phys. Rev. B **65**, 075421 (2002)
36. W.J. Kaiser, L.D. Bell, Phys. Rev. Lett. **60**, 1406 (1988)
37. M. Prietsch, Phys. Rep. **253**, 164 (1995)
38. K. Reuter, F.J. Garcia-Vidal, P.L. de Andres, F. Flores, K. Heinz, Phys. Rev. Lett. **81**, 4963 (1998)
39. M.K. Weilmeier, W.H. Rippard, R.A. Buhrman, Phys. Rev. B **61**, 7161 (2000)
40. A. Schäfer, I.L. Shumay, M. Wiets, M. Weinelt, Th. Fauster, E.V. Chulkov, V.M. Silkin, P.M. Echenique, Phys. Rev. B **61**, 13159 (2000)
41. C. Benesch, H. Merz, H. Zacharias, Phys. Rev. B **65**, 235317 (2002)
42. R. Dick, Class. Quantum Grav. **18**, R1 (2001)
43. M. Abramowitz, I.A. Stegun, *Handbook of Mathematical Functions* (United States National Bureau of Standards, Washington, 1972)