Surface resonances on transition metals as low-dimensional model systems

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Abstract. Finding and investigating low-dimensional model systems is essential to improve the understanding of metals with strong electron correlation. Here, we show that suitably chosen transition metal surfaces can provide such model systems. Comparing the band structure from density functional theory (DFT) with angular resolved photoemission (ARPES) for Pt(110), we give evidence for a low-dimensional surface resonance. Details of the band topology and fingerprints of low-dimensional behaviour are presented.

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1. Introduction

The incomplete understanding of many-body effects [1, 2] in metals with strong electron correlation represents one of the major obstacles in the effective design of new materials. Since the dimensionality of electronic states plays a major role for electron correlation [3], one possible key to the rich phase diagram of these materials is to understand the evolution of dimensionality (dimensional crossover or deconfinement [4]) with increasing subsystem coupling and decreasing temperature [5, 6]. Thus, many experimental model systems consist of three-dimensional (3D) crystals built up from weakly interacting arrays of lower-dimensional sub-units. Generally, the strong many-body response in strongly anisotropic systems is connected to the peculiar shape of the Fermi surface with either large parallel sections (nesting) [7] or a diverging density of states (DOS) at the Fermi energy $E_F$ as e.g. due to saddle points in 2D [8]. These Fermi surface topologies induce singularities in the response functions (generalized susceptibilities) which upon cooling lead to broken-symmetry phases like e.g. charge- or spin-density waves or superconductivity [7]. In the case of the cuprate superconductors, for example, it is agreed that the so-called antinodal saddle points at $(\pi, 0)$ play a dominant role in the mechanism of high-$T_c$ superconductivity [9,10]. The low-dimensional character of these materials is an important ingredient [11] and it has recently been suggested that upon entering the superconducting state a dimensional crossover from two to three dimensions occurs [12, 13]. Conductivity measurements on a number of layered metals give evidence for such a change in effective dimension, signalled by a crossover from incoherent (hopping-type) to a more coherent (Fermi-liquid or metallic) $c$-axis transport (see e.g. [12,14,15] and references therein). Partly due to the complex geometric and electronic structure of most of these model materials, however, interpretation and understanding of typical many-body effects have been very demanding or even impossible. Although intensively investigated, e.g. the out-of-plane coherence [16] of the cuprates is not yet well understood and the role of the multiple layers and its relevance to the critical temperature is not settled [9].

Single crystal surfaces as templates receive a lot of interest since various low-dimensional nanostructures can be prepared and their coupling may be changed in situ. Furthermore, quasi-1D (Q1D) model systems realized on surfaces offer a great advantage: the three experimental methods (angular resolved photo emission (ARPES), inverse photoemission (IPE) and scanning tunnelling spectroscopy (STS)) which give direct access to the single-electron spectral function, a key ingredient in many-body physics [17], are surface-sensitive rather than bulk-sensitive. Apart from investigating the surface of the bulk model systems [18], most surface studies focussed either on (i) 2D Shockley-type surface states additionally confined towards Q1D [19, 20] or on (ii) adsorption and/or self organization of 1D metallic chains on flat or vicinal substrates [21, 22]. Usually, Shockley-type states have a low electron occupancy per surface unit cell, so they are not considered to dominate the energetics of the metal surface [23]. Although examples for long range interaction mediated by Shockley surface states have been mentioned [24, 25], electronically driven phase transitions are generally not to be expected. On the contrary, so-called Tamm-type surface states on a suitably chosen transition metal surface derive from weakly dispersing d-bands and possess a high DOS at $E_F$. These surface states may influence the surface phase diagram considerably. As we have shown before, phase transitions on the Br/Pt(110) surface can indeed be related to the electronic structure at $E_F$ [13, 26, 27].

In this paper, we focus on the electronic structure of the clean transition metal surface Pt(110). Figure 1 shows the real and reciprocal space geometry of the clean Pt(110) surface. Due to the strong anisotropy of the surface, surface localized states can be expected to exhibit Q1D
Figure 1. Top: real space (top- and side-view) and reciprocal space geometry (bottom) of the unreconstructed (dotted) and the missing row reconstructed Pt(110) surface (solid). Due to the missing row reconstruction, any surface feature at $S$ (red) is repeated at $X$ (green).

As is shown below, the bulk band structure supports a Tamm-type surface resonance on the clean surface. In the ARPES spectra, we find a strong temperature-induced decay of an intense spectral feature—called the quasiparticle (QP) peak in the following—near to $E_F$. The observation of this temperature behaviour is typical for lower-dimensional systems [12, 15, 30–33]. Here, the intensity loss of the QP part of the spectral function can be—-independent of the specific kind of collective excitations in the system (phonons, spin fluctuations, charge fluctuations etc)—considered to be the general fingerprint of a dimensional crossover [12, 13]. These observations support earlier experiments on the adsorbate-covered Pt(110) surface [13, 26, 28, 29]. This is of general relevance since similar Q1D resonances are expected on surfaces of other transition metals [34] or suitably chosen compounds. In order to investigate the conditions for such low-dimensional resonances to appear on metal surfaces, we provide here data on how the Q1D surface resonance evolves from the bulk band structure and characterize it with respect to its orbital composition.

Platinum is a transition metal which does not show pronounced correlation effects like ferromagnetism, but which is (like Pd) near to ferromagnetism [35]. Both metals are interesting because of the coexistence of strong electron–phonon coupling and high d-density at the Fermi energy ($E_F$) which enhances the conduction electron susceptibility and favours a magnetic ordering. Related to the anomalously high DOS at the Fermi surface, Pt shows an anomalously
large heat capacity and magnetic susceptibility [36]. Pd and Pt are the two non magnetically ordering materials with the largest exchange enhanced Pauli susceptibility [37]. Despite their high electronic specific-heat coefficient which favours superconductivity, Pt and Pd do not become superconductive down to the micro-Kelvin range. It is generally agreed that spin fluctuations severely reduce the $T_C$ in these elements [38]. In both metals, microscopic fingerprints of strong electron–phonon coupling have been observed in the phonon dispersion relations [39]. These Kohn anomalies in 3D are related to peaks in the electron susceptibility [40]. In lower dimension, fingerprints of electron–phonon coupling were observed on the Pt surfaces Pt(100) (density wave [41]) and Pt(111) (Kohn anomaly in 2D [42]). According to recent calculations, thin films of Pt on a (001) noble metal surface are not magnetic [43]. Theoretically reducing the effective dimension further towards a free-standing chain of Pt atoms creates a van Hove singularity (vHS) at $E_F$ which is responsible for the ferromagnetic instability of a 1D Pt nanowire [44, 45]. We observe on Pt(110) a vHS at the same position in $k$-space suggesting that also the clean Pt(110) surface has a low effective dimension which promotes many-body effects. This view is supported by the fact that the experimental band structure is well described by the theoretical calculation for the free-standing Pt chain [44]–[46].

2. Experiment

The experiments were carried out in an ultra high vacuum (UHV) system with a base pressure of $5 \times 10^{-11}$ mbar. The Pt(110) crystal was cut and polished to a precision of $<0.1^\circ$. Initial cleaning of the crystal was achieved by sputtering with Ar, annealing to 1020 K and heating in oxygen. Prior to each measurement, residual carbon was eliminated by three cycles of 3 L O$_2$ adsorption at 130 K (saturation) and subsequent flash desorption (3 K s$^{-1}$) to 920 K. In the course of the experiments, three different experimental set-ups have been used. Most of the temperature-dependent and all polarization-dependent photoemission spectra were recorded in the home-laboratory in Innsbruck with photons of 21.2 eV. For the polarization dependent experiments a SPECS TMM 302 toroidal grating monochromator was used to suppress satellite lines and to yield a high degree (>90%) of linear polarization. The polarization vector of the incident radiation has been kept fixed parallel or perpendicular to the close-packed [110] rows and the angular distribution of photoelectrons has been measured by moving the analyser (energy resolution 65 meV, angular resolution 0.65$^\circ$) on a two-circle goniometer. Experiments using other photon energies were performed at the BessyII 10 m-NIM beamline (15–35 eV) using the SURICAT experimental set-up and at the VUV-beamlime at ELETTRA (26–70 eV), both using a fixed hemispherical analyser. The analyser energy resolution in all cases (65, 30 and 45 meV, respectively) was much better than the intrinsic width of the surface resonance of roughly 180 meV.

3. Experimental results

Figure 2(a) shows the bulk and surface Brillouin zones (SBZs) of an fcc crystal (without surface reconstruction). As is known from fully relativistic band calculations of bulk Pt and Pd, band no. 5 provides a large density of states near the Fermi surface, which in turn leads to the unusual bulk properties mentioned above [34]. The cut of the calculated Pt bulk band structure along the WLW line in figure 2(b) shows a fairly flat region of band no. 5 (red arrow) right below $E_F$. 

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These bulk states along the WLW line project on to the $S$ point of the (110) SBZ. As we show below, due to this special band topology, a Tamm-like surface resonance can be generated at $S$. Interactions localized at the surface do not conserve the momentum $k_z$ perpendicular to the surface. According to perturbation theory, a resonance corresponds to a coherent superposition of bulk states of similar energy with the same momentum $(k_x, k_y)$ parallel to the surface, but with different perpendicular momentum $k_z$. The $(1 \times 2)$ Fourier component of the missing row reconstruction leads to a replica of this resonance at the $X$ point of the SBZ (compare figure 1).

Evidence for the surface resonance at $S$ and $X$ is presented in figures 3 and 4. One of the necessary criteria for a surface state or a surface resonance is negligible dispersion with momentum $k_z$ perpendicular to the surface. As has been shown for the $S$ point, the comparison of energy distribution curves (EDCs) at various photon energies between 24 and 70 eV reveals in all cases a strong QP peak at $E_F$ with negligible dispersion [28]. A similar behaviour has been found at $X$, partly shown in figure 3 (left) for photon energies between 18 and 28 eV: no dispersion is observed for the sharp QP peak slightly below $E_F$. We observe roughly three maxima of the QP intensity at about 15 (not shown), 20 and 28 eV. These photon energies correspond to three different $k_z$ values in the bulk Brillouin zone, their difference not being related to the lattice periodicity in the z-direction. An intensity variation of the photoemission signal is to be expected since a surface state or resonance extends coherently over a few layers. Thus, some $k_z$ components will dominate the expansion in bulk Bloch states mentioned above. Consequently, the remainder (a ‘propensity rule’) of the momentum conservation rule in the bulk is expected to modulate the photoemmission intensities upon variation of photon energy (see e.g. [47] and references therein).

A detailed investigation of the intensity behaviour at $X$ for photon energies between 17.5 and 21 eV, partly shown in figure 3 (right), determines the absolute intensity maximum for the QP peak on the clean surface to be at 20 eV photon energy. The intensity is still reasonably
Figure 3. EDCs with respect to kinetic energy at the $X$ point for different photon energies between 18 and 28 eV (left, photon energies indicated by coloured numbers) and a zoom into the region between 17.5 and 21 eV (right). Spectra have been normalized to the lowest background signal as observed in wide kinetic energy range (12 eV) spectra. Gaussian envelopes (dotted lines) roughly indicate the intensity behaviour. Black lines: clean surface at $T = 300$ K. Red lines: hydrogen covered surface (so-called $\beta_2$-H/Pt(110) phase [48]) at $T = 120$ K.

High for the He I line at 21.2 eV, so the resonance is well suited for investigations with helium discharge sources. Furthermore, figure 3 demonstrates that the QP peak intensity is strongly influenced by adsorption (here of hydrogen), the second criterion usually invoked for surface states or resonances. We note in passing that the $(1 \times 2)$ missing row reconstruction is not affected by hydrogen absorption, whereas the interlayer distance between the outermost missing rows and the second layer is changed from 1.15 to 1.25 Å [49] (derelaxation), the bulk interlayer distance being 1.38 Å. As is obvious from figure 3, hydrogen adsorption shifts neither the kinetic energy position of the QP peak nor the intensity maximum with respect to photon energy. The first observation can be explained by the symmetry properties of the wavefunctions involved: a totally symmetric hydrogen wavefunction at the adsorption site (short bridge [49]) has zero overlap with the wavefunction responsible for the QP peak, since this is anti-symmetric with respect to the short bridge site (see below). The second observation indicates that the intensity maximum is not due to a trivial geometric effect as e.g. photoelectron diffraction between first and second layer: a 9% change of the geometry would shift the photon energy of the maximum by more than 1.5 eV, which is not the case. It is interesting to note that hydrogen usually quenches surface state intensities, here on Pt(110) the intensity rises. Taking into account the geometrical changes, namely the H-induced derelaxation of the outermost Pt rows, this behaviour could be explained by either (i) a stronger $1 \times 2$ component of the Fourier potential of the surface leading to a stronger umklapp from $\overline{S}$ to $\overline{X}$ or (ii) an increased coherence of the surface resonance leading to a stronger relative contribution of the main $k_z$ components in the Bloch expansion. Since we observe decoherence for raising temperatures in all of the variants of the Pt(110) surface (see [28] and below) we favour the second explanation.

The final criterion to establish the surface nature of the QP peak is comparing the experimental QP band topology around $\overline{S}$ and $\overline{X}$ with the corresponding bulk bands. As shown in figure 4, the experimental band topology is the same around $\overline{S}$ (lower graphs) and $\overline{X}$ (upper
Figure 4. Saddle point band topology shown by ARPES dispersion maps around $\overline{X}$ (upper panels) and $\overline{S}$ (lower panels) along the direction of the close packed rows ($k_{[1\overline{1}0]}$, left) and perpendicular to it ($k_{[00\overline{1}]}$, right). The surface resonance character of the features is evident from a comparison of experimental band topology around $\overline{X}$ and band structure cuts along the WLW line (shown for $k_{[00\overline{1}]}$ in figure 2).

Graphs). More importantly, the observed 2D band topology around $\overline{X}$ cannot be related to any flat part of the 3D bulk band structure with the same parallel momentum ($k_x = 1.13 \text{ Å}^{-1}$ and $k_y = 0 \text{ Å}^{-1}$, i.e. projecting on to $\overline{X}$) but instead agrees very well with the flat bulk band projecting on to $\overline{S}$ ($k_x = 1.13 \text{ Å}^{-1}$ and $k_y = 0.8 \text{ Å}^{-1}$). This is shown by the comparison of cuts of the theoretical bulk band structure for different $k_z$ around $\overline{S}$ (coloured lines) with the experimentally observed dispersion in the upper panels (compare also figure 2) around $\overline{X}$. All the facts presented in the figures above are only consistent with a surface resonance composed of bulk states projecting on to $\overline{S}$ which then experiences an initial state ‘umklapp’ to $\overline{X}$ mediated by the $(1 \times 2)$ Fourier component of the missing row reconstruction.

In order to investigate the properties of the surface resonance in more detail, additional photoemission experiments with respect to band dispersion and polarization dependency have been conducted at 21.2 eV. Generally, the resonance feature at $E_F$ is more pronounced on the H/Pt(110) surface while the overall observations with respect to polarization and band dispersion are identical for clean Pt(110) and H/Pt(110) [28, 29]. Figure 5 shows the band dispersion along $\overline{\Gamma X}$ in a wider range of binding energies and momenta (see also [29]). The dispersion of the
Figure 5. Comparison of ARPES band dispersion map at 21.2 eV (unpolarized light) with the DFT calculation of a single chain. The size of the symbols indicates the calculated weight of the orbital component in the charge decomposition of the electronic band. Red circles: the 5d_x^2 orbital with biggest overlap in chain direction x = [110], thus strongest antibonding along ΓX at X. Green triangles: the 5d_{x^2-z^2} and 5d_{yz} orbitals having lobes in the plane perpendicular to the chain (weakly antibonding along ΓX at X). Blue: the 5d_{yx} and 5d_{zx} orbitals having lobes which are inclined with respect to the chain direction (bonding along ΓX at X). The 10% contribution of the s-orbital to the resonance at E_F is not visible on the scale of the plot.

Surface resonance in the vicinity of X is very well described by a relativistic density functional theory (DFT) calculation [44]–[46] of a free standing atomic chain (data points). It is interesting to note that the chain calculation compares also favourably with the experiment in the other areas of the dispersion plot. This suggests that most of the features observed in this dispersion plot are localized on the surface.

Furthermore, the theoretical orbital decomposition (different symbols, see caption of figure 5) of the electronic state at X in the free standing chain of Pt atoms compares favourably with the polarization behaviour observed experimentally: according to the DFT calculation, the electronic states at X and binding energies around E_F are mainly even (ratio of even to odd components in the charge decomposition is 28:10). Figure 6 shows EDCs for the clean and H/Pt(110) surface at the X point for the polarization vector parallel and perpendicular to the close-packed row direction [110]. As predicted by the calculation, the surface resonance near E_F is mainly even, but has a small odd component. A DFT calculation without spin–orbit interaction would predict a splitting into an even resonance around E_F and a resonance of mixed symmetry at roughly 400 meV binding energy. This clearly disagrees with the experiment and hence indicates the importance of including the interaction. Generally, the band structure of the Pt chain is substantially changed by the spin–orbit interaction and the relativistic calculation shown in figure 5 provides better agreement with the data [46]. The main component of the chain state at X is the totally symmetric d_x^2 orbital in chain direction (red circles), where x refers to the [110] direction. As observed in the experiment, all components of the peaks near E_F are antibonding (with respect to the chain direction) at X, so the 1D wavefunction has a node in
Figure 6. EDCs for light polarization parallel (black) or perpendicular (red) to the close-packed [110] direction. The emission angle corresponds to the (X) point for the resonance at $E_F$. Left: clean Pt(110) at $T = 300$ K. Right: H/Pt(110) at $T = 120$ K.

between the Pt sites: an interaction with the hydrogen s-orbital at the short bridge site is not possible as has been discussed in connection with figure 3. This implies no shift of the surface resonance by hydrogen adsorption, in agreement with the experimental data presented in figure 6 (right). The polarization dependency is similar to the clean surface, and the intensity is enhanced for both polarizations. As is shown in [29] for the H/Pt(110) surface in more detail, the total dispersion of the QP peak perpendicular to the chain along $XS$ amounts to roughly 180 meV.

The same total dispersion is observed for the clean surface, indicating the highly anisotropic dispersion behaviour.

The Q1D band topology observed raises the question whether other fingerprints of low-dimensional behaviour can be observed in ARPES. Figure 7 shows the temperature dependency of the EDCs of the clean surface between 300 and 900 K near (left) and at the $S$ point (middle) in comparison with the low-dimensional surface system Br/Pt(110)−c(2 × 2) (right) [13], [26]–[28]. In the Br/Pt(110)−c(2 × 2) system, the intensity decrease at the Fermi-surface as well as the intensity transfer to the background in the region of higher binding energies up to $-0.8$ eV is most obvious [13, 28]. For the clean Pt(110) surface, at the $S$ point two components can be clearly distinguished. Whereas a sharper peak at roughly 120 meV binding energy is strongly temperature dependent similar to the QP-peak seen on Br/Pt(110)−c(2 × 2), a second, less defined component at higher binding energy seems not to be influenced. Note that the intensity of the background at higher binding energy increases with increasing temperature as seen in Br/Pt(110) as well. This intensity exchange between QP peak and less defined incoherent features or background is one of the fingerprints of correlated systems. A strong decay is also observed at $k$-values near $S$, where two components cannot be clearly distinguished. Here, the intensity loss is quite obviously not connected to the temperature dependency of the Fermi distribution, since the maxima of the intensity near $S$ is far below $E_F$. At $S$, however, a (small) correction of the QP maximum intensity by the Fermi distribution has to be taken into account, an effect of 10% for the highest temperature of 900 K. The relative height of the QP peak at $S$ after correction for the Fermi distribution and a constant background is shown in the insets of figure 7 (middle panel, symbols). Note that the evaluation of the QP peak intensity on the Br/Pt(110)−c(2 × 2)
Figure 7. Dependence of the QP peak (21.2 eV) on temperature. Left: clean surface near $S$, where the peak has broadened and is at higher binding energy. The inset shows the $k$-space position, where the two sets of spectra have been recorded. Middle: clean surface at $S$, where two components can be distinguished. The inset shows an estimate of temperature dependence of the spectral intensity near the maximum of the peak, corrected for the trivial temperature effect of the Fermi-distribution. Circles and triangles indicate two extreme assumptions for the temperature-independent background (circles: minimum background around 370 counts s$^{-1}$ as observed at higher binding energies; triangles: maximum background around 600 counts s$^{-1}$ assuming that the yellow EDC resembles the temperature independent component). Black and red symbols depict rising and falling temperatures, showing the reversibility of the intensity loss. For comparison the Debye–Waller like behaviour of the Pt(110) expected for the surface is shown by the solid line. Right: Br/Pt(110)–c(2×2) surface at $S$ shown for comparison.

System (right panel) is more accurate, since the single peak-structure allows a precise fit of the spectra with all corrections (Fermi-distribution, energy resolution of analyser, background, see [13] for details). Thus, we caution here that evaluation of the data for the clean surface (middle panel) relies on an assumption of the background (see caption). Nevertheless, even assuming the smallest possible background (circles in the inset of figure 7, middle panel), the intensity loss strongly deviates from the usual Debye–Waller behaviour based on the known Debye–Waller temperature (110 K) of the Pt(110) surface [50]. The similarities between clean and adsorbate-covered surface clearly point to a common origin: as shown above, due to the flat bulk band structure of Pt along the WLW line a surface resonance at $S$ and $E_F$ develops at both surfaces. The band topology is Q1D and consequently, the surface resonance exhibits indications of the typical dimensional crossover from the low-temperature coherent array of low-dimensional sub-units (intense QP peak) to the high-temperature incoherent array of chains. The high-temperature, more localized incoherent initial state is subject to a stronger many-body interaction which implies a distribution of the spectral weight in energy and momentum. Indications of strong many-body effects on clean Pt(110) and Br/Pt(110), namely the unusually diffuse spectral weight distribution [13] and a renormalization of the band dispersion near $E_F$ have been observed before [28]. The renormalization sets in at binding energies of a few hundred milli-electron-volt which—in a weak coupling approximation—excludes phonons as
the bosonic excitation coupling with the electrons. In a number of correlated systems, a strong-coupling, Frank–Condon-like scenario has recently been used to explain the creation of many vibrational quanta during the electronic transition (see e.g. [51]). This scenario, however, requires rather localized (0D) states whereas the electronic states on Pt(110) under consideration are well delocalized in 1D and represent a very good metal in the chain direction. Magnetic excitations could play a role, but very recent work indicates also the importance of the electron–plasmon interaction [52] and a generic renormalization for any correlated metal on the verge of localization (three-peak spectral function [53]). The above interpretation of the temperature dependency is supported by the observation of identical temperature dependencies of ARPES spectra in various 2D metals [12, 15] including high-$T_c$ superconductors (e.g. [30]) and Q1D systems [31]–[33]. As a crossover from coherent to incoherent $z$-axis transport ([14] and references therein) is observed in the 2D metals, the intensity loss observed of the QP peak at $E_F$ has been taken to be a fingerprint of this dimensional crossover [12, 13, 28]. Turning the argument around, correlated metals with low QP dispersion will show a strong temperature-induced decay of the QP intensity.

Considering the low-dimensional band topology of the Pt(110) surface which promotes many-body effects, it is interesting to note that the DFT calculations for the free standing chain [44, 45] find a ferromagnetic instability with substantial magnetic moments around $1\mu_B$ at atomic distances greater than 2.6 Å. According to the calculations, the instability is related to a divergence in the susceptibility caused by a vHS at the $\bar{X}$ point at $E_F$. In the case of the clean Pt(110) surface, the atomic distance in the close-packed rows is 2.77 Å and, as shown above, the saddle point at $\bar{X}$ or $\bar{S}$ also provides a vHS with a high DOS at $E_F$. Thus, magnetic interactions have to be seriously considered in the description of the clean surface, which is also clear from the importance of spin fluctuations even in the bulk material. If indeed some magnetic order in the chains is surviving on the surface, one could even speculate about a Kondo-like scenario, in which the magnetic moment of the chain is screened by the bulk electrons. The $d^9$-configuration of Pt would be compatible with a Kondo-resonance below $E_F$ leading to an intense peak below $E_F$ in the ARPES spectra.

4. Summary and conclusion

The unusual temperature-behaviour of a sharp QP peak near $E_F$ at $\bar{S}$ as observed in the low-dimensional surface Br/Pt(110)$-c(2 \times 2)$ is evident also on the clean Pt(110)-mr surface. This suggests a common origin and supports the assignment of the QP peak to a surface resonance deriving from the bulk bands projecting to $\bar{S}$. Consequently, we conclude that it is the band topology of bulk platinum and its projection on to Pt(110) which makes this anisotropic surface and its adsorbate-covered variants a useful Q1D model system. This observation is of general relevance since similar resonances are anticipated on surfaces of other transition metals such as Pd, thus establishing a new class of low-dimensional surface model systems. As these surfaces combine high DOS at $E_F$, a highly ordered surface, and a crystal unit cell of low complexity, experimental and theoretical investigations may lead to a better understanding of low-dimensional systems and the many-body problem in general. A comparison of Pt and Pd, for example, would be interesting because the bulk band structure is very similar, but the spin–orbit coupling in Pd is much weaker.

Comparing the EDCs and dispersion plots with calculated band structures, we show here how the surface resonance derives from the flat bulk band structure. A prominent peak in
photoemission signals a large DOS at the fermi energy $E_F$ which is related to a saddle point within the 2D band structure. Band dispersion and polarization dependency yield more information about the Pt orbitals which create this surface resonance. The photoemission intensity shows the peculiar dependency on temperature and other external changes (adsorbates) which is typical of the behaviour of QP peaks in low-dimensional and strongly correlated systems [12, 13, 15], [30]–[32], [54, 55].

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