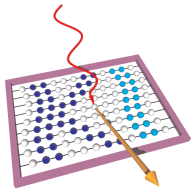

Valence band photoemission and many body effects in $TiTe_2$

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Introduction

Correlation has drawn interest to the photoemission of the two dimensional system $TiTe_2$. Especially the feature of containing one single 3d peak which is uniquelly related to a specific electronic transition allows a line shape analysis together with the investigation of a fermi liquid behaviour.

We derive the self-energy for $TiTe_2$ on the basis of the GW approximation. Results for the energy dependence as well as for the k - dependence of the matrix of Σ are presented.
We examine the influence of the optical potential on the scattering states of photoemission as well as the self-energy for the valence states derived on the basis of the GW approximation. In this contribution photoemission spectra of the (1000) surface calculated within the highly accurate one-step model are shown, demonstrating the influence of many body effects in the angular distribution and in the normal emission spectra. For comparison we also calculate photoemission spectra with a widely used energy dependent optical potential. Furthermore the influence of the GW self-energy on the electron escape depth is shown.

A second experimental tool for examining the final state band structure is the target current spectroscopy (TCS). We calculate TCS spectra for the two cases of an empirical and the GW self-energy.

In the past much work was done in mapping the Fermi surface from photoemission data. Calculating the photocurrent from the Fermi energy in a specific high symmetric direction, we present the relation between structures in the photoemission and the underlying Fermi surface.

Numerical Details:

- one- step model

initial states:

- LCAO
- Half space Green' s function

final states:

- Hamann Schlüter pseudopotential in a quasi-local representation
- time reversed LEED state

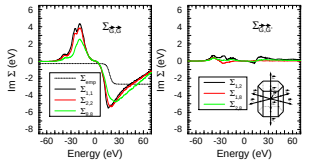
Σ in the GW approximation:

$$\Sigma_{G_1,G_2}(\vec{k},\omega) = \frac{ie^2}{(2\pi)^4\varepsilon_0}\int d\vec{w}\sum_{\vec{G}}\int d\omega' \frac{1}{(\vec{k}-\vec{k}+\vec{G}_1-\vec{G})^2+\frac{\kappa_0^2}{\varepsilon^{-1}(\vec{G})}} e^{i\omega' t} Q_{\vec{G}',\vec{G}'+\vec{G}_2-\vec{G}_1}(\vec{k},\omega+\omega')$$

URL: http://www.tp.cau.de/schattke/

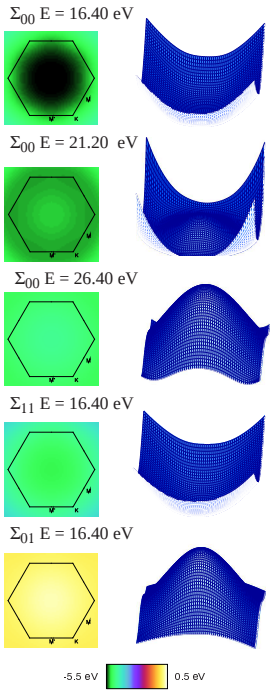
$TiTe_2$ - GW self-energy

Energy dependence of the self-energy for **k**=Γ



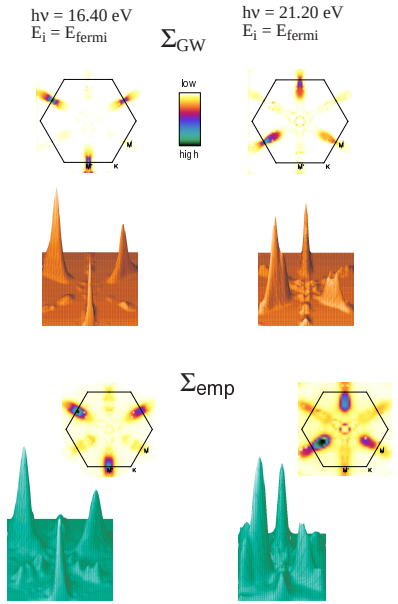
- Calculated V_{opt} shows an increased damping compared to the usual empircal fit by a function of energy
- The strongest damping appears at energies near the plasma frequency

$\mathbf{k}_{||}$ dependence of the GW self-energy for different energies



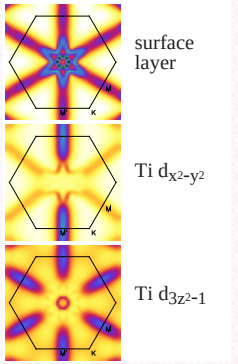
- The modulation of Σ in $k_{||}$ is of the same magnitude as the differences between the diagonal or the off- diagonal elements of Σ(E)

GW-Σ and photoemission

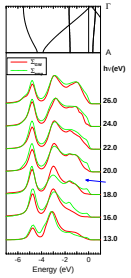


- The patterns change drastically with photon energy
- GW improves remarkably the agreement with experiment

Density of states

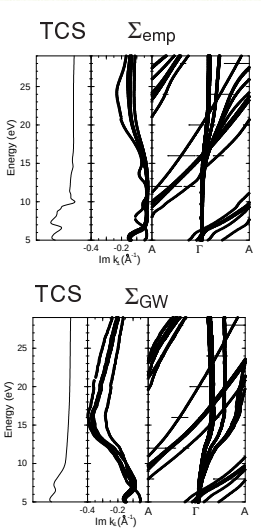


Photoemission in normal emission



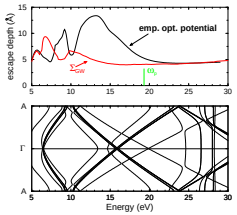
- The influence of Σ_{GW} is strongest near the plasma frequency

Complex band structure and TCS



- Σ_{GW} enhances the damping for lower final state energies
- The TCS spectra show less structure with Σ_{GW}

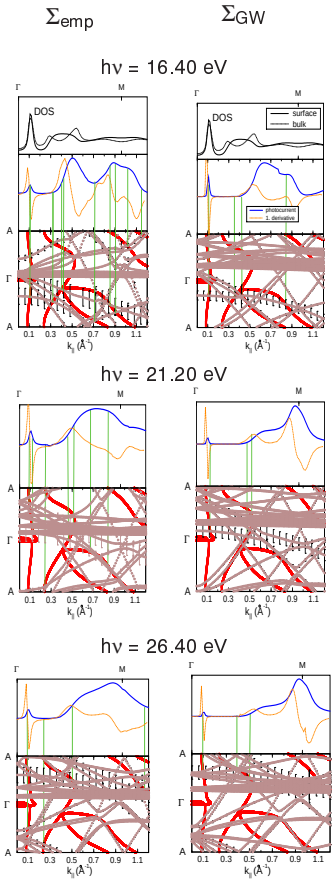
Escape Depth



- At low energies the escape depth is strongly dependent on the band structure

Mapping the Fermi surface

Comparison of the photocurrent from the Fermi energy in direction of ΓM with the direct transitions from the Fermi surface (red) to the complex final bands



- The Fermi surface is not simply mapped by the maximum in the photocurrent
- Also the maximas in the first derivative with respect to $k_{||}$ does not map the Fermi surface