AZIMUTHAL DEPENDENCE OF GAAS(110) ULTRAVIOLET PHOTOEMISSION SPECTRA

C. Solterbeck, W. Schattke

Institut für Theoretische Physik, Christian-Albrechts-Universität Kiel, Leibnizstr. 15, D-24098 Kiel, Germany

J.-W. Zahlmann-Nowitzki, K.-U. Gawlik, L. Kipp, M. Skibowski

Institut für Experimentalphysik, Christian-Albrechts-Universität Kiel, Leibnizstr. 19, D-24098 Kiel, Germany

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Theory

- The photocurrent is calculated within the one step model by a golden rule formula:

$$I \propto \kappa \sum_j \left| \langle \phi^*_{LEED} \left| \mathbf{A} \cdot \hat{\mathbf{p}} \right| \psi_j^{initial} \rangle \right|^2 \delta \left(E_j + h\nu - E_{fin} \right)$$

- With a LCAO basis of layer bloch sums and the extended Hückel theory the overlap matrix, the Hamilton matrix, the Greens matrix, and the surface density of states (SDOS) are computed for the halfspace. The initial state is described by the Greens matrix.

- The final state is a time inverted LEED state. To calculate it, the solutions of the complex band structure inside the crystal are matched to the correct asymptotic in the vacuum. In the case of the EDC, single plane waves were used for simplification.

Experiment

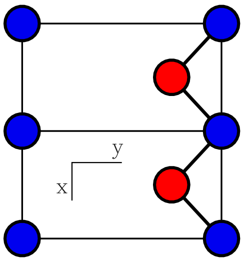
- The measurements were carried out with unpolarized HeI_α-radiation ($h\nu = 21.22\ eV$) using a spherical energy analyzer mounted on a two-axis-goniometer. The sample was kept fixed during the computer controlled rotation of the electron analyzer.
- The energy resolution of the analyzer was chosen to be 130 meV and the angular acceptance was about $\pm 0.5°$. The accuracy of the angular adjustment was $\pm 0.1°$.
- The sample was an UHV-cleaved doped GaAs single crystal.
- No background was subtracted.

Summary and Conclusions

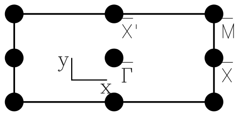
- First measurements and calculations of azimuthal valence band photoemission scans of the clean GaAs(110) surface are presented. There is an excellent agreement between experiment and theory.
- The azimuthal scans show distinct topologies. They seem to be controlled by the anisotropy of the electronic structure of the initial states. This is illustrated for the example of the dangling bond band.
- The azimuthal pattern varies strongly with the binding energy.
- The influence of different directions of the incident light is studied. It causes a modulation of the intensities, which are amplified in the forward direction of the parallel part of the incoming light.

Geometric and Electronic Structure

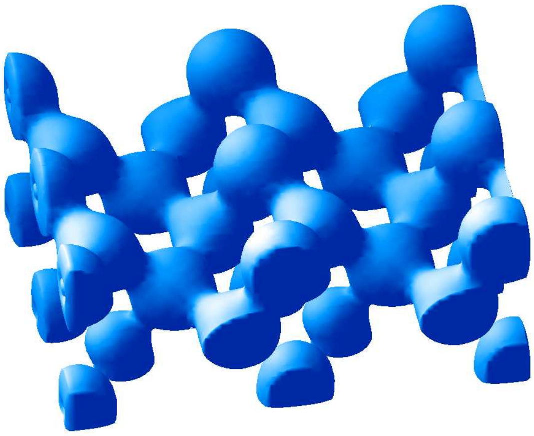
unit cells



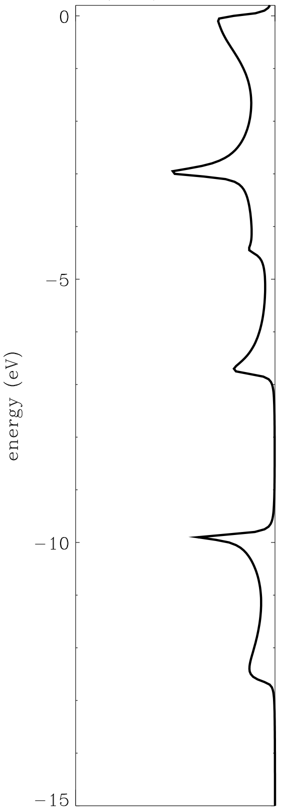
Brillouin zone



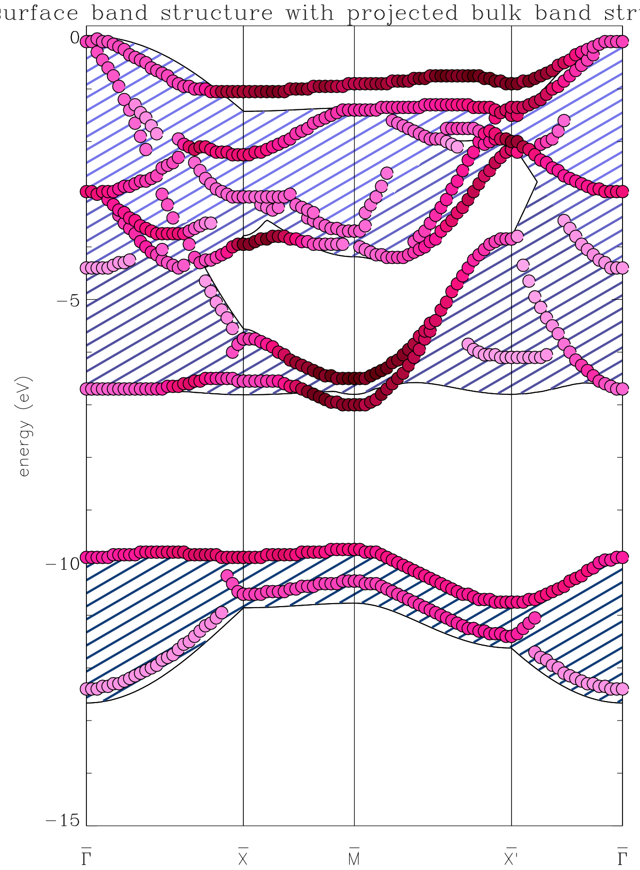
charge density

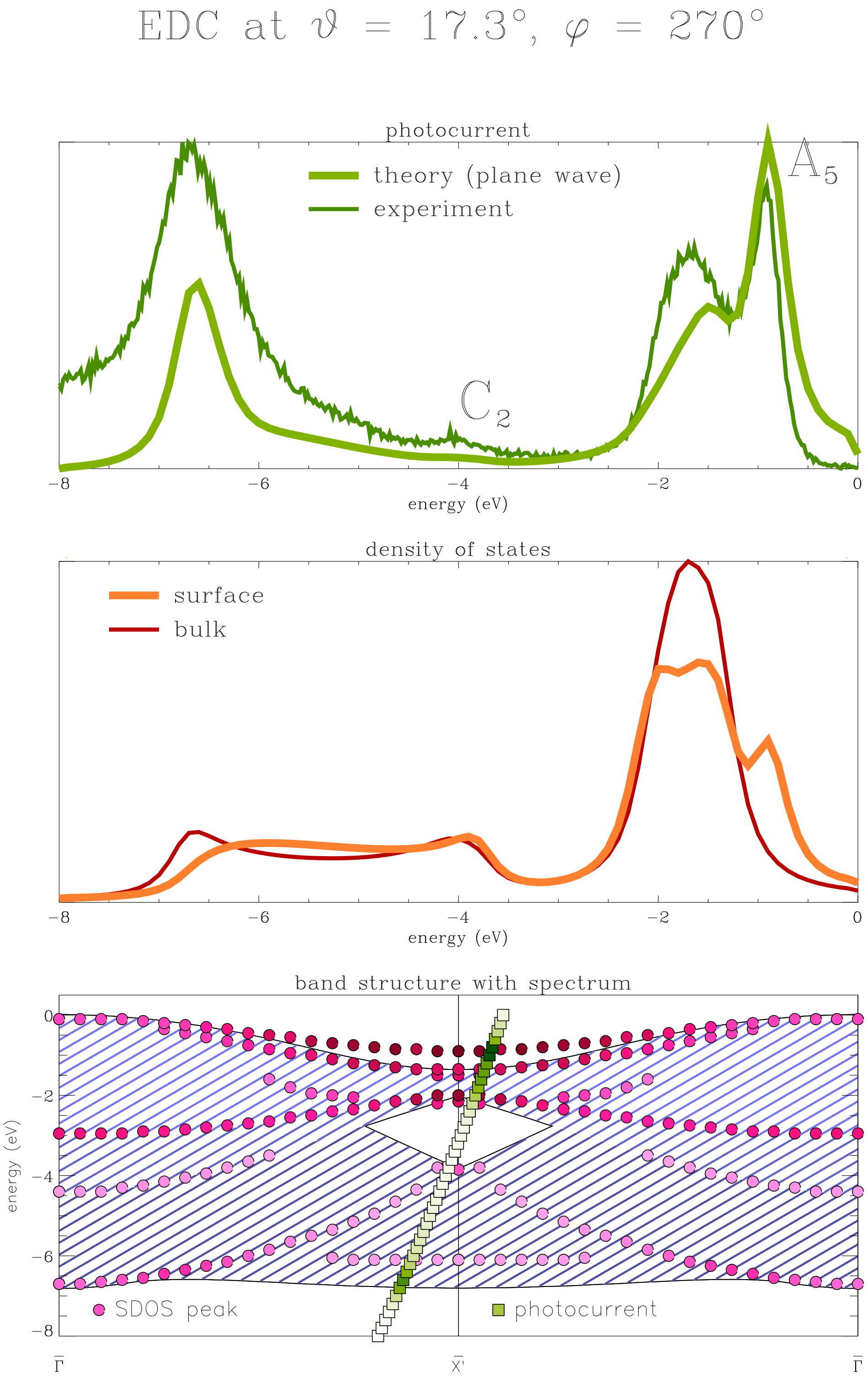


SDOS in $\overline{\Gamma}$



surface band structure with projected bulk band structure

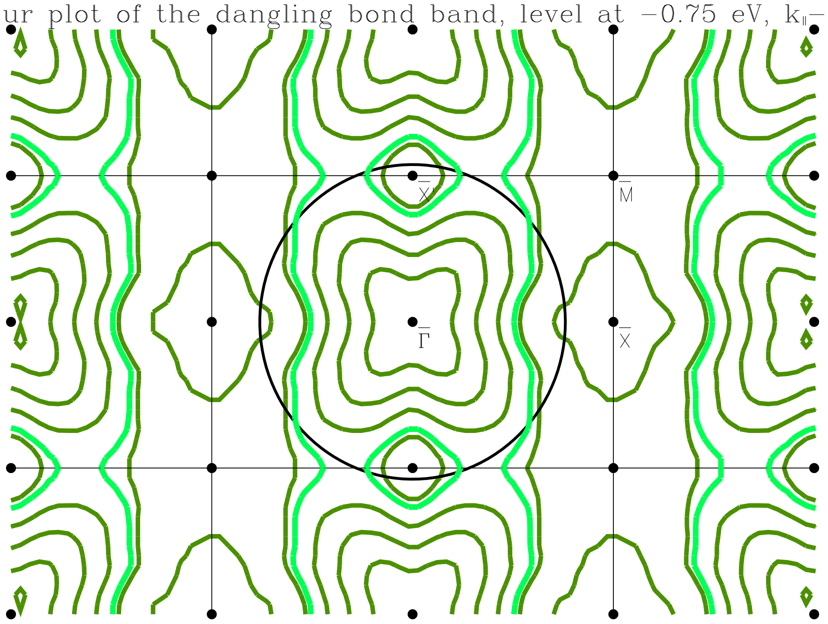




EDC at ϑ = 17.3°, φ = 270°
photocurrent
theory (plane wave)
experiment
A5
C2
−8
−6
−4
−2
0
energy (eV)
density of states
surface
bulk
−8
−6
−4
−2
0
energy (eV)
band structure with spectrum
0
−2
−4
−6
−8
energy (eV)
SDOS peak
photocurrent
Γ̄
X̄'
Γ̄

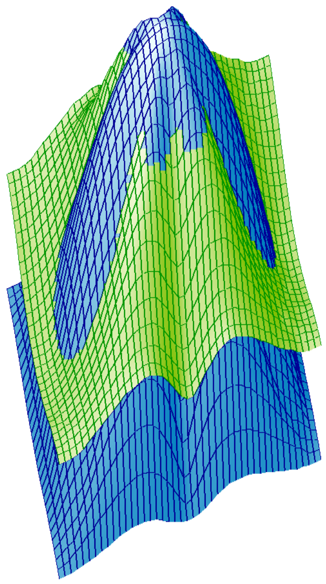
dangling bond band

contour plot of the dangling bond band, level at -0.75 eV, $k_\parallel$-values

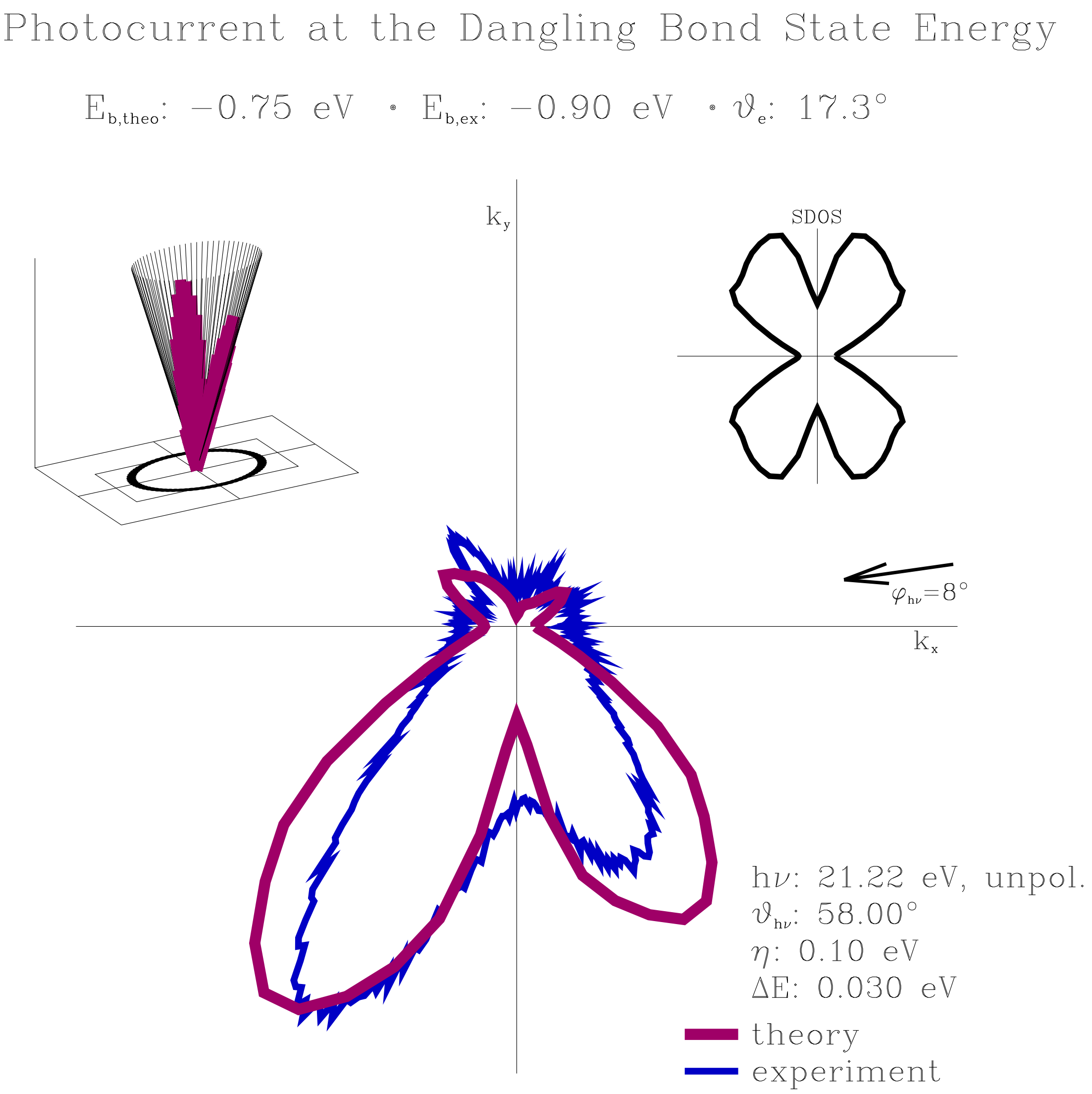


perspective view of the dangling bond band

alone



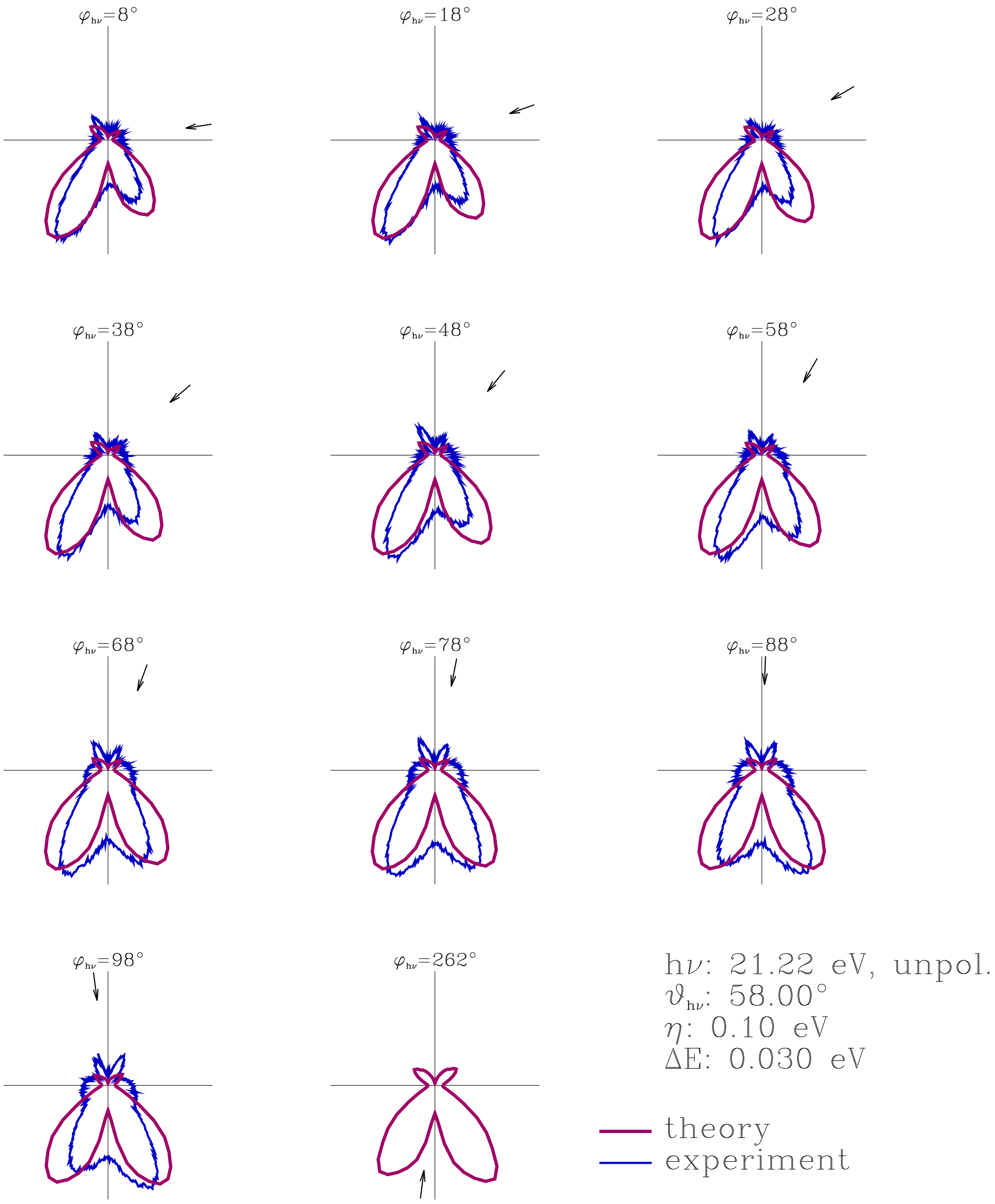
intersecting the projected bulk band structure



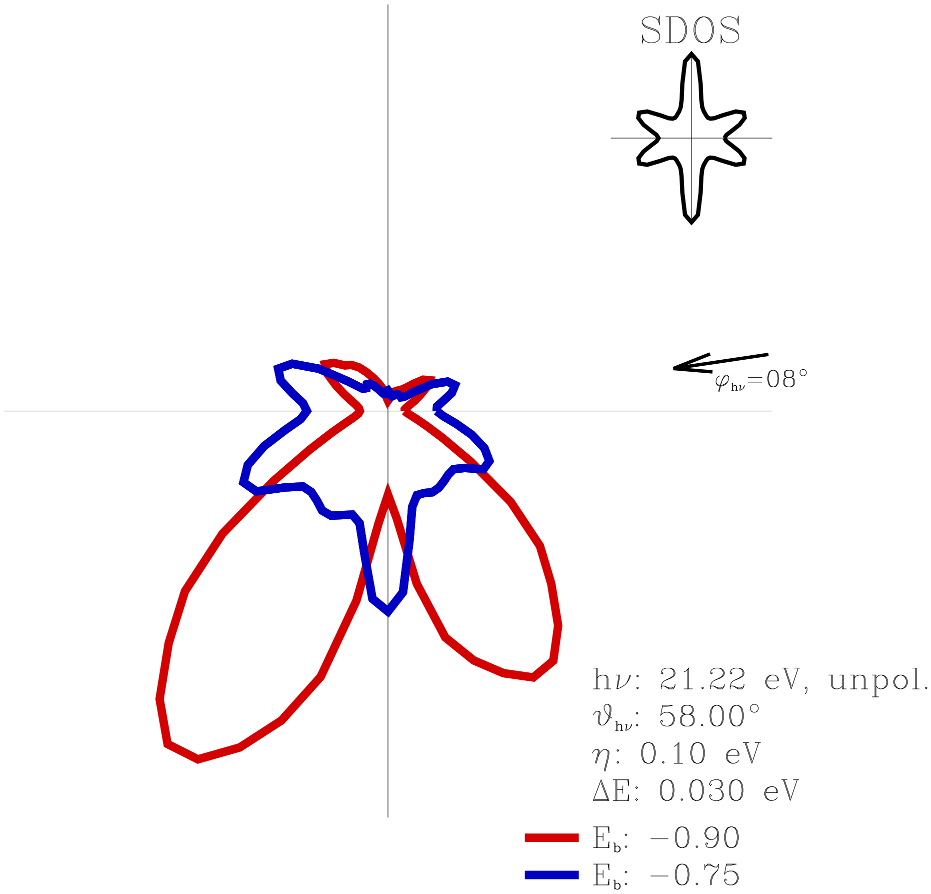
Photocurrent at the Dangling Bond State Energy
$E_{b,theo}$: −0.75 eV • $E_{b,ex}$: −0.90 eV • ϑ_e: 17.3°
k_y
SDOS
$\varphi_{h\nu}$=8°
k_x
$h\nu$: 21.22 eV, unpol.
$\vartheta_{h\nu}$: 58.00°
η: 0.10 eV
ΔE: 0.030 eV
theory
experiment

Dependence on the Incidence of Light

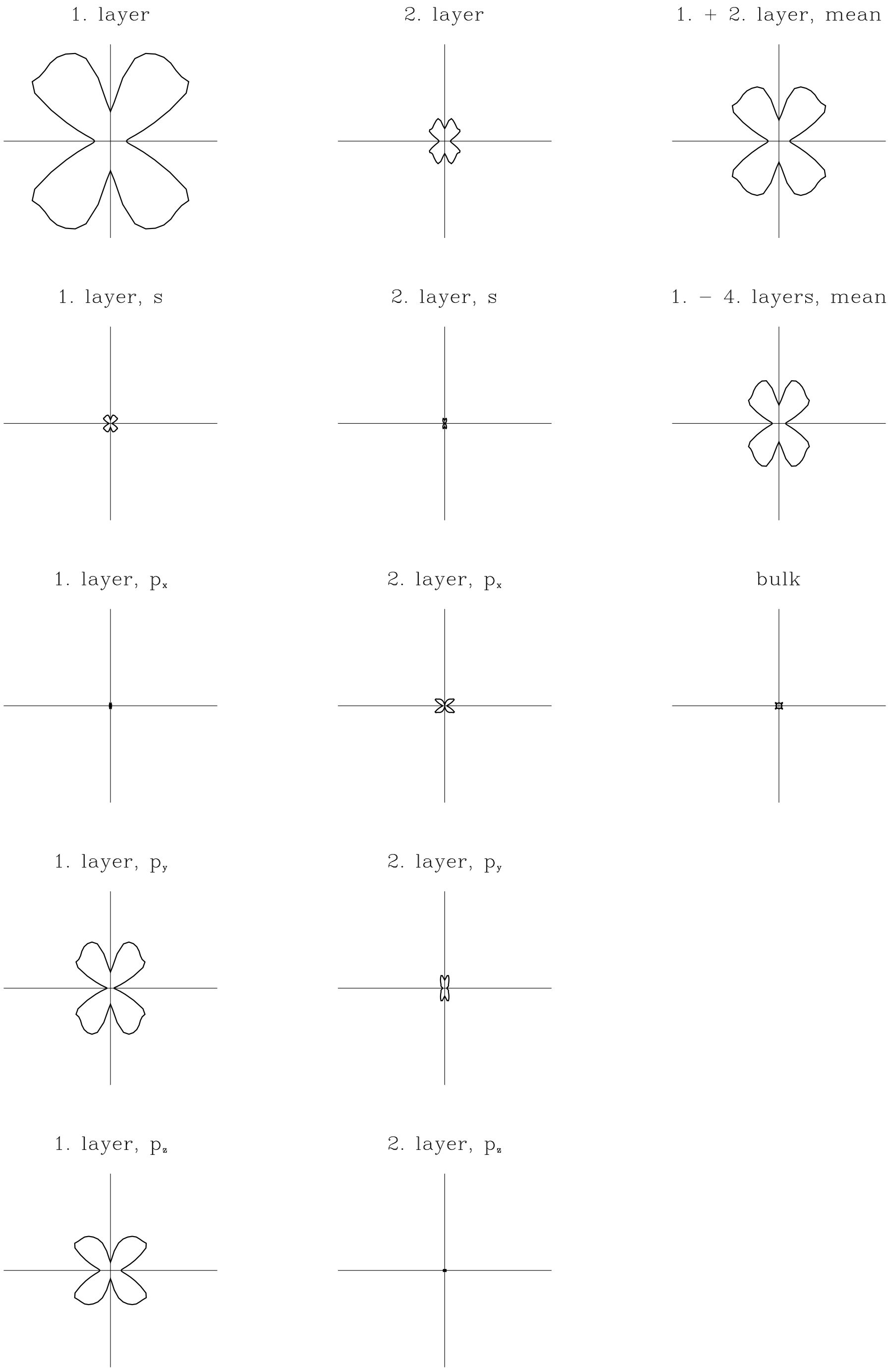
GaAs(110) • $E_{b,theo}$: −0.75 eV • $E_{b,ex}$: −0.90 eV • ϑ_e: 17.3°



Theoretical Currents at Different Energies

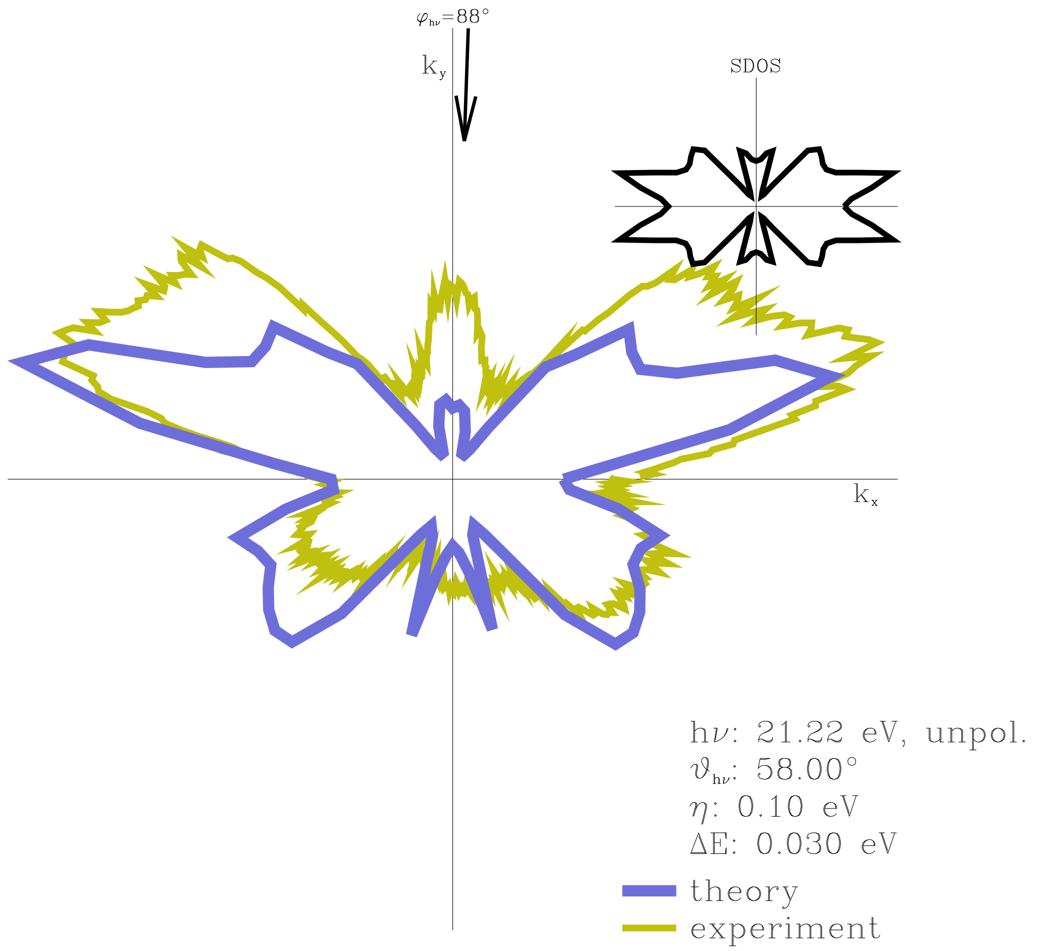


Density of States • E_b: −0.75 eV



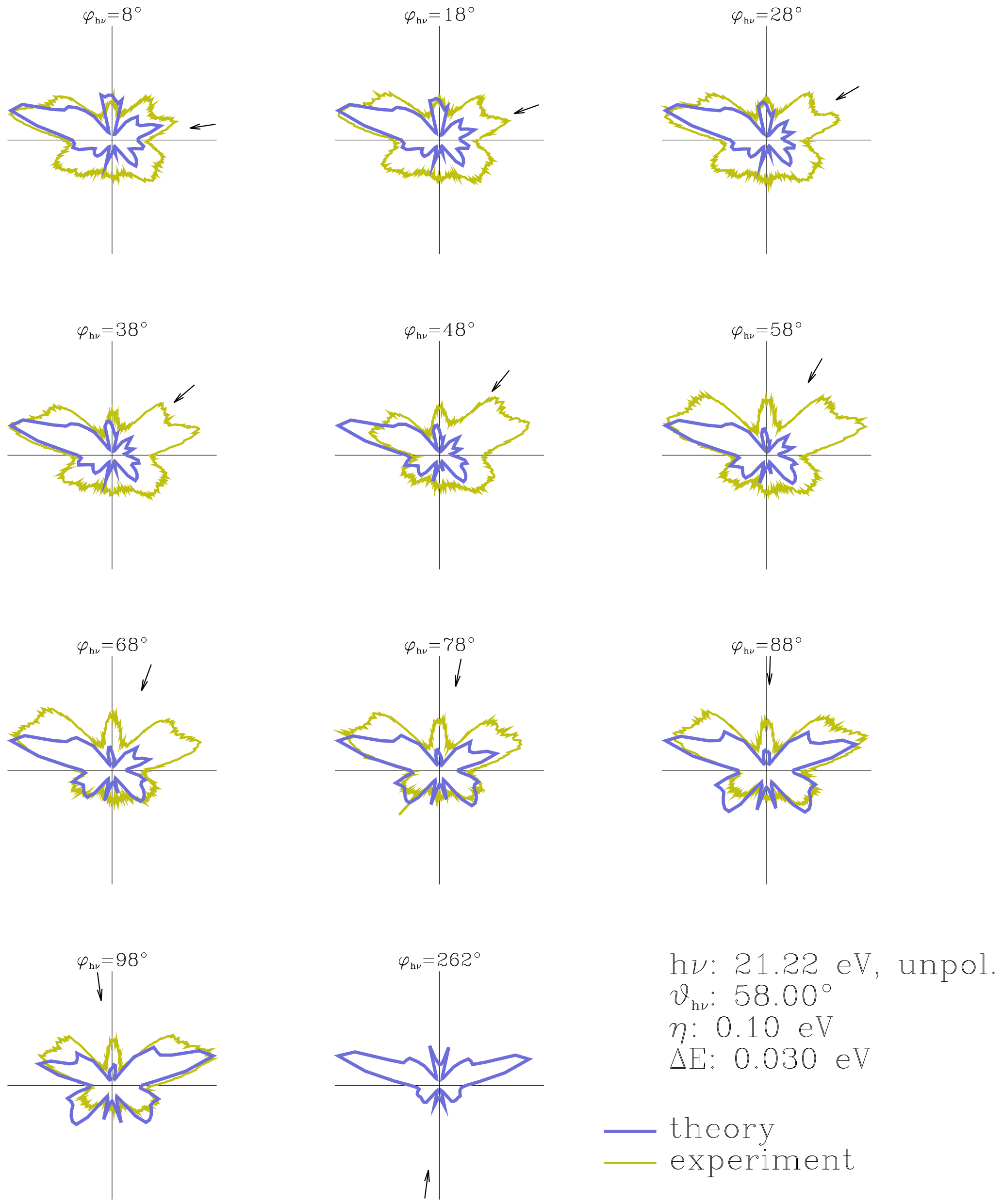
Photocurrent at the Ga Back Bond State Energy

$E_{b,theo}$: −4.00 eV • $E_{b,ex}$: −4.00 eV • ϑ_e: 19.4°



Dependence on the Incidence of Light

GaAs(110) • $E_{b,theo}$: −4.00 eV • $E_{b,ex}$: −4.00 eV • ϑ_e: 19.4°



Density of States • E_b: −4.00 eV