substance: gallium sulfide (GaS)
property: band structure, direct energy gap

The best known polytype is β-GaS.

band structure

see Fig. 1; Brillouin zone, Fig. 2; XPS-spectrum, Fig. 3.
GaS is an indirect gap semiconductor. The electronic band structure is very similar to that of GaSe. The valence band maximum is at the Γ-point The conduction band is characterized by 6 equivalent minima at the M point.

direct gap

$E_{g,dir}(\Gamma_{4v}^{-}–\Gamma_{3c}^{+})$	3.050(2) eV	T = 77 K	optical absorption	69A
	3.065 eV	T = 77 K	electroabsorption	77G

pressure coefficient of $E_{g,dir}$

$dE_{g,dir}/dp$	$-2.0(5)\cdot10^{-6}$ eV bar^{-1}	T = 77 K, p < 6 kbar	optical absorption in excitonic region	78M

References:

69A Aulich, E., Brebner, J. L., Mooser, E.: Phys. Status Solidi 31 (1969) 129.

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79A Antonangeli, F., Piacentini, M., Baizarotti, A., Grasso, V., Girlanda, R., Doni, E.: Nuovo Cimento B 51 (1979) 181.

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Fig. 1.
GaS. Empirical pseudopotential band structure for the β–polytype [81D].

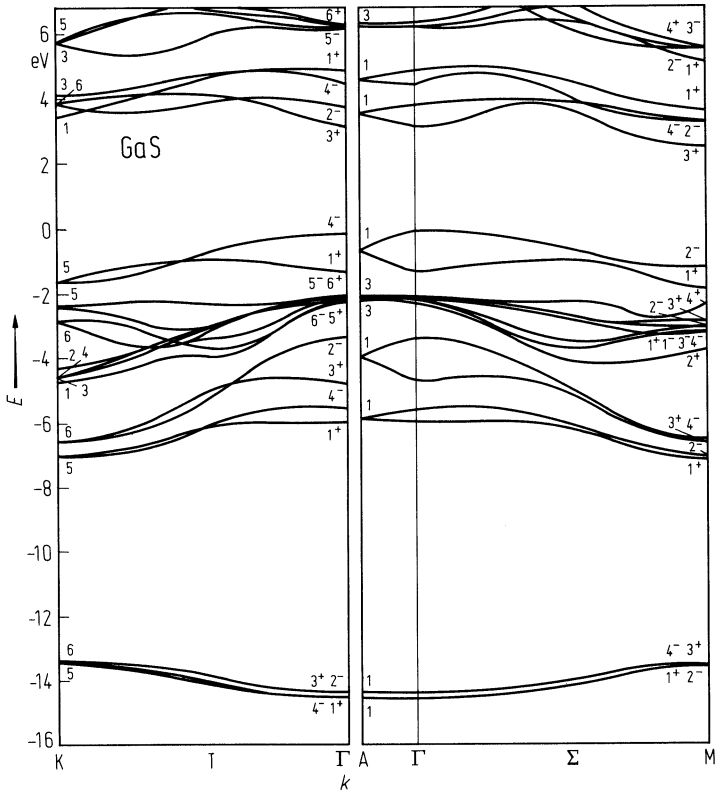

Fig. 2.
Brillouin zone for the hexagonal lattice. g_1, g_2, g_3: reciprocal basis vectors; $g_1 \parallel k_x$, $g_3 \parallel k_z$.

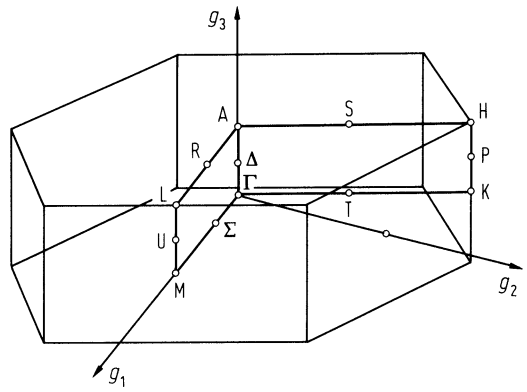

Fig. 3.
GaS, GaSe, InSe. XPS-number of electrons vs. electron binding energy. The zero of energy corresponds to the upper valence band edge. Peaks α_3 and G are spurious and most probably due to the unmonochromatized AlK_α X-ray source used in the experiment. Peak A is the contribution of the uppermost valence bands which are essentially formed by the chalcogen s–p_z-orbitals. Peak B corresponds to the contribution of the chalcogen p_{xy} states, peaks E, C to that of the cation s-states and peak F to that of the chalcogen s-electrons (S3s, Se4s) [79A].