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Electronic structure of $GeS_{0.5}Se_{0.5}$ crystal: band alignment, valence bands, and core-levels

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The GeS_xSe_{1-x} materials are semiconducting alloys considered as promising absorbers in photovoltaic.[1] Although, the high applicable potential of GeS_xSe_{1-x}, many of their fundamental optoelectronic properties are poorly explored. We present comprehensive experimental and theoretical investigations on the electronic structure of the $GeS_{0.5}Se_{0.5}$ crystal. As confirmed by transmission electron microscopy and synchrotron radiation based X-ray photoelectron spectroscopy (SR-XPS), the studied crystals, prepared by melt-growth technique, exhibit high and crystalline quality and phase purity. By combination of XPS with the optical absorption and photoreflectance spectroscopy, the band energy diagram of $GeS_{0.5}Se_{0.5}$ is driven. Herein, the ionization potential of 5.7 eV is determined based on XPS investigations, whereas the optical spectra reveal the direct character of the fundamental optical bandgap with the energy of

1.37 eV at room temperature. The optical transition is highly sensitive to the incident light beam polarization, which indicates the anisotropy of the optical properties. The total density of states obtained by calculations based on density functional theory is in a reasonable agreement with the valence band spectra measured by SR-XPS. The theoretical results highlight the presence of Ge 4s states at the valence band edge desirable for photovoltaic absorbers.

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References

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