# Electronic and optical properties of the $TlInS_2$ crystal: theoretical and experimental study

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Recently layered crystals have attracted research interest due to promising structural and physical properties. A possibility to create new multifunctional artificial materials obtained through the arrangement of several layered crystals became a new subject of studies. One of the representatives of such class of materials is a $TlInS_2$ crystal [1] which belongs to the $A^{III}B^{III}C^{VI}_2$ group of chalcogenide semiconductors, and it is regarded as a one of the highly anisotropic structures [2]. This material possesses both high- ($\beta$) and low-temperature ($\alpha$) phases [3]. Electrical measurements show its strong anisotropy of conductivity, which for $TlInS_2$ is rather temperature independent.

These features motivate us to carry out quantum mechanical calculations of physical properties of $TlInS_2$ crystal in combination with the experimental measurements of its optical characteristics. $TlInS_2$ crystal has a prominent layered structure with two layers in the unit cell which is characterized by the so-called van der Waals (vdW) gap. In this case, first principle calculations of electronic and optical properties of the $TlInS_2$ crystal have been carried out using a combination of the density functional theory (DFT) supplied with a dispersion correction (D). The DFT-D correction enables to perform geometry optimization of the considered layered structure in a correct way. In the framework of this approach, a value of the obtained band gap of $TlInS_2$ was 1.37 eV. Experimental results report the optical band gap to be $E_g^d$=2.33 eV (direct band) and $E_g^i$=2.28 eV (indirect band) [2]. In this case, to improve our bandgap calculation, the Hubbard correction was included. The Hubbard parameter was applied for *d* orbitals of Tl atom. Hence, the energy band spectra within the DFT-D+*U* approaches were calculated for the first time for this material. In experimental measurements, the spin-orbit split-off band in the valence band located at 2.87 eV at 10 K in the Γ point was observed [3]. Therefore, the spin-orbit interaction was included in our calculation. Accordingly, optical properties such as the refractive indices, dielectric constants, and absorption coefficients were calculated for the first time for the $TlInS_2$ crystal using the DFT-D+*U* approaches. The obtained results were compared with the experimentally measured optical parameters of the $TlInS_2$ crystal.

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