Comparative investigation of bulk and nanolayered properties of perspective $TlInS_2$ ferroelectric

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General information

Nanomaterials occupy one of the leading places in searching for new promising materials suitable for functional electronics and alternative energy sources. Triple thallium chalcogenides with a strongly anisotropic structure in the form of tightly bonded layer packages separated by weakly van der Waals interacted gaps, are favorable for the formation of the wide variety of nanostructures for different applications [1]. Therefore, at the stage of searching for new materials that would be characterized by predictable and controlled physical properties, we propose to investigate the evolution of electronic properties of $TlInS_2$ material depending on its thickness (the number of monolayers).

Calculation Method

Quantum-ESPRESSO program package [2], DFT-D approach / TS correction, ultrasoft Vanderbilt pseudopotentials, general gradient approximation (GGA) with the PBE parameterization

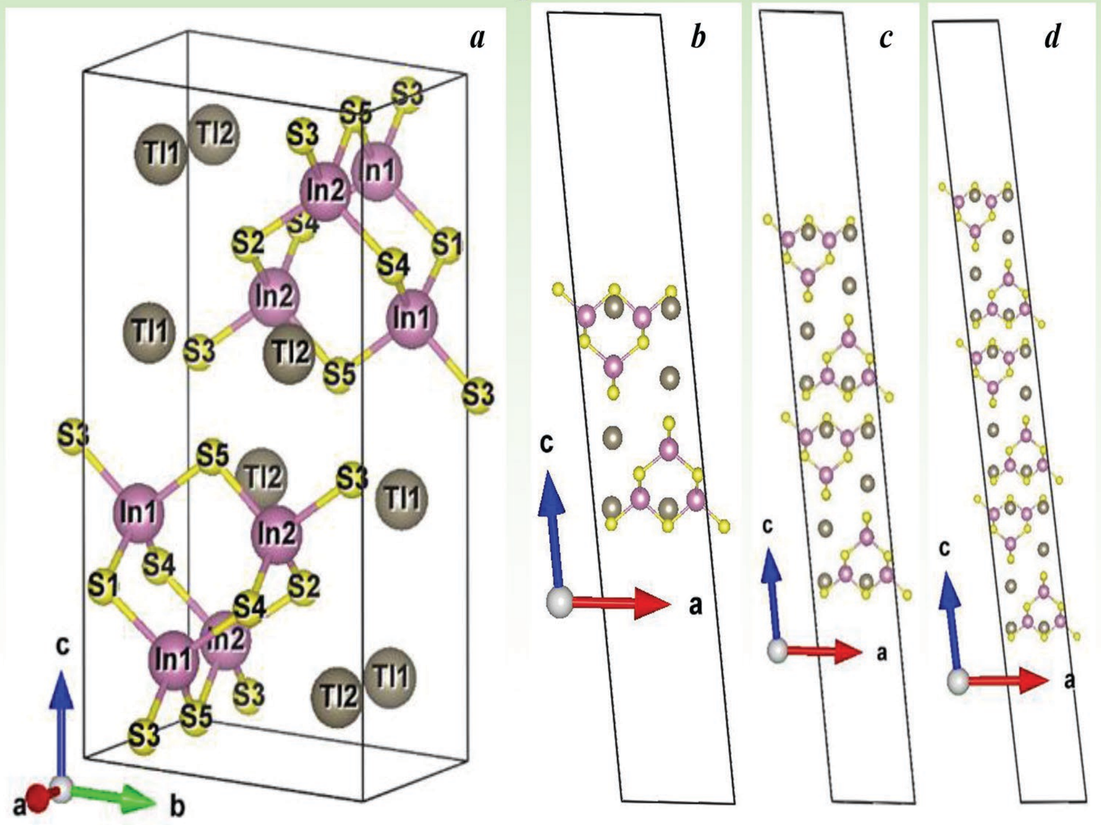
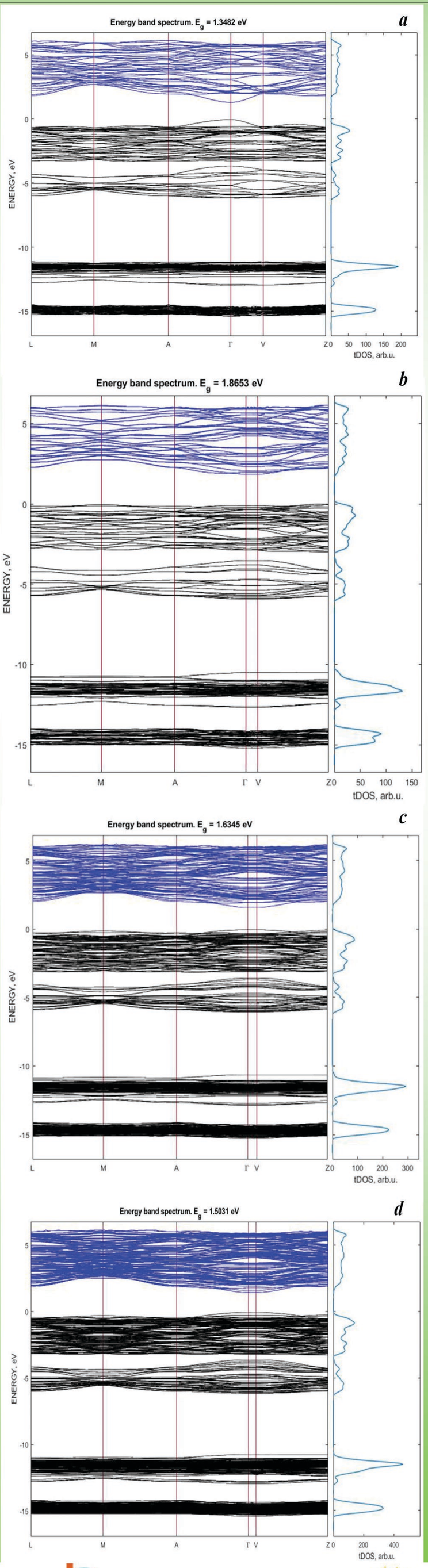


Fig. 1. Primitive cells of the bulk crystal (a) and structures with 1 (b), 2 (c) and 3 (d) layers of $TlInS_2$.

Table 1.
Parameters of $TlInS_2$ structure with different layers quantity

Structure	Num. of atoms	c, Å	V, Å^3	E_g, eV
$TlInS_2$ bulk	32	15.27	911.51	1.35
$TlInS_2$ 1 layer	32	45.56	2670.98	1.87
$TlInS_2$ 2 layers	64	60.75	3561.30	1.64
$TlInS_2$ 3 layers	96	75.93	4451.63	1.50

Fig. 2. Electronic band structures of bulk crystal (a),1 layer (b), 2 layers (c) and 3 layers (d) of $TlInS_2$ obtained in DFT(D) approach →



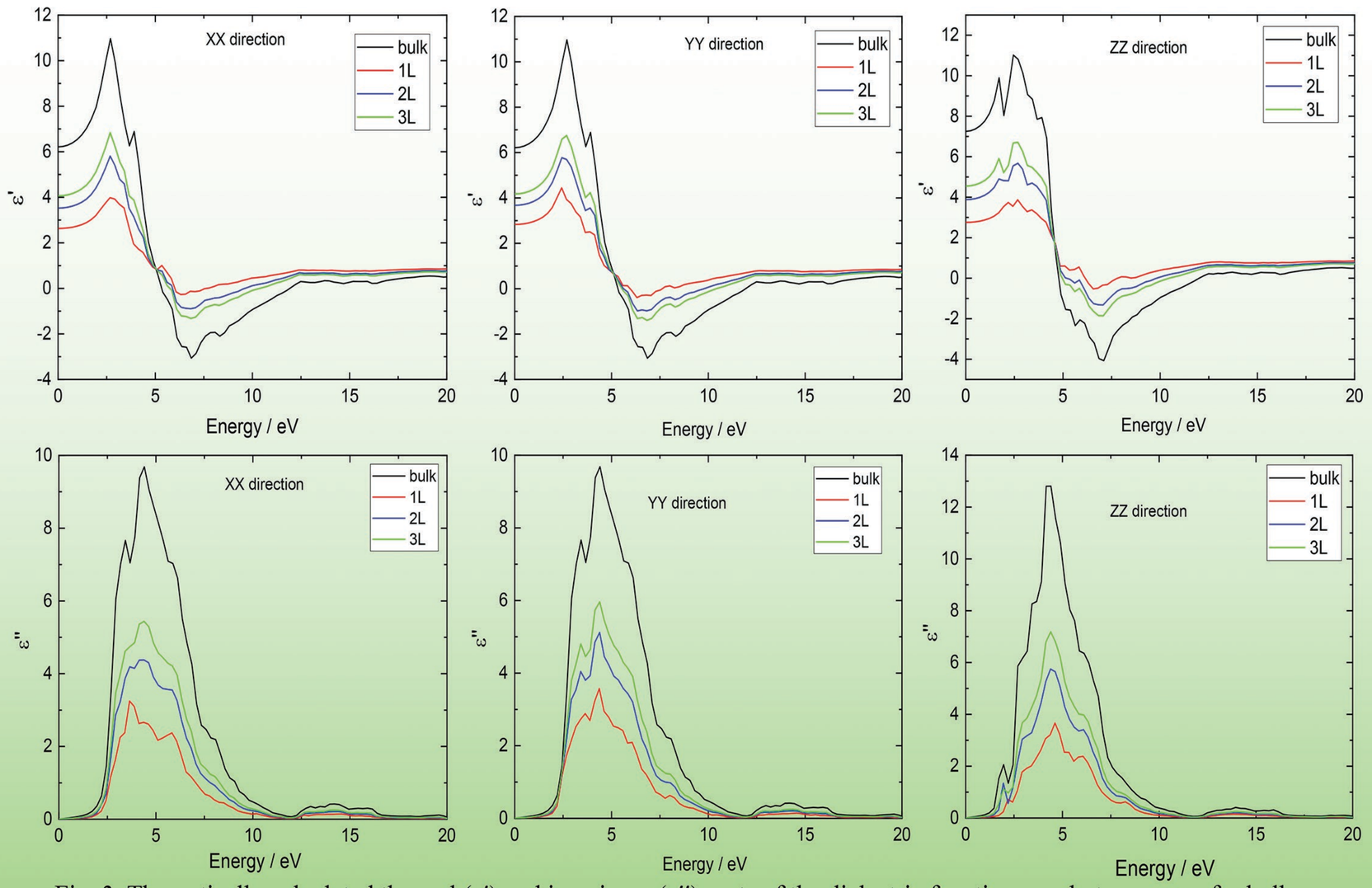


Fig. 3. Theoretically calculated the real (ε') and imaginary (ε'') parts of the dielectric function vs. photon energy for bulk, 1 layer, 2 layers and 3 layers of $TlInS_2$ in the XX, YY and ZZ directions

Conclusions. Physical properties of the $TlInS_2$ crystal in nanolayered form have been investigated theoretically using the DFT method augmented by disperssion correction are reported and the obtained results are compared to the bulk material parameters. The dependences of electronic and optical properties of the modeled material versus its thin-film thickness were simulated. The significant influence of the $TlInS_2$ slab thickness on its bandgap value was found. In addition, the real and imaginary parts of the dielectric function vs. photon energy for 1 layer, 2 layers and 3 layers of $TlInS_2$ in the XX, YY and ZZ directions were presented.

Literature

[1] Guler, I., Gasanly, N. , Thin Solid Films.-2020.-704.-p.137985.
[2] P. Giannozzi, S. Baroni, N. Bonini, et al., J. Phys.: Condens. Matter 21, 395502 (2009).