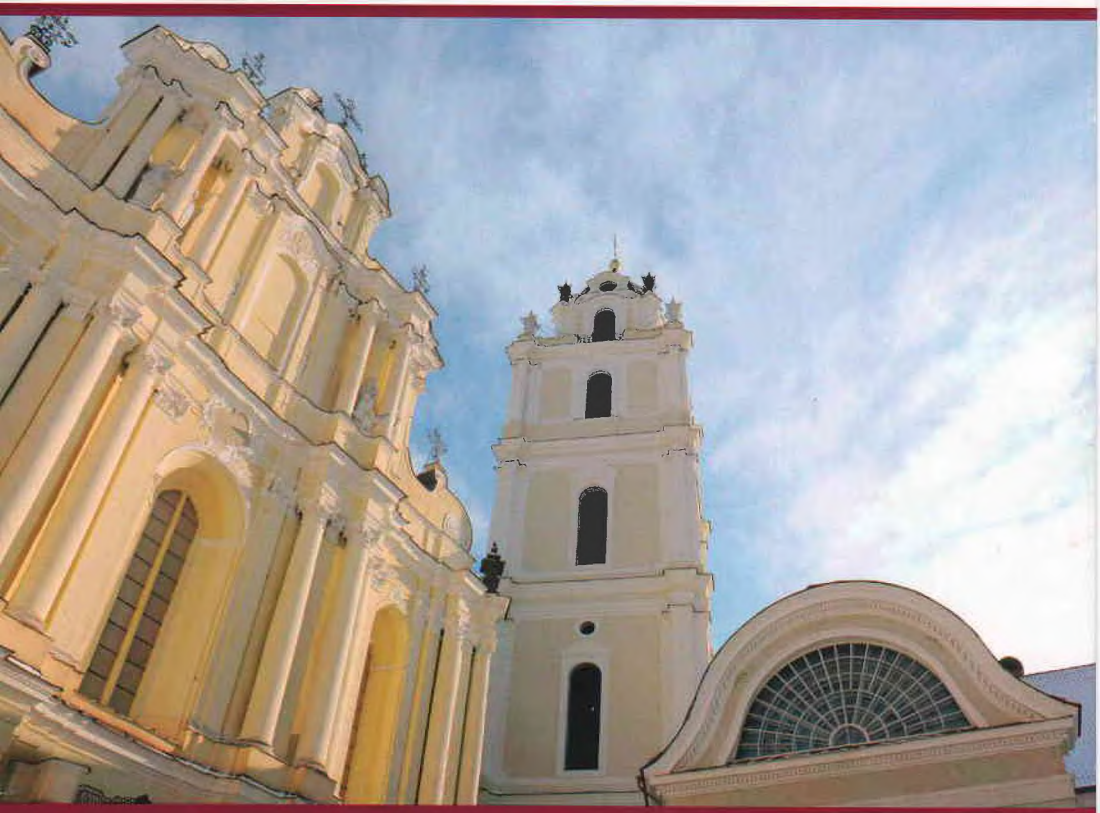
SEMINAR

NEW MULTIFEROICS AND SUPERIONIC CONDUCTORS FOR ACUSTOELECTRONICS AND SOLID STATE IONICS

PROGRAM AND BOOK OF ABSTRACTS



10 OCTOBER 2017

VILNIUS / LITHUANIA

PROGRAM

(NFTMC, Saulėtekio av. 3)

10:00–10:10 Opening remarks (prof. J. Banys)

10:10–10:30 R. Yevych, M. Medulych, I. Zamaraite, A. Dziaugys, J. Banys, **Yulian Vysochanskii**

Nonlinear dynamics of phosphorous chalcogenide ferroelectrics with many-well local potentials

10:30–10:50 **Andrius Džiaugys**, M. Chyasnavichyus, A. Belianinov, Q. He, A. Borisevich, A. N. Morozovska, E. A. Eliseev, J. Banys, Y. Vysochanskii, S.V. Kalinin, P. Maksymovych

Polarization domains in the layered ferroelectrics $CuInP_2(S,Se)_6$

10:50–11:20 **Edvardas Kazakevičius**, V. Venckutė, S. Kazlauskas, A. Kežionis, R. Korobko, T. Šalkus

High frequency impedance spectroscopy study on Gd-DOPED CeO_2 thin films

11:20–12:00 *Coffee break*

12:00–12:20 **Ihor Studenyak**, M. Luchynets, V Izai, A. Pogodin, O. Kokhan, A. Kežionis, T. Šalkus, J. Banys

Phase transitions in Cu_6PS_5Br-Cu_7PS_6 mixed crystals

12:20–12:40 I. Anusca, S. Balčiūnas, P. Gemeiner, Š. Svirskas, M. Sanlialp, G. Lackner, C. Fettkenhauer, J. Belovickis, V. Samulionis, M. Ivanov, B. Dkhil, **Jūras Banys**, V. V. Shvartsman, D. C. Lupascu

Dielectric Response of the Methylammonium Lead Halide Solar Cell Absorbers

12:40–13:00 **Saulius Kazlauskas**, E. Kazakevičius, A. Kežionis

Electrical properties of scandia- and ceria-stabilized zirconia ceramics

13:00–14:00 *Lunch*

14:00–14:20 **Alexander Grabar**, M. V. Tsyhyka, and I. M. Stoika

Dynamic interferometry using Sb-doped $Sn_2P_2S_6$ photorefractive crystals

14:20–14:40 **Ilona Zamaraite**, A. Dziaugys, J. Banys, Yu. Vysochanskii

Investigation of physical properties of phosphorous chalcogenide crystals

14:40–15:10 *Coffee break*

15:10–17:00 Poster session

17:00 *Dinner*

POSTER

PRESENTATIONS

ELECTRONIC STRUCTURE OF Cu_6PS_5I SUPERIONIC CRYSTAL

Ihor Studenyak[1], Mykhailo Bletskan[1], Vasyl Vakulchak[1], Tomas Salkus[2], Juras Banys[2]
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This paper presents the calculation results of electronic structure, total and local partial densities of states, imaginary (ε_2) and real (ε_1) parts of dielectric constant for superionic Cu_6PS_5I crystallized in the face-centered cubic lattice. The calculations were performed by the density functional theory method in the LDA+U approximation.

Valence complex of Cu_6PS_5I with total width 18 eV consists of six separate subbands divided by forbidden gaps. The analysis of partial contributions into the density of electronic states allowed to identify the genetic origin of different subbands of the valence band. In the low-energy region (from –18.00 to –16.65 eV) it is located the band of sulfur and phosphorus *s*-states. The next subband (from –14.01 to –12.76 eV) is formed by the hybridized S3*s*–P5*p*-states. There are two dispersion branches $E(\mathbf{k})$ in the central part of valence band, one of which is formed exclusively by iodine 5*s*-states and the second one is formed by sulfur 3*s*-, 3*p*-states with the insignificant impurity of phosphorus 5*p*-states. From the point of view of ionic transport, the formation nature of two upper subbands is most interesting. The subband located in the energy range from –8.45 to –4.77 eV consists of 14 dispersion branches and it is formed by the hybridized S3*p*–Cu3*d*-states with the insignificant impurity of phosphorus 5*p*-states. The uppermost subband (from –3.26 to 0 eV) is formed by the hybridized S3*p*-, I5*p*- and Cu3*d*-states with a dominant contribution of copper 3*d*-states. Electronic states in the vicinity of valence band top have a mixed anion-cation nature with approximately identical contributions of Cu3*d*-, S3*p*- and I5*p*-states.

The partial analysis of unfilled states in the vicinity of conduction band bottom shows that the conduction band is formed by the mixing of free *s*-, *p*- and *d*-states of Cu and S with an insignificant contribution of *s*-, *p*-, *d*-orbitals of P. According to performed calculations, Cu_6PS_5I is the direct-gap superionic semiconductor with the calculated value of band gap width $E_g^{calc} = 2.08$ eV, which is close to the experimental value $E_g^{opt} = 2.089$ eV [1].

References

[1] I.P. Studenyak, M. Kranjcec, M.I. Kayla, V.Yu. Izai, A.F. Orliukas, SPQEO. **16**, 146–151 (2013).

Acknowledgement

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