Appendix No. 1A to Admission rules to the Doctoral School of the Koszalin University of Technology in the academic year 2023/2024

## Application form for research topics in the field of engineering and technology for candidates to the Doctoral School in the academic year 2023/2024

Proposed subject matter of a doctorate

## Simulation studies within the density functional theory of the thermoelectric properties of semiconductor materials

Scientific discipline (delete as appropriate)

## AUTOMATION, ELECTRONICS, ELECTROTECHNICS AND SPACE TECHNOLOGIES CIVIL ENGINEERING, GEODESY AND TRANSPORT

**MECHANICAL ENGINEERING** 

Proposed doctoral thesis supervisor

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Brief description of the research topics with an indication of the scientific issues (max. 350 words)

The proposed research topic is related to the search for effective semiconductor materials for thermoelectric converters of solar energy, based on the Seebeck effect. It is known that the thermoelectric quality factor,  $ZT = \alpha^2 \sigma T/\kappa$ , is the main characteristic of a thermoelectric material ( $\alpha$  - Seebeck coefficient,  $\sigma$  - specific electrical conductivity, T - temperature,  $\kappa$  - thermal conductivity coefficient). The aim of the proposed research is to obtain these values for semiconductor materials with the argyrodite crystal structure,  $Cu_7P(S_xSe_{1-x})_6$ ,  $Ag_7P(S_xSe_{1-x})_6$ , and similar perspective substances, by performing simulation studies within the density functional theory. Finally, the substance possessing the optimal thermoelectric values will be proposed for practical applications

Justification of the purposefulness of taking up the research topics (max. 150 words)

The purpose of the proposed study is justified by the need to obtain substances for thermoelectric converters of solar energy

Proposed topics of doctoral theses within the proposed research subject matter (up to 3 topics)

Simulation studies within the density functional theory of the electrical and thermal properties of selected thermoelectric materials

The sources of financing of the research topics (the subject matter of currently implemented research grants financed from external sources or as part of subsidies)

As part of subsidies

Confirmation of the possibility of ensuring access to scientific apparatus and software necessary for the realization of the proposed research topics (*delete as appropriate*)

## FULLY/ PARTIALLY/ NONE

If the answer is PARTIALLY or NONE please indicate a type of missing scientific apparatus and/or software and the sources of financing an access to them

A list of up to 5 major supervisor's publications related to the proposed research topics, published in journals indexed in the Web of Science or Scopus for the period of the last 3 years (taking into account the IF Impact Factor and the MNiSW score)

- Electron, phonon and thermoelectric properties of Cu<sub>7</sub>PS<sub>6</sub> crystal calculated at DFT level / B. Andriyevsky, I.E. Barchiy, I.P. Studenyak, A.I. Kashuba, M. Piasecki / *Scientific Reports* 11 (2021) 19065 / 5 Year IF 4.409 / 140 pkt. /DOI: 10.1038/s41598-021-98515-6
- Growth, crystal structure and theoretical studies of energy and optical properties of CdTe<sub>1-x</sub>Se<sub>x</sub> thin films / A. Kashuba, H. Ilchuk, R. Petrus, B. Andriyevskyy, I. Semkiv, E. Zmiiovska / *Applied Nanoscience*, Springer, (2021) / 5 Year IF 3.362 / 100 pkt. /DOI: 10.1007/s13204-020-01635-0
- Impact of structure complexity on optoelectronic and non-linear optical properties in quaternary Ag(Pb)–Ga(In)–Si(Ge)–S(Se) systems / M. Piasecki, G. Myronchuk, O.Y. Khyzhun, A. Fedorchuk, B. Andryievsky, I. Barchyi, M. Brik / J. Alloys and Compounds 909 (2022) 164636 / 5 Year IF 5.155 / 100 pkt. /DOI: 10.1016/j.jallcom.2022.164636.
- Highly anisotropic layered crystal AgBiP<sub>2</sub>Se<sub>6</sub>: Growth, electronic band-structure and optical properties / V.Vu. Tuan, O.Y. Khyzhun, A.A. Lavrentyev, B.V. Gabrelian, V.I. Sabov, M.Y. Sabov, M.Y. Filep, A.I. Pogodin, I.E. Barchiy, A.O. Fedorchuk, B. Andriyevsky, M. Piasecki / *Mater. Chem. Phys.* 277 (2022) 125556 / 5 Year IF 3.984 / 100 pkt. /DOI: 10.1016/j.matchemphys.2021.125556
- 5. 5. Ab initio studies of the gas adsorption on the surface CdSe<sub>1-x</sub>S<sub>x</sub> ultra-thin films / A. I Kashuba, I. V. Semkiv, B. Andriyevsky, H. A. Ilchuk, N. Yu. Kashuba / *Applied Nanoscience* (2023) / 5 Year IF 3.362 / 100 pkt. /DOI: 10.1007/s13204-023-02771-z

A list of research grants financed by the National Science Centre, the National Centre of Research and Development and the European Research Council in which the supervisor has participated during the last 5 years

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A list of research services provided for industry related to the proposed research topics for the period of the last 5 years