2.2 Research project description template

EURIZON FELLOWSHIP PROGRAMME

“Remote Research Grants”

Valid applications need to be submitted through the website: https://indico.desy.de/event/38700/ by the Principal Investigator of the Ukrainian team before May 8th 2023 at 12:00 Pm (noon) CEST time. Before applying please read carefully the Terms of Reference (ToR).

Title[1] of the research project: *(max 30 words)*
Machine learning-based defect engineering in silicon structures for thermal management and photovoltaics

submitted by

PRINCIPAL INVESTIGATOR (PI)[2]:

First name and Family name (English)	**Oleh Olikh**

Please note that the limit in the number of words per each section of this application form constitutes one of the eligibility criteria*, so make sure that all requirements are respected. The template provided must not be modified and the formatting must be kept. All possible tables and pictures must be clearly readable.*

All fields marked with are mandatory. Other fields are optional.*

This template is part of the application package. It must be filled according to the instructions, signed by all team members, and upload it as pdf file

Table of Contents:

Please note that the limit in the number of words per each section of this application form constitutes one of the eligibility criteria.

[1] Please verify that this information corresponds to the one reported in section 1 of the online application form.
[2] Please verify this information corresponds to the one reported in the section 4 of the online application form.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

2.2 Research project´s full description* *(Max 1200 words)*

Please describe the objectives of the research, and whenever possible the methodology to be used, the instrumentation needed (if any), the implementation and timeline.

Introduction: In the last few years, materials Informatics (MI) has become one of the leading scientific paradigms, transforming the material and device development, characterization, and investigation fields by merging material property calculations/measurements with the computational power of informatics algorithms. Machine learning (ML) techniques have proven very successful within the MI, particularly in scenarios where conventional algorithm-based solutions are not readily apparent.

ML is shown [1] to be a promising direction for predicting thermal transport in solids, which is critical for various green energy solutions. Depending on the physical mechanism responsible for energy mining, it may be necessary to increase or decrease thermal transfer coefficient. Overheating is a serious problem for solar panels and requires efficient heat evacuation, while many thermoelectric applications require low thermal conductivity. Various approaches have been proposed to control thermal transport in materials, such as impurity scattering, surface roughness, alloy, and porous structures. Recently, the possibility of successfully solving thermal transport problems by coupling molecular dynamics and machine learning has been demonstrated [2], as well as the applicability of MI methods to describe the thermal properties of porous materials [3]. This project aims to use molecular dynamics-based machine learning to manage thermal properties of silicon systems with varying porosity and defects.

The other project's part deals with impurity evaluation in silicon solar cells. One of the most crucial technologies for achieving a society free of carbon emissions is solar photovoltaics (PV). It is an effective and renewable energy source, but various defects limit solar cells performance and reliability. Therefore, non-destructive methods aimed at estimating the concentration of recombination-active defects in PV structures are crucial from an applied point of view. Numerous methods have been developed to address this issue, but most involve either pre-treatment of the samples or specialized equipment. On the other hand, the measurement of current-voltage characteristics (IVCs) is a widely accepted and straightforward method for determining the parameters of photovoltaic conversion. The ways for characterizing defects from IVC measurements and Bayesian parameter estimation [4], or differential coefficients [5], were demonstrated previously. However, these approaches are too complex for practical use. The project aims to develop a machine learning-oriented express method for IVC-based impurity determination, which is highly desirable and promising for widespread use. Lately, the ML's possibility of silicon defect characterization was shown using lifetime curves [6] or ideality factor [7]. Our approach is based on using standard photovoltaic parameters as factors sensitive to the recombination centres and makes it possible to reduce the requirements for IVC measurement.

Objective: The primary objective of this research project is to develop a machine learning-based approach to defects evaluation in silicon structures that can enhance the reliability of solar modules. Another objective is to engineer phonon transport in silicon structures by combining machine learning methods, molecular dynamics simulations, and experimental measurements. Specifically, we aim to achieve the following objectives:

- Develop a ML model to predict the impact of defects on the performance of silicon structures.
- Use the ML model to design and evaluation defects that can enhance the performance of silicon structures.

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- Develop a ML based approach to extracting defect concentration from current-voltage characteristic of solar cell.
- Study the phonon transport in silicon structures of various morphologies and the development of a ML model for predicting their thermal properties.
- Synthesis of a limited series of porous silicon structures, experimental investigations of their thermal properties using photoacoustic methods, and experimental verification of theoretical models.

Methodology: The proposed research project will involve the following steps:
Step 1: Data Collection and Preparation: We will collect data on the impact of different types of defects on the performance of silicon structures for solar cells and thermal management applications. The data will be obtained through experiments and simulations. The data will be pre-processed to remove noise and outliers, and feature engineering techniques will be used to extract meaningful features. The simulations of thermal transport in silicon structures will be performed using molecular dynamics method in the LAMMPS package and/or Anharmonic Lattice Dynamics (using the kALDo software). The calculation of the current-voltage characteristics of silicon structures will be carried out using the SCAPS software. A total of 100,000 IVCs are estimated to be required to ensure high-quality ML training.
Step 2: Machine Learning Model Development: We will develop a machine learning models to predict the impact of defects on the performance of silicon structures, as well as ML models to predict the concentration of defect (iron, for example) based on the photoelectric parameters of solar cells (short-circuit current, open-circuit voltage, efficiency, and fill factor) and the set of IV curves obtained after light-induced dissociation of FeB pairs. The model will be trained and tuned on the pre-processed data collected in Step 1. To develop the model, we will explore different machine learning algorithms, including dense neural networks (DNN), random forest (RF), convolutional neural networks (CNNs). In the case of CNN, the fine-tuning of vision models (AlexNet or VGG network) will be used as well. The ML algorithms will be implemented using the TensorFlow platform, specifically the high-level Keras API.
Step 3: Defect Evaluation: We will use the developed machine learning model to evaluate defects in silicon structures that can enhance their performance. We will use an optimization algorithm, such as EBLSHADE or IJAVA, to search for the optimal defect parameters that can maximize the performance of the silicon structure. The defect parameters will be constrained by physical and material properties of the silicon structure.
Step 4: Fabrication and Testing: The porous silicon structures will be fabricated using standard processing techniques. The thermal transport properties of the fabricated structures will be evaluated using photoacoustic experiments and atomistic simulations. We will compare the performance of the synthesized structures with that of the original structures to evaluate the effectiveness of the defect engineering approach. The ability of the developed ML method of defect evaluation will be tested on actual silicon solar cells.
Expected Results: The project is expected to result in the following outcomes:

1. A machine learning model to predict the impact of defects on the performance of silicon structures for solar cells and thermal management applications.
2. A machine learning model to evaluate defect concentration in solar cells by standard photovoltaic parameters.
3. An approach to engineer phonon transport in silicon structures that can enhance their thermoelectric performance.

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4. Fabricated limited series of silicon structures including porous Si samples for experimental validation of the modelling results.
5. A better understanding of the role of defects in silicon structures for solar cells and thermal management applications.

Significance and Impact: The proposed project has significant implications for the development of efficient, reliability, and effective solar photovoltaic modules and thermal management systems. By using machine learning-based defect evaluation and phonon transport engineering techniques, we can design, characterize, and engineer silicon structures that can enhance their performance. This can lead to the development of more efficient solar cells and thermal management systems, which can have a significant impact on the energy sector. In addition, the proposed research project can contribute to the development of new materials and technologies for other applications where silicon structures are used.

2.3 COLLABORATION WITH THE EUROPEAN PARTNERS, IMPACT, DISSEMINATION

2.3.1 Description of the collaboration with the European partner(s)[3]*. *(Max 500 words)*

Please describe the expected role of the European partner and the scope of the collaboration.

The repartition of work can also be very different, with the Ukrainian team performing most of the tasks, but it is important to explain the role of the European Partners (e.g., joint analysis, support, monitoring, dissemination, etc.).

The team has longstanding collaboration with laboratory LEMTA, the join unit between University of Lorraine (UL) and CNRS, Nancy, France. Such cooperation includes exchange between students and staff, common scientific activity, preparation of the EU projects. One of the results of scientific collaboration between the project team and laboratory LEMTA is several joint publications, including: 1) Scientific Reports, 13, 5889 (2023); 2) Applied Physics Letters, 122, 172201 (2023); 3) Nanomaterials, 12, 708 (2022); 4) Journal of Applied Physics, 126, 055109 (2019); 5) Applied Physics Letters, 115, 021902 (2019).

In frames of the current project, LEMTA will support with computational facilities by providing access to the mesocentre for calculations EXPLOR (https://explor.univ-lorraine.fr/) of UL. The latter will give the possibility to the team members launch time consuming simulations and to be independent from electricity interruptions.

LEMTA will also provide the support in the analysis of the calculated data concerning thermal transport properties of the exanimated systems, and it will provide support in cross-validation and verification of the data received during the project.

It should be also noted that the members of LEMTA have well-developed network at French national level (like GDR "NAME", French Society of Thermic (SFT), ICEEL Carnot, etc.), EU, and worldwide. Specifically, LEMTA is also active in two joint programs of the European Energy Research Alliance (EERA), one concerning materials and processes for energy applications (AMPEA), the other fuel cells and hydrogen (FCH). It will use this network to help dissemination of the received results, which will help increase the visibility of the team.

[3] The name and contact details of the European partners are to be mentioned in the Application form (Section 3).

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LEMTA will also welcome the young researchers from Kyiv University in frames of existing projects (like ERAMSUS+, Lorraine University of Excellence (LUE) program, bilateral agreements) for performing characterization of the samples with use of facilities of LEMTA, like optical characterization tool, Raman approach, scanning thermal microscopy, etc.

2.3.2 Expected outcomes of the research project*. *(Max 300 words)*

Please highlight the possible positive impact of your research project. Please also highlight if the project could (i) support the operations and/or reconstruction and/or long-term sustainability of Ukrainian RIs and/or (ii) boost possible future collaboration and partnership opportunities with European Research Institutes.

1. Development of advanced algorithms: The project aims to develop advanced machine learning algorithms for thermal management and defect evaluation in silicon structures. These algorithms could potentially enhance the performance and efficiency of photovoltaic and thermoelectric devices. This is particularly important because the restoration of Ukraine's energy system, which was significantly damaged by Russian's aggression, will largely depend on renewable technologies.
2. Enhanced device performance: The research could lead to the identification of defects that could affect the performance of photovoltaic and thermoelectric devices. This could result in the production of more efficient and reliable devices.
3. Creating of data collection: The big data array, obtained through experiments and simulations, will be in open access at GitHub and may be used by other researchers.
4. Improved manufacturing processes: The machine learning algorithms developed in this project could be used to improve the manufacturing processes of photovoltaic and thermoelectric devices. This could lead to the production of high-quality devices at lower costs.
5. Positive impact on the environment: The use of photovoltaic and thermoelectric devices could reduce the dependence on fossil fuels, leading to a positive impact on the environment. The improved efficiency and reliability of these devices could further promote their use.

Regarding the project's potential impact on Ukrainian RIs and European research institutes, it could:
(i) The development of advanced algorithms and improved manufacturing processes has the potential to positively impact the sustainability and competitiveness of Ukrainian RIs. Additionally, new technologies and processes developed through the project could improve the performance of photovoltaic and thermoelectric devices in Ukraine.
(ii) The project's development of advanced machine learning algorithms and improved manufacturing processes may also attract European research institutes, creating opportunities for collaborations and partnerships that could benefit both parties and promote scientific advancements.

2.3.3 Dissemination of the results*. *(Max 200 words)*

Please describe how you plan or would like to disseminate the results of the research project.

Disseminating the results of the research is crucial for maximizing the impact of the project. Here are some ways in which we plan to disseminate the results of the research project:

1. Conference Presentations: We plan to present the results of the research project at least three relevant conferences in the fields of materials science, semiconductor engineering, solar cell technology, and thermal management. This will provide an opportunity to share

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the findings of the research with a wider audience and receive feedback from experts in the field.

2. Journal Publications: Based on the results of the research project, we plan to prepare at least 4 articles for publication in Scopus-indexed peer-reviewed journals. This will ensure that the findings are widely disseminated to the scientific community and can be cited by other researchers.
3. Social Media: We plan to use social media platforms such as Facebook, Instagram, or Telegram to disseminate the research findings to a wider audience. We will create posts and updates highlighting the key findings of the research and share links to the conference presentations and journal publications.

2.3.4 Possible references related to the research proposal (optional) . *(Max 300 words)*

Citations used in the proposal text have to be listed here. References should be consecutively numbered using the format:

[1] A. Author, B. Author, and C. Author, Title, Phys. Rev. B 50, pages (year). (DOI as hyperlink, if applicable)

[1] X. Qian, R. Yang, Machine learning for predicting thermal transport properties of solids, Materials Science & Engineering R 146, 100642 (2021) (https://doi.org/10.1016/j.mser.2021.100642)

[2] K. Xu, T. Liang, Y. Fu et al., Gradient nano-grained graphene as 2D thermal rectifier: A molecular dynamics based machine learning study, Appl. Phys. Lett. 121, 133501 (2022) (https://doi.org/10.1063/5.0108746)

[3] Y. Yang, Y. Zhao, and L. Zhang Machine learning boosting the discovery of porous metamaterials with an abnormal thermal transport property, Appl. Phys. Lett. 122, 144102 (2023) (https://doi.org/10.1063/5.0137665)

[4] R. Kurchin, J. Poindexter, V. Vahanissi et al., How much physics is in a current-voltage curve? Inferring defect properties from photovoltaic device measurements, IEEE J. Photovolt 10, 1532-1537 (2020). (https://doi.org/10.1109/JPHOTOV.2020.3010105)

[5] S. Bulyarskiy, A. Lakalin, M. Saurov, and G. Gusarov, The effect of vacancy-impurity complexes in silicon on the current–voltage characteristics of p–n junctions, J Appl. Phys. 128, 155702 (2020). (https://doi.org/10.1063/5.0023411)

[6] Y. Buratti, J. Dick, Q. Gia, and Z. Hameiri, Deep Learning Extraction of the Temperature-Dependent Parameters of Bulk Defect, ACS Appl. Mater. Interfaces 14, 48647-48657 (2022). (https://doi.org/10.1021/acsami.2c12162)

[7] O. Olikh, O. Lozitsky, and O. Zavhorodnii, Estimation for iron contamination in Si solar cell by ideality factor: Deep neural network approach, Prog. Photovolt. Res. Appl. 30, 648-660 (2022).(https://doi.org/10.1002/pip.3539)

2.4 RESEARCH TEAM DESCRIPTION and FINANCIAL PLAN

2.4.1 Description of the roles within the research team*. *(Max 500 words)*

Please describe what are the roles, availabilities and tasks of each of the research team members within the research project. *Please note that the qualification, expertise, effort and roles of the members within the research project must be in line with the financial plan of the team. Each team member should have a meaningful role in the project.*

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The following are the roles, availabilities, and tasks of each team member:

1. Principal Investigator (Oleh Olikh): The PI is responsible for supervising the entire project and ensuring that it meets the objectives. He is also responsible for interacting with stakeholders, and managing the research team. The PI will be available full-time throughout the project's duration. His tasks include directing the project's overall strategy, developing the methodology of machine learning models using, and overseeing data collection and machine learning code writing. Additionally, he will develop a model for simulating solar cells, analyze the data, and review & editing scientific papers and reports.
2. Researcher 1 (Vasyl Kuryliuk): The researcher 1 will be available full-time throughout the project's duration. He will have expertise in molecular dynamics modeling of thermal transport. His tasks include performing simulations, data collection, models development, and contributing to publications and presentations.
3. Researcher 2 (Pavlo Lishchuk): The researcher 2 will be full-time and will work closely with the principal investigator and researcher 1. His tasks include running experiments to measure the transport properties of silicon structures by photoacoustic technique, assisting in manuscript preparation, and providing general support for the research team.
4. Graduate Student 1 (Oleksii Zavhorodnii): The graduate student 1 will spend 75 % of the working time for the project and will work closely with the principal investigator. His tasks include collecting and processing experimental data relating to solar cells, implementing and testing machine learning models, and contributing to the draft of papers and presentations.
5. Graduate Student 2 (Lesia Chepela): The graduate student 2 will spend 75 % of the working time for the project and will work closely with the researcher 2. Her tasks include synthesis and characterization of porous silicon, implementing photoacoustic experiments, and contributing to the draft of papers and presentations.
6. Student (Nataliia Kyrychenko): The student will spend 50 % of the working time for the project. She will carry out debugging software to perform MD calculations on grid clusters and experimental installations for the measure thermal conductivity of silicon structures, will conduct primary processing of experimental and theoretical data.

2.4.2 Financial plan*. *(Max 500 words)*

Please describe how the team suggests to distribute the monthly grants within the team members. *Please kindly note that the monthly grant amount per each team member should reflect on his/her qualifications, years of experience, planned effort and role within the suggested research project*[4] [5] [6]

Please indicate for your research team what are the <u>wished estimated monthly grants per each member</u> *(within the maximum and minimum amounts described in the ToR):*

[4] Each team member will receive a constant amount of monthly grant during the whole duration of the fellowship.

[5] Candidates that are not in a vulnerable condition or that are already beneficiaries of other support grants/ fellowships (above 1,000 Euro) can participate in the programme but are not entitled to receive the monthly grant.

[6] Teams should be composed by 2-5 Members (including the PI). Teams can include more than 5 Members, but the maximum monthly grant available for the research project will not exceed 6,500 Euro.

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Role	*Name and Surname (English)*	*Euro per Month*
PI:	**Oleg Olikh**	***1300***
Team Member 2: Researcher 1	**Vasyl Kuryliuk**	***1300***
Team Member 3: Researcher 2	**Pavlo Lishchuk**	***1300***
Team Member 4: Graduate Student 1	**Oleksii Zavhorodnii**	***950***
Team Member 5: Graduate Student 2	**Lesia Chepela**	***950***
Team Member 6: Student	**Nataliia Kyrychenko**	***700***

If your team is composed by more than 5 Members please add new table lines.

2.4.3 Research team members information

The information of the Principal Investigator (considered as Team Member 1) is already included in the online application form, no need to repeat them here.

Team Member 2 – information

First name ENG[7]*	Vasyl
Family name ENG*	Kuryliuk
Date of Birth*	23/07/1982
Gender*	M
Phone number(s)	
E-mail address(es)*	kuryliuk@knu.ua
Institute of affiliation[8]*	Taras Shevchenko National University of Kyiv
Affiliation Institute address	Volodymyrska Street 64/13, Kyiv, 01601, Ukraine
Current position[9]*	Head of the Department of Metal Physics, Faculty of Physics
Country of permanent residence*	Ukraine
Country of current residence*	
Citizenship	Ukraine
Knowledge of English *	Good
Highest level of instruction achieved*	PhD in Solid State Physics

Team Member 3 – information

First name ENG[10]*	Pavlo
Family name ENG*	Lishchuk

[7] As mentioned in the ID document, please use English alphabet;
[8] Please mention if you are still affiliated to that institute or until when you were affiliated;
[9] Please mention if you are still in the same position or until when you held it;
[10] As mentioned in the ID document, please use English alphabet;

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Date of Birth*	*12/07/1992*
Gender*	*M*
Phone number(s)	
E-mail address(es)*	*pavel.lishchuk@knu.ua, pavel.lishchuk@gmail.com*
Institute of affiliation[11]*	*Taras Shevchenko National University of Kyiv*
Affiliation Institute address	*Volodymyrska Street 64/13, Kyiv, 01601, Ukraine*
Current position[12]*	*Assistant at the general physics department, Faculty of Physics*
Country of permanent residence*	*Ukraine*
Country of current residence*	
Citizenship	*Ukraine*
Knowledge of English *	*Very good*
Highest level of instruction achieved*	*PhD in Solid State Physics*

Team Member 4 – information

First name ENG[13]*	Oleksii
Family name ENG*	Zavhorodnii
Date of birth*	07/12/1998
Gender*	M
Phone number(s)	
E-mail address(es)*	nevermor464@gmail.com
Institute of affiliation[14]*	Taras Shevchenko National University of Kyiv
Affiliation Institute address	Volodymyrska Street 64/13, Kyiv, 01601, Ukraine
Current position[15]*	PhD at the general physics department, Faculty of Physics
Country of permanent residence*	Ukraine
Country of current residence*	
Citizenship	Ukraine
Knowledge of English *	Good
Highest level of instruction achieved*	Master in Physics of Nanosystems

Team Member 5 – information

First name ENG[16]*	Lesia
Family name ENG*	Chepela
Date of birth*	13/06/1997

[11] Please mention if you are still affiliated to that institute or until when you were affiliated;
[12] Please mention if you are still in the same position or until when you held it;
[13] As mentioned in the ID document, please use English alphabet;
[14] Please mention if you are still affiliated to that institute or until when you were affiliated;
[15] Please mention if you are still in the same position or until when you held it;
[16] As mentioned in the ID document, please use English alphabet;

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Gender*	F
Phone number(s)	
E-mail address(es)*	Lesia.chepela97@gmail.com
Institute of affiliation[17]*	Taras Shevchenko National University of Kyiv
Affiliation Institute address	Volodymyrska Street 64/13, Kyiv, 01601, Ukraine
Current position[18]*	PhD at the general physics department, Faculty of Physics
Country of permanent residence*	Ukraine
Country of current residence*	
Citizenship	Ukraine
Knowledge of English *	Good
Highest level of instruction achieved*	Master in Physics of Nanosystems

Team Member 6 – information

First name ENG[19]*	Nataliia
Family name ENG*	Kyrychenko
Date of birth*	08/09/2001
Gender*	F
Phone number(s)	
E-mail address(es)*	natalija.kyrychenko@gmail.com
Institute of affiliation[20]*	Taras Shevchenko National University of Kyiv
Affiliation Institute address	Volodymyrska Street 64/13, Kyiv, 01601, Ukraine
Current position[21]*	Student in the Department of Metal Physics, Faculty of Physics
Country of permanent residence*	Ukraine
Country of current residence*	
Citizenship	Ukraine
Knowledge of English *	Good
Highest level of instruction achieved*	Bachelor in Physics

2.5 SIGNATURES

After completing all the chapters of this form, it shall be signed by the PI and by all research team members, then the PI should upload it together with all other relevant documents (indicated in the Terms of Reference of the call) in the online application form.

Please remember that the limit in the number of words per each section of the application form constitutes one of the eligibility criteria, so make sure that all requirements are respected.

[17] Please mention if you are still affiliated to that institute or until when you were affiliated;
[18] Please mention if you are still in the same position or until when you held it;
[19] As mentioned in the ID document, please use English alphabet;
[20] Please mention if you are still affiliated to that institute or until when you were affiliated;
[21] Please mention if you are still in the same position or until when you held it;

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Privacy Notice

Please, be informed: when applying for the EURIZON Remote Research Grant Fellowship, you agree that the personal data and documents that you provide to the EURIZON Secretariat and Review Panel will be stored and processed for the purpose of participating in the EURIZON Remote Research Grant application procedure. The personal data and documents from all applicants will be stored and processed according to DESY data privacy policy : https://www.desy.de/data_privacy_policy/index_eng.html

Signature of the PI: ______________________ ***Date:*** *04/05/2023*

Signatures of all other team members:

Name, Family name(English)	*Signature*
Vasyl Kuryliuk	
Pavlo Lishchuk	
Oleksii Zavhorodnii	
Lesia Chepela	
Nataliia Kyrychenko	

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