**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/**](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]](#footnote-2)of the research project:** *(max 30 words)*  **Machine learning-based defect engineering in silicon structures for thermal management and solar cells applications**  **Як варіант**  **Machine learning-based thermal management and defect evaluation in silicon structure for photovoltaics and ???? application** |

submitted by

***PRINCIPAL INVESTIGATOR (PI)[[2]](#footnote-3):***

|  |  |
| --- | --- |
| *First name and Family name (English)* |  |

***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*

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

**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.

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| Пропоную структурувати текст за таким шаблоном:  **Introduction: ….**  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 in SCs. The ways for characterizing defects from IVC measurements and Bayesian parameter estimation [1], or differential coefficients [2], were demonstrated previously. However, these approaches were too complex for practical use. Therefore, an express IVC-based method of impurity determination is very desirable and extremely promising for wide use.  **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 ~~performance~~ reliability of solar modules ~~cells~~ and thermal management applications. Specifically, we aim to achieve the following objectives:   * Develop a machine learning (ML) model to predict the impact of defects on the performance of silicon structures for solar cells and thermal management applications. * Use the machine learning model to design and engineer defects that can enhance the performance of silicon structures. * Develop a machine learning based approach to extracting defect concentration from current-voltage characteristic of solar cell. * Fabricate the engineered silicon structures and evaluate their performance.   **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. *Можливо, додати конкретику? На кшталт* Simulation will be done by using molecular dynamics calculation and 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 defect concentration from solar cell photovoltaic parameters. The model will be trained on the pre-processed data collected in Step 1. To develop the model, we will explore different machine learning algorithms, including ~~deep learning algorithms such as~~ dense neural networks (DNN), random forest (RF), convolutional neural networks (CNNs) and recurrent neural networks (RNNs) *(точно часові послідовності будуть?)* ~~to develop the model~~. 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 Engineering: We will use the developed machine learning model to engineer defects in silicon structures that can enhance their performance. We will use an optimization algorithm, such as a genetic algorithm (*?? вже користувалися?*) or differential evolution algorithm, 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, Testing and Evaluation: The engineered silicon structures will be fabricated using standard semiconductor processing techniques. *(реально створити сонячні елементи я не бачу можливості – є готові, на яких можна тестувати методи оцінки дефектів)* The performance of the fabricated structures will be evaluated using experiments and simulations. We will compare the performance of the engineered 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 proposed research 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 defects in silicon structures that can enhance their performance. 4. Fabricated silicon structures with engineered defects that demonstrate enhanced performance. 5. A better understanding of the role of defects in silicon structures for solar cells and thermal management applications.   **Significance and Impact:** The proposed research project has significant implications for the development of efficient, reliability, and effective solar ~~cells~~ photovoltaic modules and thermal management systems. By using machine learning-based defect 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.  The other project’s part deals with impurity evaluation in silicon solar cells (SSCs). One of the most crucial technologies for achieving a society free of carbon emissions is 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 in SCs. The ways for characterizing defects from IVC measurements and Bayesian parameter estimation [1], or differential coefficients [2], were demonstrated previously. However, these approaches were too complex for practical use. Therefore, an express IVC-based method of impurity determination is very desirable and extremely promising for wide use. The project's purpose is the development of a machine learning (ML) based approach to extracting defect parameters from IVC.  The research will focus on the application of the mentioned approach for the evaluation of iron contamination. Iron is a typical impurity in silicon solar cells, and its properties are well-studied. In particular, the iron atom is known to form a complex with the acceptor, and this pair can be easy dissociated, for example, due to illumination. It is envisaged to use two ways to determine the defect concentration.  In the first one, the standard photovoltaic parameters (short-circuit current, open-circuit voltage, efficiency, and fill factor) will be used as factors sensitive to the recombination centers and input parameters for ML algorithms. Lately, the ML's possibility of silicon defect characterization was shown using lifetime curves [3] or ideality factor [4]. Our approach makes it possible to reduce the requirements for IVC measurement. Changes in photovoltaic parameters after the Fe-acceptor pair breakdown will be used to separate the iron from other recombination channels. The defect concentration will be determined as a regression result of neural networks and random forest.  We will consider the IVCs measured during pair association in the second case. Then, we will convert this set of IVCs into an image and use it as training data for a convolutional neural network based on either the AlexNet or VGG network.  The project implementation requires the generation of training and test datasets through the simulation of IVC of solar cells using various combinations of parameters. The SCAPS software will be utilized for modeling, with varied parameters, including cell temperature, illumination condition, base doping degree and thickness, and iron concentration A total of 100,000 IVCs are estimated to be required to ensure high-quality ML training. The hyperparameter tuning of the ML algorithms will also be necessary. The neural network and random forest will be implemented using the TensorFlow platform, with the high-level Keras API being used for the former. Testing of the ML algorithms on real SSCs will also be conducted to evaluate their effectiveness. |

**2.3 COLLABORATION WITH THE EUROPEAN PARTNERS, IMPACT, DISSEMINATION**

**2.3.1 Description of the collaboration with the European partner(s)[[3]](#footnote-4)\*.** *(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.).*

|  |
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| *Please indicate what kind of collaboration is foreseen and if there are specific contributions and/or external funding available for the actions requested (e.g. European partner willing to perform an experiment at their facilities and/or to host and contribute to travel and accommodation expenses of Ukrainian team members).* |

**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.

|  |
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| Due to Russia's aggression, Ukraine's energy system has been significantly impacted. Obviously, its restoration will depend heavily on renewable technologies, such as photovoltaics. This project aims to develop the physical foundations for an express method of assessing the content of electrically active defects in silicon solar cells using photovoltaic parameter values. This method will be used to evaluate the performance and reliability of solar cells. Moreover, a database containing around 100,000 current-voltage characteristics of silicon solar cells with varied parameters will be made publicly accessible. This dataset is suitable for training various artificial neural networks by other researchers. |

**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.

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| This project will prepare at least two papers to be published in Scopus-indexed journals and at least three presentations at international conferences. |

**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] 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*](https://doi.org/10.1109/JPHOTOV.2020.3010105)*)*  *[2] 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*](https://doi.org/10.1063/5.0023411)*)*  *[3] 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*](https://doi.org/10.1021/acsami.2c12162)*)*  *[4] 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*](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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**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]](#footnote-5) [[5]](#footnote-6) [[6]](#footnote-7)*

|  |  |  |
| --- | --- | --- |
| **Please indicate for your research team what are the wished estimated monthly grants per each member** *(within the maximum and minimum amounts described in the ToR ):* | | |
| ***Role*** | ***Name and Surname (English)*** | ***Euro per Month*** |
| **PI:** |  | *Min 700 Max 1,600* |
| **Team Member 2:** |  |  |
| **Team Member 3:** |  |  |
| **Team Member 4:** |  |  |
| **Team Member 5:** |  |  |
|  |  |  |

*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]](#footnote-8)\*** |  |
| **Family name ENG\*** |  |
| **Date of Birth\*** | *Dd/mm/yyy* |
| **Gender\*** | *M / F / Non-binary* |
| **Phone number(s)** |  |
| **E-mail address(es)\*** |  |
| **Institute of affiliation[[8]](#footnote-9)\*** |  |
| **Affiliation Institute address** | *Street name and street number, city, postal address, country* |
| **Current position[[9]](#footnote-10)\*** |  |
| **Country of permanent residence\*** |  |
| **Country of current residence\*** | *Only if different from permanent residence. In case you live in a different country now, please specify since when.* |
| **Citizenship** |  |
| **Knowledge of English \*** | *Please select between:*  *Excellent – Very good – Good – Fair - Basic* |
| **Highest level of instruction achieved\*** | *e.g. PhD, Master, Bachelor in …(please specify the field)* |

**Team Member 3 – information**

|  |  |
| --- | --- |
| **First name ENG[[10]](#footnote-11)\*** | 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[[11]](#footnote-12)\*** | *Taras Shevchenko National University of Kyiv* |
| **Affiliation Institute address** | *Street name and street number, city, postal address, country*  *Volodymyrska Street 64/13, Kyiv, 01601, Ukraine* |
| **Current position[[12]](#footnote-13)\*** | *Head of Department of Metal 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 4 – information**

|  |  |
| --- | --- |
| **First name ENG[[13]](#footnote-14)\*** |  |
| **Family name ENG\*** |  |
| **Date of birth\*** | *Dd/mm/yyyy* |
| **Gender\*** | *M / F / Non-binary* |
| **Phone number(s)** |  |
| **E-mail address(es)\*** |  |
| **Institute of affiliation[[14]](#footnote-15)\*** |  |
| **Affiliation Institute address** | *Street name and street number, city, postal address, country* |
| **Current position[[15]](#footnote-16)\*** |  |
| **Country of permanent residence\*** |  |
| **Country of current residence\*** | *Only if different from permanent residence. In case you live in a different country now, please specify since when.* |
| **Citizenship** |  |
| **Knowledge of English \*** | *Please select between:*  *Excellent – Very good – Good – Fair - Basic* |
| **Highest level of instruction achieved\*** | *e.g. PhD, Master, Bachelor in …(please specify the field)* |

**Team Member 5 – information**

|  |  |
| --- | --- |
| **First name ENG[[16]](#footnote-17)\*** |  |
| **Family name ENG\*** |  |
| **Date of birth\*** | *Dd/mm/yyyy* |
| **Gender\*** | *M / F / Non-binary* |
| **Phone number(s)** |  |
| **E-mail address(es)\*** |  |
| **Institute of affiliation[[17]](#footnote-18)\*** |  |
| **Affiliation Institute address** | *Street name and street number, city, postal address, country* |
| **Current position[[18]](#footnote-19)\*** |  |
| **Country of permanent residence\*** |  |
| **Country of current residence\*** | *Only if different from permanent residence. In case you live in a different country now, please specify since when.* |
| **Citizenship** |  |
| **Knowledge of English \*** | *Please select between:*  *Excellent – Very good – Good – Fair - Basic* |
| **Highest level of instruction achieved\*** | *e.g. PhD, Master, Bachelor in …(please specify the field)* |

**Team Member 6 – information**

|  |  |
| --- | --- |
| **First name ENG[[19]](#footnote-20)\*** |  |
| **Family name ENG\*** |  |
| **Date of birth\*** | *Dd/mm/yyyy* |
| **Gender\*** | *M / F / Non-binary* |
| **Phone number(s)** |  |
| **E-mail address(es)\*** |  |
| **Institute of affiliation[[20]](#footnote-21)\*** |  |
| **Affiliation Institute address** | *Street name and street number, city, postal address, country* |
| **Current position[[21]](#footnote-22)\*** |  |
| **Country of permanent residence\*** |  |
| **Country of current residence\*** | *Only if different from permanent residence. In case you live in a different country now, please specify since when.* |
| **Citizenship** |  |
| **Knowledge of English \*** | *Please select between:*  *Excellent – Very good – Good – Fair - Basic* |
| **Highest level of instruction achieved\*** | *e.g. PhD, Master, Bachelor in …(please specify the field)* |

***If you wish to add more team Members, please copy this table, paste it below and add the details of the additional team member(s).***

**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.***

***Disclaimer on Intellectual Property Rights and Copyright****: A proposal for the EURIZON Fellowship programme must respect the fundamental ethical principles for scientific research. EURIZON Secretariat condemns the replication of ideas, data, results without due permission and acknowledgement. Please make sure that the ideas developed in this research proposal are yours (and/or of the people mentioned in the paragraph 2 “Research team”) and that you own or have received the necessary authorizations from the intellectual property rights holders to validly use data and materials that you include in the Application form.*

***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*](https://www.desy.de/data_privacy_policy/index_eng.html)

***Signature of the PI: Date:*** *dd/mm/yyyy*

***\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_***

***Signatures of all other team members:***

***Name, Family name(English) Signature***

***\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_***

***Name, Family name(English) Signature***

***\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_***

***Name, Family name(English) Signature***

***\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_***

***Name, Family name(English) Signature***

***\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_*** ***\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_***

***Name, Family name(English)***  ***Signature***

***\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_*** ***\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_***

***Please note that this document must be signed by all team members, so if your team is composed by more than 5 members, please add their signatures here below.***

1. Please verify that this information corresponds to the one reported in section 1 of the online application form. [↑](#footnote-ref-2)
2. Please verify this information corresponds to the one reported in the section 4 of the online application form. [↑](#footnote-ref-3)
3. The name and contact details of the European partners are to be mentioned in the Application form (Section 3). [↑](#footnote-ref-4)
4. Each team member will receive a constant amount of monthly grant during the whole duration of the fellowship. [↑](#footnote-ref-5)
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. [↑](#footnote-ref-6)
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. [↑](#footnote-ref-7)
7. As mentioned in the ID document, please use English alphabet; [↑](#footnote-ref-8)
8. Please mention if you are still affiliated to that institute or until when you were affiliated; [↑](#footnote-ref-9)
9. Please mention if you are still in the same position or until when you held it; [↑](#footnote-ref-10)
10. As mentioned in the ID document, please use English alphabet; [↑](#footnote-ref-11)
11. Please mention if you are still affiliated to that institute or until when you were affiliated; [↑](#footnote-ref-12)
12. Please mention if you are still in the same position or until when you held it; [↑](#footnote-ref-13)
13. As mentioned in the ID document, please use English alphabet; [↑](#footnote-ref-14)
14. Please mention if you are still affiliated to that institute or until when you were affiliated; [↑](#footnote-ref-15)
15. Please mention if you are still in the same position or until when you held it; [↑](#footnote-ref-16)
16. As mentioned in the ID document, please use English alphabet; [↑](#footnote-ref-17)
17. Please mention if you are still affiliated to that institute or until when you were affiliated; [↑](#footnote-ref-18)
18. Please mention if you are still in the same position or until when you held it; [↑](#footnote-ref-19)
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21. Please mention if you are still in the same position or until when you held it; [↑](#footnote-ref-22)