1.1 Title of the research project

Machine learning-based defect engineering in silicon structures for thermal management and photovoltaics

1.3 Research Project duration

12 Month duration

1.4 Keywords (up to 5 keywords)

Silicon structure, machine learning, thermal management, defect engineering

1.5 Research thematic area

◉ 5-PHYSICAL SCIENCES & ENGINEERING;

2.1 Brief outline of the research project (abstract) *(max. 250 words)*

Materials informatics is a scientific paradigm that combines material property calculations and measurements with the computational power of informatics algorithms. In particular, machine learning (ML) techniques have proven to be highly effective in predicting the properties of solids and designing materials. The first project aims to develop a molecular dynamics-based ML approach for the thermal management of silicon systems. The other project aims to develop an ML-based method to extract defect concentration from the current-voltage characteristics of solar cells. The projects involve data collection and preparation, machine learning model development, and experimental investigations. Data will be collected from simulations. The simulation of thermal transport in silicon structures will be performed using the molecular dynamics method in the LAMMPS package and/or kALDo software. The current-voltage characteristics of silicon solar cells will be calculated using SCAPS software. Machine learning models will be developed using various algorithms, including dense neural networks, random forest, and convolutional neural networks, implemented using the TensorFlow platform. Photoacoustic experiments will be used to evaluate the thermal transport properties of the fabricated porous silicon. The developed method for defect evaluation will be tested on actual silicon solar cells. The expected outcomes of the proposed research project are the development of ML

models for thermal management and defect evaluation, the creation of open-access data collection, and an approach to enhance thermoelectric performance in silicon structures. These results are significant for the development of efficient and reliable solar photovoltaic modules and thermal management systems.

3. European Partner(s)

3.1 European partner(s) first name and last name

3.2 European partner(s) e-mail address

3.3 Name, address and/or website of the European RIs/Institute(s) of affiliation of the European Partner

Full name in English, address, country, website

3.4 Have you already contacted the suggested partners?

- ○ No, I still have to contact the suggested partners
- ◉ Yes, I have already contacted them

3.5 (optional) Supporting document from European partners

If you have already connected with the intended European partners you would like to involve in the research project (strongly recommended option!), you can upload any supporting declaration/document from the European partners about their willingness to take part in the research project

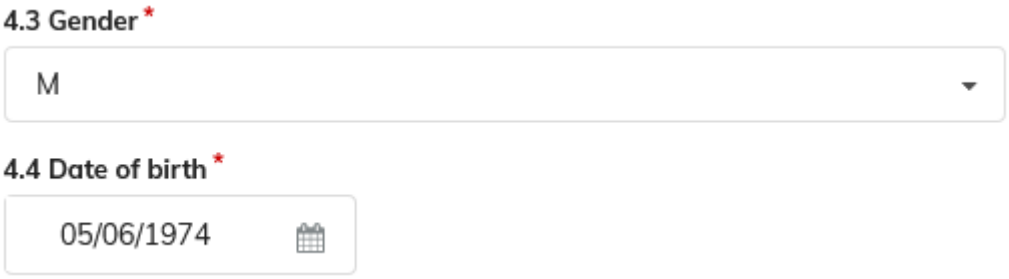
4. Principal Investigator (PI)

4.1 First Name (English alphabet)

Oleh

4.2 Family Name (English alphabet)

Olikh



4.5 Citizenship

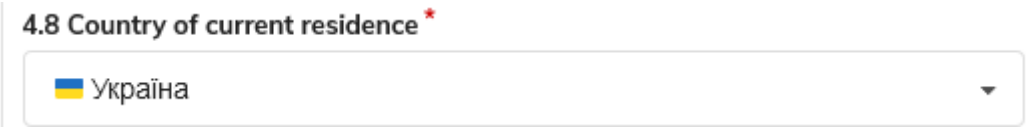
Ukraine

4.6 Email Address

olegolikh@knu.ua

4.7 Current personal address

Mayakovskogo Prospect 32, ap.280, Kyiv, 02222, Ukraine



4.9 Phone Number

+380673169020

4.10 Affiliation Institute

Please mention if you are still affiliated to the institute or until when you were affiliated.

Taras Shevchenko National University of Kyiv,

I am still affiliated to the institute.

4.11 Affiliation Institute address

Volodymyrska Street 64/13, Kyiv, 01601, Ukraine

4.12 Affiliation institute website

https://knu.ua

4.13 Position

Please mention if you are still in the same position or until when you held it.

Professor at Department of General Physics,

I am in the same position.

4.14 Knowledge of English *

- [ ] Excellent
- [ ] Very Good
- [x] Good

4.15 Details of the doctoral degree

Field and Year of graduation

Dr. Hab., Physics and Mathematics, solid-state physics specialty, thesis «Acoustically and radiation induced phenomena in surface barrier silicon and gallium arsenide structures», 2018

4.16 Institute of graduation

Taras Shevchenko National University of Kyiv,

Volodymyrska Street 64/13, Kyiv, 01601,

Ukraine