LITHUANIAN ENERGY INSTITUTE

ADMISSION TO PHD STUDIES FOR THE YEAR 2025

DOCTORAL RESEARCH TOPIC:

Investigation of heat and mass transfer processes by Molecular Dynamics methods

RESEARCH FIELD:

Energetics and Power Engineering (T 006)

BRIEF DESCRIPTION OF RESEARCH TOPIC:

We invite students to choose PhD studies focused on the Molecular Dynamics (MD) computer simulations of heat and mass transfer processes. The MD is used to numerically simulate the movement of individual atoms/molecules in the considered system, which can bridge the gap between molecular movements and macroscopic measurements and provide useful insights in small scales hardly accessible by experimental procedures. The students will have an opportunity to apply MD method and work on one of the following topics:

- investigation of evaporation/condensation processes at nanoscales;
- investigation of heat and mass transfer processes inside nanochannels;
- investigation of appearance and breakup of larger-scale structures due to hydrogen bond interactions among multiple water molecules
- investigation of the influence of hydrogen and helium on the structure and properties of materials;
- investigation on the catalytic chemical reactions at solid-liquid and solid-gas interfaces, such as hydrogen production during methane pyrolysis.

The PhD student will perform MD simulations, analyse the obtained data and disseminate findings in international conferences abroad and scientific journals. During the studies, the PhD student will hone his/her skills in problem solving, data analysis, scientific writing and results dissemination. Furthermore, the student will also have the opportunity to spend some time and improve or learn coding skills with chosen programming language as it is beneficial for the analysis of the simulation data.

The research team offering these topics has over 10 years of experience in the field, so they are ready to assist, advice, and motivate.

Young scientists interested in pursuing doctoral studies in these areas are encouraged to contact the project supervisor for further information.

SCIENTIFIC SUPERVISOR:

Dr. Gediminas Skarbalius
Laboratory of Heat-Equipment Research and Testing

Lithuanian Energy Institute
Breslaujos 3, 44403 Kaunas
Lithuania

Gediminas.Skarbalius@lei.lt

More information and the full list of offered PhD topics available at our website

https://www.lei.lt/en/phd-studies/