**ERC Starting Grant 2020**
**Research proposal [Part B1]**[1]
***(Part B1 is evaluated both in Step 1 and Step 2,***
***Part B2 is evaluated in Step 2 only)***

# Forward thermal transport manipulation at solid/liquid interface

# THERMINATOM

**Cover Page:**

- Name of the Principal Investigator (PI): Mykola ISAIEV
- Name of the PI's host institution for the project: CNRS
- Proposal duration in months: 60

Advances in nowadays fabrication processes allow us to manipulate systems with the sizes up to several nanometres. This opens the possibility for engineering of new high-efficient and ultrafast devices for energy exchange/convert/store that can be found in data storage centres, nanoreactors, biotechnologies, etc. One of the common issues to all these domains is overheating, and thermal management can be improved by liquid cooling. In the last decade, significant progress has been made in the finding of scaling laws for solid/liquid interfacial transport description. However, we are still far from clear understanding of the microscopical mechanisms of thermal transport properties variations in the systems with significant interfacial area.
ThermInAtom aims to provide a deep physical insight regarding thermal transport properties across the solid/liquid interface, and, consequently, to propose unexplored pathways for improving thermal management in the systems were solid meets liquid at the nanoscale. To fulfil this complex goal, the PI addresses following objectives: i) investigations of liquid properties in the vicinity of a solid depending on the morphology of the interface with use of atomistic simulation; ii) study of the heat carrier's scattering processes at the solid/liquid interface; iii) beyond the state-of-the-art, development of innovative experimental tools based on the photothermal methods and scanning thermal microscopy for the study of heat transfer across solid/liquid interface; iv) finding optimal design of the solid/liquid interface based on the experimental and theoretical results to enhance thermal transport. Addressing these objectives will finally bring answers to the fundamental questions "How does heat transfer from solid into liquid?" and "How can we control it?". Therefore, TermInAtom will push the frontier of knowledge on solid/liquid interface at the nanoscale and lead to design optimized systems dedicated to energy applications.

Explain and justify the cross-panel or cross domain nature of your proposal, if a secondary panel is indicated in the online proposal submission forms. There is a limit of 1000 characters, spaces and line breaks included.

[1] Instructions for completing Part B1 can be found in the '*Information for Applicants to the Starting and Consolidator Grant 2020 Calls'*.

## Section a: Extended Synopsis of the scientific proposal

### a.1 Context and state of the art

Continuous miniaturisation of the various devices and components leads to the overheating due to hotspots and thermal interface effects that started to be a bottleneck to improve their stability and reliability. Therefore, tuning heat transfer have a significant importance for a wide range of applied fields. Specifically, thermal transport across the solid/liquid interface is a key issue for energy applications, materials production, solidification/melting processes, cooling applications, etc. Especially, such processes started to be more important at the nanoscale when the surface-to-volume ratio is significant. In the latter, interface often defines the properties of the whole system. One of the most remarkable manifestation of this feature is an outstanding 100% enhancement of the energy transfer in a porous silicon when the latter is filled by a liquid (experimentally observed by PI[1,2]). Such significant enhancement of the thermal conductivity of the porous silicon filled by the liquid in comparison with the liquid-free matrix was confirmed with molecular dynamics (MD) simulations[3]. The above-mentioned variations of the thermal properties could not be addressed by the simple effective media approaches, and the explanation requires more accurate microscopic considerations.

But what do we exactly know about the specificity of energy transport across the solid/liquid interface at the nanoscale? Despite the significant applied and fundamental interest to this issue, mechanisms that rule thermal conductance close to the interface are still unclear. Particularly, the origin of thermal transport in nanofluids, with significant densities of interfaces are still under debates[4]. Several mechanisms that allow us to explain heat transfer enhancement in nano-systems such as influence of Brownian motion of nanoparticles, nanoparticle aggregation and cluster formation, impact of specific surface of the suspended nanoparticles, nanoparticle size, and effects of interfacial layer were proposed[5]. However, the models based on these mechanisms cover only a limited number of experimental situations. These examples of the thermal transport in systems with important solid/liquid interface density show the necessity to change our mind on this topic and elaborate new pathways for understanding accurately the interfacial heat transfer at small scales.

Consequently, **the current project will be focused on the understanding of physical features of thermal transport properties close to the interfacial area from microscopic point of view**. In the same time, while conventional microscopic approaches are mainly based on the examination of the impact of few parameters[6] (work of adhesion, wetting properties, etc), we will rather consider more complex processes involving several multi-physical and multiscale approaches. This requires development of innovative tools for the description of the properties of liquids as well as solids, and their modification in vicinity the interface. Further, special attention will be paid to the accurate consideration of the elementary excitations transfer across and along the interface. We will therefore be offering unprecedented prospects for integration and scalability to improve thermal management of systems for energy application, consumption and harvesting.

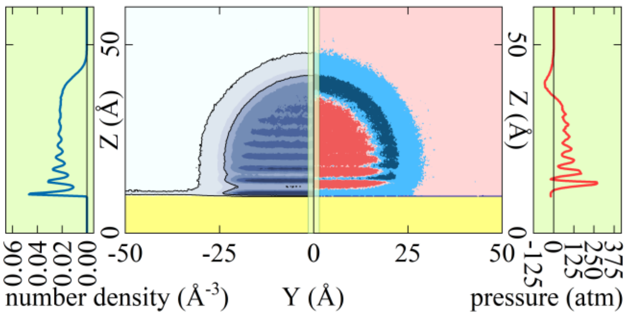


**Fig. 1.** Results from the MD simulations that will be published in ongoing paper of PI: (left side) number density map of a nanoscale droplet and the density profile in the middle of the droplet; (right side) pressure map in the droplet and pressure profile in the middle of the droplet. Such droplet represents difficulties in the defining of solid/liquid and gas/liquid interfaces

Our consideration of the thermal transport through interfaces will start by the addressing the following question – “what is an interface at the nanoscale?”. This question naturally arises because an interface can be defined in several ways based on the atom’s concentration or pressures. It is important to note that such interfaces may be different while we increase the curvature of the interface. As an example, a well-known phenomenon is the size dependence of the surface tension that arises due to the difference between equimolar surface and surface of tension[7]. The clear difference in density and pressure maps/profiles for nanoscaled droplet located on the solid substrate is demonstrated in **Fig. 1**.

Such difference between the interfaces defined in different manner have a significant impact on the description of the thermal exchange between different species. For instance, mass transfer of the individual atoms/molecules will act on the equimolar interface, while the surface of tension is responsible for the arising of collective modes. It is a reason of the existing debates regarding the need or not of different parameters for thermal transport models in these systems. Understanding the fundamental principles of such interactions at molecular level on specific heat carriers at an interface will give us the possibility to propose “universal patterns” for the phenomena description. In this framework, rather than conventional approaches using various parameters to describe heat transfer across the interface we will go deeper in the physical understanding of the interface’s features based on the precise consideration of the interfacial properties. This will naturally provide answers on how we should tailor the interface to obtain a maximum efficiency for energy transfer. These results will initiate new research pathways for further manipulations of the heat/mass transfer at the nanoscale.

The PI can address this ambitious program as this project lies on his different skills and expertise. He is familiar with the theory and models related to thermal transport and solid/liquid interfaces. Furthermore, he has significant experimental background in characterisation of thermal properties of nanostructured materials with the use of photothermal approaches (Raman and photoacoustic). He has already started the examination of interfacial thermal transport with the use of scanning thermal microscopy (SThM) and modulated laser thermoreflectance (FDTR). Thus, the project naturally will combine his experimental and theoretical skills.

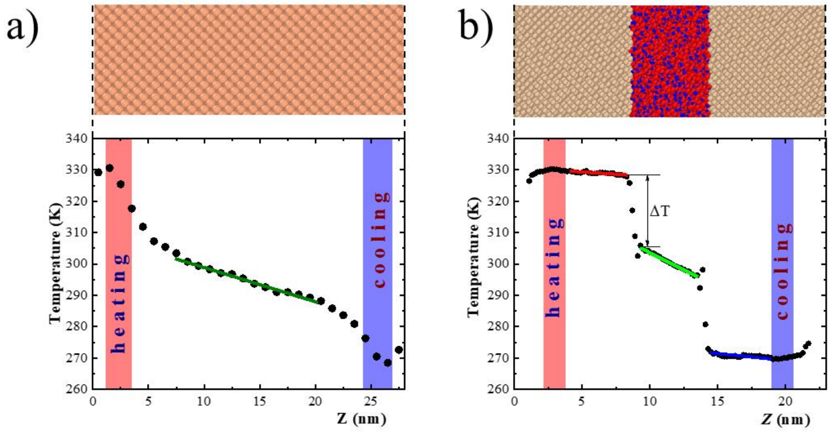


**Fig. 2.** Atomistic view of temperature profiles in a homogeneous material (left) and a three-layer “solid-fluid-solid” system (right) simulated by molecular dynamics. Thermal resistances to the heat flow clearly rise at the solid/liquid interface in the multilayer system.

Let us firstly summarize recent advances in theoretical and simulation studies regarding thermal transport across an interface. Using this knowledge and improving it above the current state-of-the-art, the PI intends to answer the question – “what is happening on the interface during thermal transport?” Heat transfer in the absence of mass flow at the macroscopic level can be described in the frame of Fourier law, which lead to the linear temperature profile between point-like heat source and heat think in one dimensional case (see **Fig. 2A**). In the case of multiphase systems, an additional temperature drop ($\Delta T$) appears at the interface (see **Fig. 3**) separating the phase media. This temperature drop (see **Fig. 2B**) is defined in terms of an interfacial thermal resistance, $R = \Delta T / J_i$ (Kapitza thermal resistance), where $J_i$ is the heat flux across the interface with respect to its normal $n_i$. The presence of this resistance is known to significantly influence the thermal transport in systems where there is an important surface-to-volume fraction. The value of the interfacial resistance depends on the interactions between atoms of solid and fluid at the interface[8,9]. Specifically, well-pronounced dependence of the interfacial thermal resistance on the wetting angle was found[10,11]. Based on the spectral analysis of the heat flow in the silicon-based systems with solid/liquid interface, it was shown that the scaling law with wetting angle is not universal[6,12], and liquid density depletion layer thickness[13,14] was shown to be more universal. C. Ulises Gonzalez-Valle and Bladimir Ramos-Alvarado[13] also showed that out-of-plane modes (perpendicular to the surface) of the substrate contribute more significantly than in-plane-modes (parallel to the surface) to the thermal transport across the interface. It was also shown the dependence of boundary resistance with the confined liquid slab thickness[15,16] and the curvature of the interface[17]. In such simulations, one needs to know exactly the location of the interface to define the temperature difference there. However, it is not a trivial issue (see **Fig. 1**), hence we should know which interface exactly to choose. In literature, this issue is often ignored which may be a source of errors.

The dependence of the Kapitza resistance on the interactional parameters (wetting angle, depletion length, work of adhesion) forms the significant difference from the solid/solid interface, where it mostly depends on bulk properties of materials[18]. Thus, we will develop models which considers interactions between atoms of solids and liquid.

The paragraph above presents a brief overview of the state-of-the-art and shows that significant efforts are paid for inductive observation. Yet, such approaches are not always relevant and sometimes fail to explain unexpected heat transport behavior. For example, the interfacial boundary resistance reduces thermal transport, and the current studies could not address thermal conductivity enhancement in nanofluids and porous systems filled by liquids. Further understanding of what is happening at the interface requires deeper analysis, and only limited number of studies start to consider microscopical features mainly from the solid side[9,12,13]. However, one needs to develop additional cutting-edge approaches from both solid and liquid sides as well as new models to fully understand their interactions. In the current project we will pay a significant attention to the impact of the specie's property modification arising at the contact of the solid and liquid interface. As an example of such modifications, there is the "solid-like" behavior of the adsorbed water nanofilm[19].

#### a.2 Novelty and specific objectives

**The ThermInAtom project aims to study and provide new pathways to control energy and mass transfer across the liquid/solid interfaces.** When convenient approaches are mainly based on the finding of scaling laws using parameters (work of adhesion, wetting angle, depletion length, etc) for heat transport modelling, the ThermInAtom project goals are to find the physical principles and to understand the thermal transport across the solid/liquid interface in a general framework. To this aim, PI will proceed series of molecular dynamics simulations to obtain knowledge regarding the properties of the liquid close to the solid interface. This first stage will give us insights and useful inputs to develop analytical models of thermal transport across the solid/liquid interface at small scales, which consider the presence of the adsorbed layer on the interfacial boundary resistance. In the second step, these models will be tested at different spatial and timescales with cutting edge experiments based on photothermal phenomena and scanning thermal microscopy.

Fulfilling this innovative project requires to carefully address many objectives: i) investigations of liquid properties in the vicinity of the solid substrate depending on the morphology of the interface with use of atomistic simulation; ii) study of the phonon scattering processes at the solid liquid/interface; iii) developments of experimental tools based on the photothermal methods and scanning thermal microscopy (SThM) for the study of heat transfer across solid/liquid interface; iv) formulation of new models, which take into account the presence of adsorbed film, describing thermal transport across solid/liquid interface based on the experimental results and results of simulations; v) optimal design of the solid/liquid interface based on the experimental and theoretical results to enhance thermal transport.

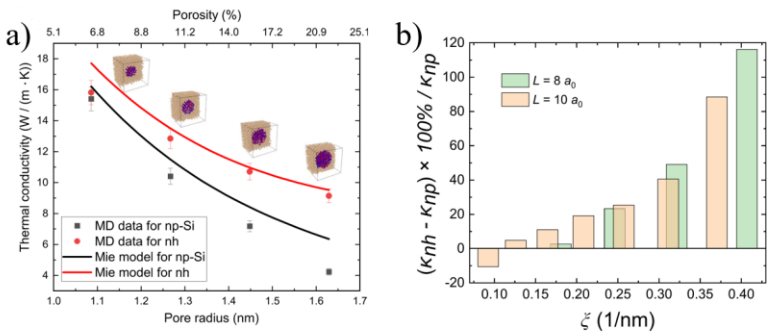


**Fig. 3** a) Thermal conductivity in empty porous silicon (np-Si) and porous silicon water nanohybrid (nh) as a function of a pore size and porosity; b) Thermal conductivity enhancement in nh in relation to the np-Si as function of the pore specific surface area. Thermal conductivity of bulk water 0.86 W/(m×K) for the considered water model

Achieving these objectives is ambitious, and requires significant skills in different domains of materials research, thermal transport, liquids, interfaces etc. Nevertheless, latest results and expertise of PI make such challenge possible. As an example of these latest results, we have proposed an efficient technique for the parametrisation of interaction potential due to the minimisation of the line tension impact[20]. The anomalous enhancement of thermal conductivity of porous silicon filled by liquid compared to the empty one was studied both experimentally[2] and with the use of simulation approach[3] (see **Fig. 3**). Different tendencies in the size dependence of the surface tension of the water droplet depending on their morphology were found[7]. Experimental photoacoustic approaches were developed for the characterisation of thermal transport in nanofluids[21], heat fluxes across nanostructured solid liquid interfaces[22] as well as interfacial boundary resistance in nanostructured materials[23]. SThM was tested in a vacuum environment for further examination of the heat fluxes at the nanoscale due to the presence of adsorbed liquid film[24]. Raman approach was advanced for the study of the anisotropy of thermal transport in nanomaterials[25].

### a.3 Methodology

All theoretical and experimental inputs are the corner stones for further studies going beyond the current state-of-the-art in the examination of thermal transport across the solid/liquid interface. This will allow us further to accurately control and tune processes related to thermal transport (see **Fig. 4**).

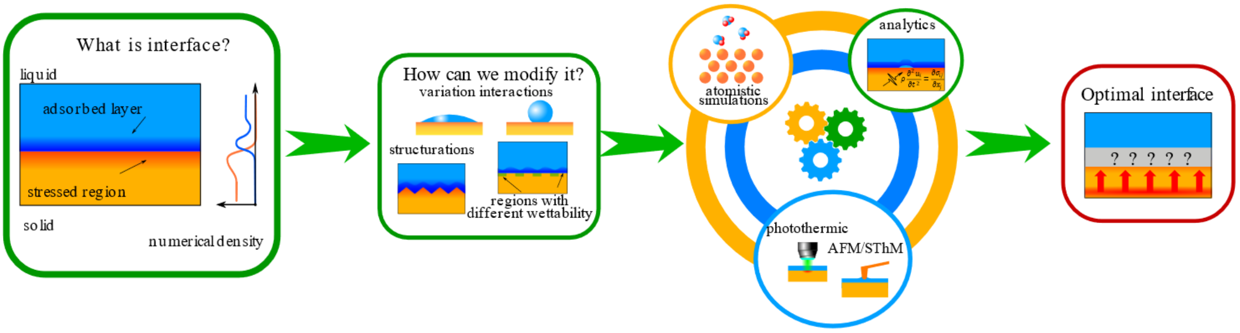


**Fig. 4.** Microscopic insight for thermal transport management

The research program is organized with the 4 interconnected work-packages (WP):

**WP 1.** *Solid/liquid interface characterization.* This WP will be devoted to the study of the liquid and solid properties in vicinity to the interface, and it will be implemented in respect to the following tasks:

1.1. Modules will be developed for the calculation of the static and the dynamical structure factors. Radial distribution function, velocity autocorrelation function, mean square displacements, density fluctuation, etc. will be examined in equilibrium for different parametrization of the solid/liquid interaction.

1.2. Wetting angle, adsorption energy and forces, solid/liquid surface tension will be evaluated for different morphologies of the interface. Impact of the surface structuration and presence of the heterogenous regions on the solid substrate will be examined for the parameters mentioned above.

1.3. Experimental studies of the wetting angle of a droplet that is in contact with a solid with various surface morphologies and its functionalization. Additional attract-approach curves measurements with use of atomic force microscopy (AFM) built inside a controlled environment chamber, where the surrounding gas or pressure can be controlled, will be carried out to verify simulations received in Tasks 1.1 and 1.2.

**WP 2.** *Dynamical response of the solid/liquid interface.* This WP will be devoted to the investigations of the solid/liquid phases in response to dynamical actions:

2.1 MD simulations of the solid/liquid interface behavior will be examined under action of the pulsed and periodic force with different spatial distributions. Additionally, the transfer of phonon wave-packet across the interface will be examined. Spectral characteristic of the wave-packet will be chosen based on the data obtained in Task 1.1. This will give us the possibility to examinate precisely phonon scattering conditions at the solid/liquid interface. The received data will be important because they will highlight the process of transmission of the elementary excitations from the solid in the liquid.

2.2 Development of the analytical acoustical models that consider the adsorbed film presence with the input parameters from Tasks 1.2 and 2.1. This will give us the possibility to estimate interfacial boundary resistance based on the model.

2.3 Photothermal experiments, based on thermoreflectance and/or photoacoustic methods, with different excitation sources will be carried out to examine experimentally dynamical impact on the systems with significant solid/liquid interface. Photothermal in frequency domain can be used to precise measurements of the thermal conductivity of the sample under test (liquid or solid) and thermal interface resistance. The optical sampling by using ultrashort pulsed lasers will give access to vibrational modes and acoustical coupling between liquid and solid phases. The results will probe the elastic and thermophysical properties of the considered systems that can be compared with MD simulations.

**WP 3.** *Thermal transport across the solid/liquid interface.* This WP consists of the several tasks:

3.1 Thermal transport studies across solid/liquid interface with the use of non-equilibrium molecular dynamics (NEMD). This task will give us the possibility to verify the acoustical-based model for the interfacial boundary resistance (Task 2.2).

3.2 NEMD simulations of the thermal transport across nanostructured the solid/liquid interface. During this task we will demonstrate dependence of the interfacial boundary resistance on the size (or curvature). SThM measurements of the thermal resistance between a nanoscale tip and a water adsorbed film. The obtained results will be correlated with the deliverables of Tasks 2.2 and 3.1.

3.3 Implementation of the equilibrium molecular dynamics methods for the investigation of the heterogenous systems (with the atoms of solids and liquids). Examination of anisotropy of the thermal transport at the solid/liquid interface. Raman measurements of the thermal transport anisotropy in porous silicon and silicon nanowires arrays that are empty/filled by liquid. Afterwards, the evaluation of thermal conductance in interfacial boundary layer and further comparison with equilibrium molecular dynamics results will be performed.

**WP 4.** *Heat transport across the interface tuning for energy applications.* This work package will summarize all the results received in WPs 1-3, and the WP 4 implementation will significantly depend on the previous steps. Nevertheless, in frames of this WP:

4.1 As a result of the previous steps implementation, we will verify our hypotheses that explain thermal transport modification close to the solid/liquid interface. Some examples of such hypothesis: i) the presence of a liquid on a solid substrate modifies scattering condition of phonons at the interface, and thus impacts on their mean free path; ii) the solid/liquid interface supports surface waves that carry energy and contribute to thermal transport; iii) the pore acts as "nanochannel" that may change the diffusivity of water molecules; iv) the adsorbed layer of a liquid on a solid substrate has significant thermal conductivity because of the crystal-like behavior due to local increase of liquid density.

4.2 The analytical model will be developed to describe thermal transport modifications at the solid/liquid interface with respect to the identified physical insight in T. 4.1.

4.3 The optimal design of the solid/liquid interface will be proposed to enhance/reduce impacts of different mechanisms on the thermal transport across the solid/liquid interface.

## a.4 Risk and mitigation plan

The implementation of the project with respect of the presented WPs will give us the possibility to obtain a clear view about the phenomena that appear at the solid/liquid interface during thermal transport processes and thus, to precisely control them to tailor thermal transport. Nevertheless, there are significant risks regarding the chosen methods and pathways. Therefore, we have also developed forward-back solutions for each identified risk. Classical MD, which will be one of the main tools, is based on the usage of predefined potentials. For example, in semiconductor and metallic materials, the bending of electronic states close to the surface significantly perturb interaction between the atoms. This effect cannot be simply addressed with classical MD[26] without a complex parametrization of the properties of the system. Therefore, if this such parametrization is found to be impossible, we will use ab-initio technique (developed in our teams) as a *plan B* to feed the molecular dynamics input parameters. In this case, the forces are calculated from quantum mechanics, and the electronic effects are included naturally. In **WP 2**, there is a risk that the Kapitza resistance will not be accessible with photoacoustic experiments, which is quite desirable value to be compared with MD simulations to gain the project goal. However, the use of different photothermal approaches (as thermoreflectance) will minimize this risk. One of the main deliverables from **WP 4** (the optimal interface to heat transfer) will significantly depend on the developed analytical models in **WP 2** and **WP 3**. There is a risk that the model will be complicated, and it will be hard to perform optimization. In this case, we will increase variation of configuration in atomistic simulations, and we will use additionally numerical optimization methods[27–29].

## a.5 Impact

The project will obviously culminate in the demonstration of the possibility of the heat fluxes manipulation at the solid/liquid interfaces. Since it will give the open new routes to improve thermal transport in the system where solid and liquid eventually met this fundamental project will impinge on different fields. The straightforward example that can be mentioned is the common situation for harvesting heat from solid systems surrounded by liquid cooling to further storage and use. Such examples can be mentioned in the context of actual heat capacitors, fuel cells, solar cells, electrics components in datacenters, etc. Thus, it will contribute to optimization of the actual heat exchanger systems, specifically for the various cooling/heating applications. The results of the project will give us the relevant insight for elaboration of the components in the systems at various scales when intensification of the thermal transport is desirable. But the ThermInAtom project is also built around several intermediate outcomes. Particularly, **WP 1** is more general and deals with different aspects of interfacial science. The implementation of this WP will provide us innovative solutions in other crucial domains such as intensified chemical reactors, membranes separation technologies, nanofluids, etc.

(1) Andrusenko, D.; Isaiev, M.; Tytarenko, a.; Lysenko, V.; Burbelo, R. Size Evaluation of the Fine Morphological Features of Porous Nanostructures from the Perturbation of Heat Transfer by a Pore Filling Agent. *Microporous Mesoporous Mater.* **2014**, *194*, 79–82. https://doi.org/10.1016/j.micromeso.2014.03.045.

(2) Lishchuk, P.; Andrusenko, D.; Isaiev, M.; Lysenko, V.; Burbelo, R. Investigation of Thermal Transport Properties of Porous Silicon by Photoacoustic Technique. *Int. J. Thermophys.* **2015**, *36* (9), 2428–2433. https://doi.org/10.1007/s10765-015-1849-8.

(3) Isaiev, M.; Wang, X.; Termentzidis, K.; Lacroix, D. Thermal Transport Enhancement of Hybrid Nanocomposites; Impact of Confined Water inside Nanoporous Silicon. *Appl. Phys. Lett.* **2020**, *117* (3), 033701. https://doi.org/10.1063/5.0014680.

(4) Ali, N.; Teixeira, J. A.; Addali, A. A Review on Nanofluids: Fabrication, Stability, and Thermophysical Properties. *J. Nanomater.* **2018**, *2018*. https://doi.org/10.1155/2018/6978130.

(5) Taha-Tijerina, J. J. Thermal Transport and Challenges on Nanofluids Performance. In *Microfluidics and Nanofluidics*; InTech, 2018; pp 1–15. https://doi.org/10.5772/intechopen.72505.

(6) Ramos-Alvarado, B.; Kumar, S.; Peterson, G. P. Solid-Liquid Thermal Transport and Its Relationship with Wettability and the Interfacial Liquid Structure. *J. Phys. Chem. Lett.* **2016**, *7* (17), 3497–3501. https://doi.org/10.1021/acs.jpclett.6b01605.

(7) Burian, S.; Isaiev, M.; Termentzidis, K.; Sysoev, V.; Bulavin, L. Size Dependence of the Surface Tension of a Free Surface of an Isotropic Fluid. *Phys. Rev. E* **2017**, *95* (6), 062801(1-5). https://doi.org/10.1103/PhysRevE.95.062801.

(8) Merabia, S.; Shenogin, S.; Joly, L.; Keblinski, P.; Barrat, J. L. Heat Transfer from Nanoparticles: A Corresponding State Analysis. *Proc. Natl. Acad. Sci. U. S. A.* **2009**, *106* (36), 15113–15118. https://doi.org/10.1073/pnas.0901372106.

(9) Frank, M.; Drikakis, D. Thermodynamics at Solid-Liquid Interfaces. *Entropy* **2018**, *20* (5), 1–11. https://doi.org/10.3390/e20050362.

(10) Acharya, H.; Mozdzierz, N. J.; Keblinski, P.; Garde, S. How Chemistry, Nanoscale Roughness, and the Direction of Heat Flow Affect Thermal Conductance of Solid-Water Interfaces. *Ind. Eng. Chem. Res.* **2012**, *51* (4), 1767–1773. https://doi.org/10.1021/ie2010274.

(11) Shenogina, N.; Godawat, R.; Keblinski, P.; Garde, S. How Wetting and Adhesion Affect Thermal Conductance of a Range of Hydrophobic to Hydrophilic Aqueous Interfaces. *Phys. Rev. Lett.* **2009**, *102* (15), 1–4. https://doi.org/10.1103/PhysRevLett.102.156101.

(12) Ramos-Alvarado, B.; Kumar, S. Spectral Analysis of the Heat Flow Across Crystalline and Amorphous Si-Water Interfaces. *J. Phys. Chem. C* **2017**, *121* (21), 11380–11389. https://doi.org/10.1021/acs.jpcc.7b01689.

(13) Gonzalez-Valle, C. U.; Ramos-Alvarado, B. Spectral Mapping of Thermal Transport across SiC-Water Interfaces. *Int. J. Heat Mass Transf.* **2019**, *131*, 645–653. https://doi.org/10.1016/j.ijheatmasstransfer.2018.11.101.

(14) Gonzalez-Valle, C. U.; Paniagua-Guerra, L. E.; Ramos-Alvarado, B. Implications of the Interface Modeling Approach on the Heat Transfer across Graphite-Water Interfaces. *J. Phys. Chem. C* **2019**, *123* (36), 22311–22323. https://doi.org/10.1021/acs.jpcc.9b05680.

(15) Masuduzzaman, M.; Kim, B. Scale Effects in Nanoscale Heat Transfer for Fourier’s Law in a Dissimilar Molecular Interface. *ACS Omega* **2020**, *5* (41), 26527–26536. https://doi.org/10.1021/acsomega.0c03241.

(16) Alosious, S.; Kannam, S. K.; Sathian, S. P.; Todd, B. D. Prediction of Kapitza Resistance at Fluid-Solid Interfaces. *J. Chem. Phys.* **2019**, *151* (19). https://doi.org/10.1063/1.5126887.

(17) Alosious, S.; Kannam, S. K.; Sathian, S. P.; Todd, B. D. Nanoconfinement Effects on the Kapitza Resistance at Water–CNT Interfaces. *Langmuir* **2021**. https://doi.org/10.1021/acs.langmuir.0c03298.

(18) Zhang, Y.; Ma, D.; Zang, Y.; Wang, X.; Yang, N. A Modified Theoretical Model to Accurately Account for Interfacial Roughness in Predicting the Interfacial Thermal Conductance. *Front. Energy Res.* **2018**,

*6* (JUN), 1–6. https://doi.org/10.3389/fenrg.2018.00048.

(19) Montazeri, K.; Abdolhosseini Qomi, M. J.; Won, Y. Solid-like Behaviors Govern Evaporative Transport in Adsorbed Water Nanofilms. *ACS Appl. Mater. Interfaces* **2020**, *12* (47), 53416–53424. https://doi.org/10.1021/acsami.0c13647.

(20) Isaiev, M.; Burian, S.; Bulavin, L.; Gradeck, M.; Lemoine, F.; Termentzidis, K. Efficient Tuning of Potential Parameters for Liquid–Solid Interactions. *Mol. Simul.* **2016**, *42* (11), 910–915. https://doi.org/10.1080/08927022.2015.1105372.

(21) Dubyk, K.; Isaiev, M.; Alekseev, S.; Burbelo, R.; Lysenko, V. Thermal Conductivity of Nanofluids Formed by Carbon Flurooxide Mesoparticles. *SN Appl. Sci.* **2019**, *1* (11), 1440. https://doi.org/10.1007/s42452-019-1498-9.

(22) Dubyk, K.; Nychyporuk, T.; Lysenko, V.; Termentzidis, K.; Castanet, G.; Lemoine, F.; Lacroix, D.; Isaiev, M. Thermal Properties Study of Silicon Nanostructures by Photoacoustic Techniques. *J. Appl. Phys.* **2020**, *127* (22), 225101. https://doi.org/10.1063/5.0007559.

(23) Dubyk, K.; Chepela, L.; Lishchuk, P.; Belarouci, A.; Lacroix, D.; Isaiev, M. Features of Photothermal Transformation in Porous Silicon Based Multilayered Structures. *Appl. Phys. Lett.* **2019**, *115* (2), 021902. https://doi.org/10.1063/1.5099010.

(24) Pernot, G.; Metjari, A.; Chaynes, H.; Weber, M.; Isaiev, M.; Lacroix, D. Frequency Domain Analysis of 3ω-Scanning Thermal Microscope Probe—Application to Tip/Surface Thermal Interface Measurements in Vacuum Environment. *J. Appl. Phys.* **2021**, *129* (5), 055105. https://doi.org/10.1063/5.0020975.

(25) Isaiev, M.; Didukh, O.; Nychyporuk, T.; Timoshenko, V.; Lysenko, V. Anisotropic Heat Conduction in Silicon Nanowire Network Revealed by Raman Scattering. *Appl. Phys. Lett.* **2017**, *110* (1), 011908. https://doi.org/10.1063/1.4973737.

(26) Sakong, S.; Groß, A. The Electric Double Layer at Metal-Water Interfaces Revisited Based on a Charge Polarization Scheme. *J. Chem. Phys.* **2018**, *149* (8), 084705. https://doi.org/10.1063/1.5040056.

(27) Grasedyck, L.; Kressner, D.; Tobler, C. A Literature Survey of Low-Rank Tensor Approximation Techniques. *GAMM-Mitteilungen* **2013**, *36* (1), 53–78. https://doi.org/10.1002/gamm.201310004.

(28) Kargas, N.; Sidiropoulos, N. D. Supervised Learning and Canonical Decomposition of Multivariate Functions. *IEEE Trans. Signal Process.* **2021**, *69*, 1097–1107. https://doi.org/10.1109/TSP.2021.3055000.

(29) Fasshauer, G.; McCourt, M. *Kernel-Based Approximation Methods Using MATLAB*; Interdisciplinary Mathematical Sciences; WORLD SCIENTIFIC, 2015; Vol. 19. https://doi.org/10.1142/9335.

**Section b: Curriculum vitae (max. 2 pages)**

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- **EDUCATION**

| | |
|---|---|
| 2014 | PhD-student, Field: Solid State Physics, Faculty of Physics, Taras Shevchenko National University of Kyiv, Kyiv (Ukraine); Topic: **"Peculiarities of photothermal and photoacoustic transformation in silicon-based heterogeneous structures"**; PhD Supervisor: Roman Burbelo; |
| 2010 | MSc in Physical Science, Speciality: Material Research, Taras Shevchenko National University of Kyiv, Kyiv, Ukraine (degree with distinction) |

- **CURRENT POSITION(S)**

| | |
|---|---|
| 2019 – | CNRS permanent researcher (CNRS recruitment is a national competition with a selection on CV, research project and adequacy with host laboratory), Section 10 – Fluid and reactive media: transport, transfers, transformation processes, Laboratory LEMTA (UMR 7563), CNRS, University of Lorraine; |

- **PREVIOUS POSITIONS**

| | |
|---|---|
| 07.2018 –31.12.2018 | Associate Professor of General Physics Department, **Faculty of Physics,** Taras Shevchenko National University of Kyiv, Ukraine; |
| 03.2018 – 31.12.2018 | Researcher (partial time), **Faculty of Physics,** Taras Shevchenko National University of Kyiv, Ukraine; |
| 04.2017-07.2018 | Director of R&D (partial time), "Research Assist" LLC, start-up company, Kyiv; |
| 03.2017-09.2018 | Researcher (partial time), **Corporation "Scientific Parc Taras Shevchenko University of Kyiv"**, Kyiv, Ukraine; |
| 09.2010 –06.2018 | Assistant Professor of General Physics Department, **Faculty of Physics**, Taras Shevchenko National University of Kyiv |
| 06.2016-10.2016<br>01.2015-09.2015 | Postdoctoral researcher, **LEMTA (UMR-7563),** University of Lorraine, CNRS, Nancy, France |

- **FELLOWSHIPS AND AWARDS**

| | |
|---|---|
| 2006 – 2007 | Awarded by the Kyiv Mayor's grant |
| 2009 – 2010 | Awarded by M. Maksymovych grant of the Taras Shevchenko National University of Kyiv |
| 2010 | Awarded by M. Bilyi Honorary Prize and Medal of the Faculty of Physics of Taras Shevchenko National University of Kyiv |
| 2017 | Awarded by The Taras Shevchenko Prize and Medal of Taras Shevchenko National University of Kyiv |
| 2017 | Awarded by The Honorary Diploma of the Presidium of National Academy of Science of Ukraine |
| 2018 | Ministry of Education and Science of Ukraine, (2018 – 2020). Competition of Projects of Scientific Works of Young Scientists 2017 (5th among 59 in section). Features of photothermal and photoacoustic processes in low dimensional silicon-based semiconductor systems (project leader). |

- **SUPERVISION OF GRADUATE STUDENTS AND POSTDOCTORAL FELLOWS**

| | |
|---|---|
| 2010 – 2019 | Scientific advisor of 7 Master Students, Faculty of Physics, Taras Shevchenko National University of Kyiv; |
| 2015 – 2019 | Supervision of 3 master students in LEMTA, University of Lorraine |
| 2015 – 2019 | Participation in supervision of 3 PhD students (Pavlo Lishchuk and Sergii Burian are currently an assistant prof., and Kateryna Dubyk is a researcher in Kyiv); Faculty of Physics, Taras Shevchenko National University of Kyiv; |

2021 Supervision of a postdoc in LEMTA (UMR-7563), University of Lorraine, CNRS, Nancy, France

- **TEACHING ACTIVITIES**

2010 – 2019 Associate/Assistant Professor of General Physics Department, Faculty of Physics, Taras Shevchenko National University of Kyiv (600 – 700 teaching hours per year);

- **ORGANISATION OF SCIENTIFIC MEETINGS**

2015 International Conference Nanoscale and Microscale Heat Transfer V - Eurotherm Seminar No 108, September 26-30, 2016, Santorini, Greece

2020 Physics of Liquid Matters: Modern Problems 2020, May 22-26, 2020, Kyiv, Ukraine (postponed to 2021)

- **INSTITUTIONAL RESPONSIBILITIES**

2012 – 2018 Advisor of the Dean of the Faculty of Physics / periodically was taken responsibility as the deputy dean for educational work, Taras Shevchenko National University of Kyiv, Kyiv (Ukraine)

2011 Member of the Jury Committee (district level) of National Research Paper Defense Competition among pupils of school organized by the Junior Academy of Sciences of Ukraine;

2012 – 2014 Organisation member of the Student Conferences in the Faculty of Physics, Taras Shevchenko National University of Kyiv, Kyiv (Ukraine);

2010 – 2018 Organisation member of the Olympiad in physics for Physical Faculty Entrants

2015 Scientific popular lecture in Physics for the pupils of school in Kreminsk area of Lugansk region (region under conflict) in Ukraine organized by the Junior Academy of Sciences

- **REVIEWING ACTIVITIES**

2020 – Guest Editor of the special issue "Photoacoustic and Photothermal Phenomena in Nanomaterials" of the journal Nanomaterials (IF 4.324)

2010 – Review of different journals: Journal of Applied Physics, Thermochimica Acta, International Journal of Thermophysics, Journal of Chemistry, Applied Optics, Phys Rev Letters

- **MEMBERSHIPS OF SCIENTIFIC SOCIETIES**

2014 – in Mendeley Advisor Team

2019 – Member of Marie Curie Alumni Association

2020 – Member of National Research Group (GDR) “NAME” CNRS, France

- **MAJOR COLLABORATIONS**

Several Departments in Faculty of Physics, on fundamental aspects of interfacial science and solid-state physics, Taras Shevchenko National University of Kyiv, Kyiv, Ukraine;

Dr. Ali Belarouci, Dr. Tetiana Nychyporuk, Dr. Vladimir Lysenko on materials fabrication, INSA Lyon, Lyon, France;

Prof. Olivier Bourgeois and Dr. Dimitri Tainoff on sample deposition and growth, Néel Institute, Grenoble, France

Prof. Stefan Dilhaire and Stéphane Grauby for experimental characterizations if needed, LOMA, University of Bordeaux, France.

Prof. Ali Shakouri, Energy harvesting applications, Birck Nanotechnology Center, Purdue, U.S.

Prof. Je-Hyeong Bahk, energy applications and modelling, University of Cincinnati, U.S.

Prof. Vladimir Sivakov, Functional Interfaces, Leibniz IPHT, Jena, Germany

Dr. Yurii Ryabchikov, nanoparticles fabrications, HiLASE Center, Institute of Physics of the Czech Academy of Sciences, Scientific Laser Application department

Dr. Yuriy Lyulin, on heat and mass transfer across solid/liquid interfaces, Center for Energy Science and Technology, Skolkovo Institute of Science and Technology, Skolkovo, Russia

Prof. Joseph Kioseoglou, Department of Physics, Aristotle University of Thessaloniki, GR-54124 Thessaloniki, Greece

***Appendix: Current research grants and any on-going applications related to the proposal of the PI (Funding ID)***

<u>*Mandatory information*</u> *(does not count towards page limits)*

**Current grants (Please indicate "No funding" when applicable):**

| *Project Title* | *Funding source* | *Amount (Euros)* | *Period* | *Role of the PI* | *Relation to current ERC proposal*[2] |
|---|---|---|---|---|---|
| HOTLINE | ANR (French National Research Agency), France | 378001 | 12/2019-12/2022 | Responsible for matching of atomistic simulations with macroscale experiments | HOTLINe is mainly focused on thermal transport in porous media filled by liquids, while ThermalTune is more wide dealing with interfaces. Some preliminary results were obtained in frames of the project. The samples with chemically functionalised interfaces will be obtained in frames of HOTLINE project for ThermalTune. |
| DROPSURF | ANR (French National Research Agency), France | 518854 | 10/2020-10/2024 | Responsible for WP with atomistic and coarse-grained simulations of thermal transport with liquid-gas phase transition | This project also deals with thermal transport across solid/liquid interface, but due to nucleate boiling. Nevertheless, some experimental approaches will give the insight for ThermalTune. |
| VAPEURS | International Emerging Action CNRS | 13 700 | 01/2020-01/2021 | PI of the project. | This project deals with heat transfer due to droplet evaporation on the overheated substrate. |

[2] Describe clearly any scientific overlap between your ERC application and the current research grant or on-going grant application.

**On-going and submitted grant applications (Please indicate "None" when applicable):**

| *Project Title* | *Funding source* | *Amount (Euros)* | *Period* | *Role of the PI* | *Relation to current ERC proposal*[2] |
|---|---|---|---|---|---|
| Convinces | ANR (French National Research Agency), France | 590 000 | 48 months (with the start close to November 2021) | Responsible for Raman characterisation of phase transition solid/liquid in phase changed materials | None |
| | | | | | |
| | | | | | |

**Section c: Early achievements track-record (max. 2 pages)**[3]

**34 publications in international peer-review journals** + 7 articles in national journals
21 are as lead author (*first or last author*)
**3 book chapters**
**2 national patents**
**10 conference proceedings**
**130 citations** (without self-citations)

My early work (PhD) was focused on the development of the analytical models for the description of photothermal and photoacoustic transformation in the heterogenous materials for the experimental results analysis. During my postdoctoral stay in LEMTA, I switched to the study of the interfacial phenomena with the atomistic approaches. My research activity as assistant/associate professor at the Faculty of Physics in Taras Shevchenko National University of Kyiv (Ukraine) was directed towards the experimental study of thermal properties in the porous systems empty/filled by liquids with the use of photothermal approaches. This work on photothermal methods for thermal transport properties evaluation in complex media has earned me 2 invited talks/lectures as a main author and speaker. My research activities on thermal transport characterisation across the solid/liquid interface and on impact of the interfacial boundary resistance on thermal transport in porous systems and gave me the opportunity to develop two national Ukrainian patents for utility models. My current activity gains a new dimension with microscopic description of the thermal transport at the solid/liquid interfaces using both atomistic simulation approaches and cutting-edge experiments achievable thanks to scientific autonomy granted to me upon my recruitment at CNRS.

During these periods, I proposed the approach for an efficient procedure to tune interactional parameters between a solid and a liquid based on the wetting angle [1] and the adsorption [2]. Additionally, since interface by its definition is mechanically stressed region, I investigated of the impact of the potential on thermal conductivity in materials under the strain [3]. As a continuation of my experimental involvement, a photoacoustic approach for the evaluation of boundary resistance between porous silicon layers with different porosities was proposed [4], and the unique method for thermal transport properties evaluation in anisotropic materials was developed based on the Raman approach [5]. During my research activity I was involved in numerous national (Ukrainian and France) and international (Marie Skłodowska-Curie Actions, H2022 and International Emerging Actions of CNRS) projects, and in 4 projects I was a project leader. In such way I have early stood as an independent researcher in the domain of thermal transport in complex media.

**<u>Selected publications:</u>**

1. **Isaiev, M.**; Burian, S.; Bulavin, L.; Gradeck, M.; Lemoine, F.; Termentzidis, K. Efficient Tuning of Potential Parameters for Liquid–Solid Interactions. Mol. Simul. 2016, 42 (11), 910–915. https://doi.org/10.1080/08927022.2015.1105372. – **21 citations**
2. **Isaiev, M.**; Burian, S.; Bulavin, L.; Chaze, W.; Gradeck, M.; Castanet, G.; Merabia, S.; Keblinski, P.; Termentzidis, K. Gibbs Adsorption Impact on a Nanodroplet Shape: Modification of Young–Laplace Equation. J. Phys. Chem. B 2018, 122 (12), 3176–3183. https://doi.org/10.1021/acs.jpcb.7b12358. arXiv:1707.08844 – **8 citations**
3. Kuryliuk, V.; Nepochatyi, O.; Chantrenne, P.; Lacroix, D.; **Isaiev, M.** Thermal Conductivity of Strained Silicon: Molecular Dynamics Insight and Kinetic Theory Approach. J. Appl. Phys. 2019, 126 (5), 055109. https://doi.org/10.1063/1.5108780. arXiv:1904.10204 – **5 citations**
4. Dubyk, K.; Chepela, L.; Lishchuk, P.; Belarouci, A.; Lacroix, D.; **Isaiev, M.** Features of Photothermal Transformation in Porous Silicon Based Multilayered Structures. Appl. Phys. Lett. 2019, 115 (2), 021902. https://doi.org/10.1063/1.5099010. arXiv:1907.02875 – **8 citations**
5. **Isaiev, M.**; Didukh, O.; Nychyporuk, T.; Timoshenko, V.; Lysenko, V. Anisotropic Heat Conduction in Silicon Nanowire Network Revealed by Raman Scattering. Appl. Phys. Lett. 2017, 110 (1), 011908. https://doi.org/10.1063/1.4973737. arXiv:1609.08133 – **17 citations**

**<u>Book chapters:</u>**

Co-author of 3 book chapters dealing with different aspects of my research profile – simulations [1], experimental approaches for thermal properties evaluation [2], porous silicon fabrication and characterisation [3]:

[3] Please list the order of authors as indicated in the original publication.

1. M. Isaiev, G. Castanet, M. Gradeck, F. Lemoine, K. Termentzidis. – Microscopic study of solid/fluid interface with Molecular Dynamics. – Modern Problems of the Physics of Liquid Systems, Springer Proceedings in Physics 223. – 2019. – pp. 73–89
2. A. Assy, S. Gomès, P. Lishchuk, M. Isaiev. Chapter 17: Thermal wave methods. – Nanostructured Semiconductors: Amorphisation and Thermal Properties. – Pan Stanford Publishing. – K. Termentzidis ed. – 2017. – 564 p. – pp. 493-516
3. M. Isaiev, K. Voitenko, D. Andrusenko, R. Burbelo. Chapter 5: Methods of Porous Silicon Parameters Control. – Porous Silicon: From Formation to Application: Formation and Properties. – Volume one. – edited by G. Korotcenkov. – CRC Press, Taylor & Francis Group. – 2016. – 423 p. – pp.129-153

**National (Ukrainian) patents:**
1. R. Burbelo, K. Dubyk, and M. Isaiev, "An approach for evaluation of heat capacity and thermal conductivity of nanostructured materials with photoacoustic method," u201803640, 2018.
2. R. Burbelo, P. Lishchuk, and M. Isaiev, "An approach for reduction of thermal conductivity of semiconductor nanostructures based on silicon," u201804935, 2018

**Invited conferences:**
1. Photoacoustic effects in two phase solid-fluid composite media // CTCT2015 – Current Trends in Cancer Theranostics, June 1-3, 2015, Jena, Germany. (keynote speaker)
2. Photoacoustic and Photothermal Phenomena in Nanomaterials with Solid/Fluid Interfaces // 4th BIATRI workshop 2020, 09 Dec 2020 - 10 Dec 2020, Prague, Czechia

Also, I was invited on **International Material Research Congress** organised by Material Research Society (15-20 August 2020) to give an invited talk *"Thermal transport characterisation with molecular dynamics of solid/liquid interface"* in section "F9. Interfacial Heat Transfer in Small Scale Systems: Solids, Liquids, Gases and their Interfaces" https://www.mrs-mexico.org.mx/imrc2021/symposium-F9

**Major/significant projects**

-International Emerging Action CNRS (01/2020-01/2021) "VAPEURS" collaborative project with Center for Energy Science and Technology, Skolkovo Institute of Science and Technology, Skolkovo, Russia (**as project leader in France**)

-French Research Agency (ANR) project (2020-2024): "Rational design of enhanced heat transfer surfaces for droplet and spray cooling systems" (Dropsurf) – responsible for work package dedicated to atomistic simulations

-French Research Agency (ANR) project (2019-2023): "Thermal transport across nanostructured solid/liquid interface (HotLine)" – responsible for macroscale and coarse-grained modelling

-CNRS Energy unit PEPS ENERGIE 2019 exploratory Project, Funding for young researchers t "" Improvement of heat exchange surfaces by nanostructuration: an atomistic simulation approach"(ImHESurNaASA) (**as project leader**)

-EMPP pole of University of Lorraine (2019) Project of young researchers "Heat and mass transfer across nanostructured interface" (**as project leader**)

- HORIZON-2020(2016-2019) Marie Skłodowska-Curie Research and Innovation Staff Exchange (RISE),. Carbon-based nano-materials for theranostic application. – responsible for photoacoustic approaches

-Ministry of Education and Science of Ukraine, (2018 – 2020). Competition of Projects of Scientific Works of Young Scientists 2017. Features of photothermal and photoacoustic processes in low dimensional silicon-based semiconductor systems (**as project leader**).

-CARNOT Institute (ICEEL project) (2015-2016) Control and Amelioration of the transfer by structuration of the exchange surfaces (CAMTRASTE)

- State Fund for Fundamental Research of Ukraine. Project F-64 (2016). Photothermoacoustic transformation in heterogeneous silicon-based structures under laser irradiation.

- State Fund for Fundamental Research of Ukraine. Project F-64 (2015). Photothermoacoustic transformation and high-rate mass transfer in Silicon and Cadmium telluride under laser irradiation by the nanosecond short pulses.