

Rozstrzygnięcie konkursu PLL/2025/08 na granty obliczeniowe dla naukowców z Polski realizowane na superkomputerze LUMI
Settlement of competition PLL/2024/07 for for scientists from Poland computational grants implemented on the LUMI supercomputer

Zgodnie z Regulaminem konkursu na granty obliczeniowe dla naukowców z Polski realizowane na superkomputerze LUMI na podstawie przedstawionych recenzji Panel Ekspertów zakwalifikował do realizacji następujące projekty:

In accordance with the Rules of the competition for computing grants for Polish scientists implemented on the LUMI supercomputer, on the basis of the submitted reviews, the Expert Panel qualified the following projects for implementation:

Projekt Project		
1.	Tytuł projektu Title of the project	High-Throughput Atomistic Simulations and AI-Enabled Inverse Design of Quantum Nanostructures on LUMI
	Wnioskodawca Applicant	Michał Zieliński (Uniwersytet Mikołaja Kopernika w Toruniu / Wydział Fizyki, Astronomii i Informatyki Stosowanej)
	Streszczenie Abstract	The primary objective of this proposal is to harness high-throughput, atomistic simulations on the LUMI supercomputer to generate high-fidelity training data for AI-driven inverse design of nanowire quantum dots and quantum dot molecules. Our research will focus on single, double, and triple nanowire quantum dot molecules, exploring various chemical compositions and compositional profiles. By integrating our advanced simulation tools with neural network training, we aim to develop predictive models that accelerate the optimization and engineering of quantum dot-based devices for applications in quantum information and optoelectronics. This project builds upon our extensive publication record in leading journals. It leverages our state-of-the-art hybrid MPI/OpenMP computational framework to address the complexity inherent in these nanostructured systems.
	Ocena Rating	4,79

2.	Tytuł projektu <i>Title of the project</i>	<i>Argon cluster scattering as a tool for measuring surface stiffness and roughness</i>
	Wnioskodawca <i>Applicant</i>	Michał Kański (Uniwersytet Jagielloński w Krakowie / Wydział Fizyki, Astronomii i Informatyki Stosowanej)
	Streszczenie <i>Abstract</i>	The goal of this project is to help in understanding how argon cluster scattering depends on surface properties, such as its roughness and Young modulus. These properties are crucial in any branch of science which employs surfaces and thin (nanometric) films, such as catalysis, solar cell research or studying the interactions between surfaces and microorganisms. Normally, such data are obtained using atomic force microscopy (AFM), which require long time to perform a single measurement and the measured area is limited to micrometres. In contrary, this novel approach allows for rapid measurement of the mentioned surface attributes, which should allow to create 2D maps of local surface roughness and stiffness (with micrometre lateral resolution). The main idea is that the amount of scattered argon dimers and trimers detected after a cluster projectile hits the sample depends on the surface properties, such as Young modulus and its roughness. If this relationship is quantified, it would create a new, powerful method of determining surface properties.
	Ocena <i>Rating</i>	4,79
3.	Tytuł projektu <i>Title of the project</i>	<i>Graph-based methods for modeling and prevention of spreading threats</i>
	Wnioskodawca <i>Applicant</i>	Krzysztof Michalak (Uniwersytet Ekonomiczny we Wrocławiu / Wydział Zarządzania)
	Streszczenie <i>Abstract</i>	The purpose of the proposed research is to develop methods allowing for better understanding and prevention of various threats modeled using graph-based formalism. Studied phenomena include epidemics, waves of bankruptcies and others. The completion of the proposed works will result in more effective optimization of preventive actions used to stop the aforementioned threats from spreading. Because previous research shown that combining metaheuristic optimization

		with lightweight machine learning models was a successful approach, it is expected that with more computing power it will be possible to employ modern ML models such as Graph Neural Networks or other deep learning (DL) models to achieve even better results. The other expected outcome is reaching the ability to handle very large real life networks, such as the animal transports network in Italy consisting of about 250 000 vertices and 6 500 000 edges. Apart from large graph size, the studies based on this dataset face additional challenges such as the network being dynamic (transports occur only at certain moments in time) and thus the need to discover temporal patterns and to predict future transports. Last, but not least, developments towards better explainability and interpretable models are envisioned. Some possible approaches are listed in the above paragraph (i.e. pattern discovery and edge prediction), others involve obtaining human-readable description of the threat propagation mechanism, which is important for tackling poorly studied and new diseases, improving the understanding of dynamics of financial crises, etc.
	Ocena Rating	4,58
4.	Tytuł projektu Title of the project	<i>Calculating predictions for EIC physics</i>
	Wnioskodawca Applicant	Piotr Korcyl (Uniwersytet Jagielloński w Krakowie / Wydział Fizyki, Astronomii i Informatyki Stosowanej)
	Streszczenie Abstract	The project is devoted to the numerical investigations of high-energy nuclear matter. The theory of strong interactions making nucleons and nuclei stable is Quantum Chromodynamics (QCD). The QCD is a complicated theory of interacting quarks and gluons and can be studied only in specific conditions. One of such interesting regime is the high energy limit, namely the situation when two very energetic nucleons (or nuclei) collide. Various predictions can be done using QCD for such collisions, but not all of them are experimentally confirmed. One of the least known phenomenon is the saturation, where the density of gluons inside the nucleus is so high that they recombine. The purpose of this project is to investigate saturation using state-of-the art numerical methods and data from collider experiments. We are planning to provide unified description of several collision processes, which was never achieved within frameworks with saturation included. This provides new tools to study different aspects of saturation

		and connections to other properties of nucleons at high energy. In our work we will concentrate on processes that are planned to be measured at the future Electron-Ion Collider that is being constructed at the Brookhaven National Laboratory in USA. Thanks to our innovative numerical methods and implementations (we use automatic differentiation in our solvers, we plan to leverage machine learning methods to optimize the cost of simulations through simulation-based inference methods) we are able to improve on previous work and perform comparisons with various experimental data simultaneously (called combined fit to several observables). Our results will provide other groups with more realistic models of initial conditions describing the nuclei, and henceforth allow them to perform better predictions of future experiments.
	Ocena Rating	4,5
5.	Tytuł projektu Title of the project	Phase diagram of gallium nitride — towards closing the gap?
	Wnioskodawca Applicant	Jacek Piechota (Instytut Wysokich Ciśnień Polskiej Akademii Nauk)
	Streszczenie Abstract	The aim of this project is to resolve critical uncertainties in the high-pressure–high-temperature phase diagram of gallium nitride (GaN), a semiconductor central to advanced optoelectronic and high-power/high-frequency devices. Although GaN technology has reached impressive levels due to its superior figures of merit, key aspects of its phase behavior remain unresolved—particularly the mechanisms governing congruent melting versus thermal decomposition. Recent ab initio molecular dynamics studies (Piechota et al., Chem. Mater. 2023) have demonstrated that GaN exhibits dual melting behavior. At pressures of 7 GPa and below, GaN decomposes upon heating, leading to the formation of N₂ molecules and an atomic Ga:N liquid solution. In contrast, at pressures near 15 GPa, the evolution of N₂ is suppressed, and GaN melts congruently into a stoichiometric atomic liquid. Moreover, these studies suggest that the intersection of the decomposition and melting curves—and thus the location of the wurtzite–rocksalt–liquid triple point—occurs within this pressure range.

		In our project, we will extend these investigations to even higher pressures (above 50 GPa), where the rocksalt phase becomes increasingly significant. By employing extensive ab initio DFT molecular dynamics simulations, we will analyze the temporal evolution of GaN under extreme conditions to accurately determine the pressure–temperature coordinates of the triple point. The integration of our simulation results with existing experimental data will provide a coherent and predictive model for GaN's phase transitions, ultimately guiding improvements in crystal growth techniques and device fabrication.
	Ocena Rating	4,38

Projekty niezakwalifikowane do realizacji:

Lp.	Projekt	
1.	Tytuł projektu <i>Title of the project</i>	3D numerical simulations of collapsing stars and their gravitational radiation
	Wnioskodawca <i>Applicant</i>	Gerardo Urrutia (Centrum Fizyki Teoretycznej Polskiej Akademii Nauk)
	Streszczenie <i>Abstract</i>	Long Gamma-Ray Bursts (GRBs) are emitted by the energy dissipation of relativistic jets that originate during the collapse of massive stars. However, due to the high opacity of the progenitors, the early jet interaction cannot be directly observed through electromagnetic signals. Understanding this early dynamics is crucial, as the main physical properties of such jets are acquired during their interaction with the star. The early jet dynamics should be observed by the gravitational wave (GW) emission and enhancing our understanding of the origin and propagation of GRBs. Numerical simulations are an appropriate technique for studying the described physical scenarios. However, fully simulating the jet dynamics from its production at the black hole (BH) horizon to its escape from the progenitor star is computationally demanding. Additionally, achieving more realistic results requires three-dimensional simulations. These demanding tasks are planned to be performed using special and general relativistic magnetohydrodynamics codes that employ adaptive mesh

		refinement and MPI parallelization to ensure high-performance computing. The storage requirements for simulation dumps used in post-processing analysis are typically enormous due to the high-precision details of the dynamical evolution. The LUMI supercomputer allocation represents a crucial opportunity for advancing this project. The main outcome of this project is to report the gravitational wave signal generated by jets in collapsars during different evolution's stages: acceleration in a turbulent environment, the accretion process, and propagation at relativistic velocities. Subsequent outcomes will arise from the high-precision simulation data, which will be useful for estimating energy dissipation in different fluid structures. These insights will contribute to a more accurate explanation of electromagnetic counterparts and improve predictions of transients generated by failed jets or subrelativistic ejections.
	Ocena Rating	4,17
2.	Tytuł projektu Title of the project	2D materials for photo(electro)catalysis
	Wnioskodawca Applicant	Silvio Osella (Uniwersytet Warszawski / Centrum Nowych Technologii Uniwersytetu Warszawskiego)
	Streszczenie Abstract	With this project, we will study a hybrid photo(electro)catalyst that combines solar energy harvesting and N₂/CO₂ conversion into one single compact unit based only on environmentally friendly and non-critical low dimensional materials. To this aim, we propose a novel approach for catalyst design, combining (i) the highly efficient, robust, and tunable light absorption of graphene quantum dots (GQDs) with (ii) the superior electronic properties of 2D materials (2DMs), and (iii) 2D metal organic frameworks as catalyst (2D-MOF). We orient the research program towards a material-by-design approach, which allows the selection of different low dimensional materials to obtain efficient and selective catalysis toward the generation of ethylene and ethanol, as well as energetic tuning guiding the synthesis to tune the optoelectronic properties of the different materials. For that, computational methods will be first applied to screen NBBs from the perspectives of their optical, electrical and catalytic properties. Thanks to the modular nature of the NBBs, different assemblies can be produced, to obtain the

		optimal catalytic device for maximizing the CO₂ reduction and the production of complex chemicals with additional carbon atoms (C₂, C₃, termed C₂₊ hereafter). The peculiar electronic properties of these NBBs, being either <i>optically active (objective 1)</i>, <i>electrically conductive (objective 2)</i>, or <i>catalytically active (objective 3)</i> are rationally combined in a “bottom-up” fashion at the nanoscale to address these challenges. We will foster the production of solar fuels by means of reduction of CO₂ through (photo)catalysis at a ternary interface of GQDs, 2D materials, and 2D-MOF. The precise architectures will further ensure sufficiently large surface areas to favor interfacial processes and CO₂ adsorption. By considering all these aspects, we will go considerably beyond the state-of-the-art in the design and production of photocatalytic devices.
	Ocena Rating	2,88