Rozstrzygnięcie konkursu PLL/2026/10 na granty obliczeniowe dla naukowców z Polski realizowane na superkomputerze LUMI

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:

Lp.	Projekt	
1.	Tytuł projektu	***Ergodicity breaking in many-body dynamics: quantum complexity in localization***
	Wnioskodawca	Jakub Zakrzewski (Uniwersytet Jagielloński w Krakowie / Wydział Fizyki, Astronomii i Informatyki Stosowanej)
	Abstrakt	The project aims to improve the understanding of ergodicity-breaking transitions in quantum systems. Despite more than 20 years of many-body localization studies, the existence of a stable localized phase in the thermodynamic limit remains an open question. We intend to continue our studies on disordered one-dimensional quantum spin chains, where recent results indicate that very strong disorder may be required to sustain localization. One reason for this has been attributed to rare, long-range correlated events that may destabilize localization, with the most correlated states forming cat-state pairs absent in noninteracting systems. One objective is to uncover the mechanism underlying cat-state formation in Anderson insulators upon introducing interactions of different types, offering a new understanding of localization in the thermodynamic limit. Correlated projects will also consider disorder distributions with fat tails. Unlike standard Gaussian or box distributions, fat-tailed disorder may suppress the formation of system-wide resonances by reducing the probability of atypically weak disorder regions, potentially stabilizing the MBL phase even at moderate interaction strengths. We also intend to study spin systems with off-diagonal disorder, representing a

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		new class of models that reveal ergodicity breaking. They exhibit unconventional localization properties, as we recently demonstrated. Such systems can be realized using Rydberg atoms trapped in tweezers. Due to the long-range, power-law-decaying interactions inherent to Rydberg atoms, the corresponding Hamiltonian matrices are less sparse than usual, leading to increased computational costs for diagonalizations. We also intend to continue investigating the interplay between entanglement and other measures of quantum complexity, such as nonstabilizerness (i.e., quantum magic), particularly in the context of ergodicity and resource generation.
	Ocena	4,88
2.	Tytuł projektu	***How can glycosylation influence thermal stability?***
	Wnioskodawca	Alexis Descamps (Uniwersytet Jagielloński w Krakowie / Małopolskie Centrum Biotechnologii Uniwersytetu Jagiellońskiego)
	Abstrakt	Without proper glycosylation of your proteins, you would not be able to read this proposal. The importance of this process gave rise to glycobiology. Yet, how glycans influence proteins and their environment remains largely unknown. Do they simply guide protein folding, or do they also affect conformational equilibria, as observed for the SARS-CoV-2 Spike protein? It is still unclear whether these effects are mainly enthalpic and attractive, or dominated by entropy. This uncertainty limits the development of glycan-aware drug design and personalized medicine. Addressing these questions requires close interaction between experiments and theory. The work proposed here will tackle key aspects of this challenge.
	Suma punktów	4,67
3.	Tytuł projektu	***GRMHD simulations of BH accretion and jets***
	Wnioskodawca	Krzysztof Nalewajko (Centrum Astronomiczne im. Mikołaja Kopernika Polskiej Akademii Nauk)

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	Abstrakt	We plan to perform general-relativistic magneto-hydro-dynamical (GRMHD) numerical simulations in 3D of magnetized accretion onto spinning black holes described by the Kerr metric using the GPU code H-AMR. We plan to investigate extended accretion systems by modifying the initial conditions used to simulate quasi-spherical “Bondi” accretion flows with low angular momentum (LAM). We plan to explore conditions leading to the production of relativistic jets powered by Poynting fluxes from spinning black holes. In order to simulate large systems extending to ~1000 r_g, we need a large resolution of 1464x512x512 cells. With our current allocation on the Helios computer at Cyfronet, we can only run simulations at a smaller resolution of 732x256x256 cells. We plan to perform a series of 4 simulations: H1) the reference case of quasi-symmetric LAM flow; H2) a moderately flattened equatorial LAM flow; H3) a tilted flattened LAM flow; H4) flattened equatorial LAM flow with azimuthal asymmetry. We also plan to use CPU code KORAL to conduct high magnetization (the ratio of magnetic to plasma enthalpy densities) simulations via its hybrid GRMHD/GRFFE (force-free electrodynamics) module. These results will be compared with outputs produced by KHARMA (existing data sets) through standard GRMHD simulations to investigate physical discrepancies in high magnetization regions. We will model 2D and 3D magnetically arrested disks (MAD) with thick tori and strong jets, exploring the effects of limiting maximum magnetization. The main aim is to perform at least 2 long (up to t ~ 50 000 r_g/c) 3D simulations with 256x256x128 cells that extend to 1000 r_g. Thus we plan to perform 3 sets of simulations: K1) suites of high-resolution 2D simulations; K2) 3D hybrid simulation with unlimited magnetisation; K3) 3D hybrid simulation with magnetisation limited to 10^5.
	Ocena	4,54
4.	Tytuł projektu	***Real-time Bethe-Salpeter equation and random-phase approximation for the multiphoton excitations and light-intensity dependent refracting index in rare-earth doped ZrO2, as a model for the transverse-mode instability in fiber-glass laser***

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	Wnioskodawca	Małgorzata Wierzbowska (Instytut Wysokich Ciśnień Polskiej Akademii Nauk)
	Abstrakt	This project is a continuation of the pllglass project. The main aim is to understand the transverse mode instability in fiber lasers. This effect stops development of the high-power lasers since 2010. Previous grant enabled to obtain the absorption spectra of Eu doped ZrO2 with oxygen vacancies as a model of glass doped with rare earths. The light intensity was moderate so that the standard Bethe-Salpeter equation (BSE) was used. This grant will focus on extreme light intensity effect on the plausible multiphoton absorption and changes of the refracting index. The studied system will be ZrO2 doped with lanthanides from Nd to Lu. In the same time, the AI simulations for the quasi-periodic glass are conducted at AGH by the PhD student of Prof. Horzyk. We plan to combine our studies for the rare earths in glass. Nonlinear optics in this system shows up in many ways. Multiphoton absorption might lead to upconversion and multimodal instabilities. While refracting index in fibers should be constant for the operation conditions, but it is not. Extreme intensity leads to light leakage. Gaussian shape of the beam causes a spectrum of the refracting index for the largest intensity and two tails. This leads to a curvature of the refracting called “self-focusing”. The real-time BSE will be used for the absorption and real-time random-phase approximation (RPA) for the refracting index via Kramers formula applied to the components of the dielectric function. The approach is called Baym-Kadanoff and operates in the real space. However, after transformation to the momentum space, it leads to the Bethe-Salpeter result that depends on the intensity and shape of the optical-pumping electromagnetic field. At the end, all results obtained from quantum-mechanical simulations will serve as a dataset for the classical device simulations.
	Ocena	4,5
5.	Tytuł projektu	***Towards better accuracy: AI trained across quantum chemical methods***
	Wnioskodawca	Ireneusz Grabowski (Uniwersytet Mikołaja Kopernika w Toruniu / Wydział Fizyki, Astronomii i Informatyki

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		Stosowanej)
	Abstrakt	Atomistic simulations are essential tools in chemistry, materials science, and molecular modeling, but their predictive power is limited by the accuracy and cost of the quantum-chemical (QM) methods. That has stimulated the development of artificial intelligence (AI) and machine learning (ML) approaches, which can reproduce reference QM results for atomistic simulations at much lower cost. The ML interatomic potentials (MLIPs) and related AI models have emerged as powerful surrogates of QM calculations, reaching CCSD(T)/CBS accuracy on benchmark sets when carefully trained on large, high-quality datasets. However, all existing universal ML models share a fundamental limitation: their accuracy, by construction, cannot exceed that of the QM methods used to generate the training data, because they interpolate within chemical compound space at a fixed QM level. The central scientific objective of this project is to develop and rigorously test new extrapolation strategies, both classical and AI-based, that: • Systematically improve upon the accuracy of the QM levels explicitly used in the calculations, or in the training data, and • They are transferable across chemical compound space, basis sets, and QM method hierarchies. We focus on three main research questions: • How can we design modern, benchmarked extrapolation schemes for basis-set and coupled cluster (CC) truncation sequences that approach the Full Configuration Interaction (FCI) and complete basis set (CBS) limit in a controlled and transferable way? Can we construct AI models that explicitly encode the QM method and basis level, thereby extrapolating in QM-method space (towards FCI/CBS) rather than only in chemical space? These questions are formalized into four main goals: (1) extrapolation towards FCI/CBS based on CC and basis-set hierarchies, (2) a universal MLIP approximating exact potential-energy surfaces.

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	Ocena	4,5
6.	Tytuł projektu	***High-Throughput First-Principles Design of 2D Photocatalysts and M–Si–O Materials for Energy Applications***
	Wnioskodawca	Magdalena Popielska (Uniwersytet Warszawski / Wydział Fizyki)
	Abstrakt	Today's global economy relies heavily on non-sustainable fossil fuels, which are expected to be depleted within the coming decades and contribute to environmental problems such as water pollution and global warming [1–3]. Solar energy is clean and virtually inexhaustible and is widely regarded as a promising alternative to address global energy challenges. Photocatalytic water splitting uses sunlight and semiconductor catalysts to produce hydrogen, a clean and sustainable fuel. However, conventional metal oxides suffer from large band gaps (Eg>3eV), photocorrosion, and low quantum efficiency (<10%)[4–6]. Two-dimensional (2D) materials, particularly transition metal dichalcogenides (TMDCs), have emerged as promising candidates due to suitable band gaps, strong optical absorption, and large surface area [7–10], but their performance is limited by fast charge recombination and poor stability. In parallel, amorphous M–Si–O systems (M=transition or selected metals) are promising for electronic and energy applications, including transparent conducting oxides, yet their thermodynamic stability and electronic properties remain poorly understood. This project aims to perform computational screening of functional materials. TMDC-based van der Waals heterostructures, including alloyed and doped systems, will be investigated to identify efficient photocatalysts. In parallel, the thermodynamic stability of transition metals in amorphous M–Si–O systems will be studied using ab initio molecular dynamics and electronic structure methods. Screening criteria include band gaps, band alignment, redox potentials, and stability against decomposition. For M–Si–O systems, metal incorporation in amorphous Si–O matrices will be evaluated. Degradation mechanisms, including photocorrosion and surface hydrophilicity, will also be analyzed.

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	Ocena	4,25
7.	Tytuł projektu	***Large-scale molecular dynamics simulations of RNA, DNA, and nucleic acid–protein complexes for ensemble-based structure and interaction modeling***
	Wnioskodawca	Nithin Chandran (Uniwersytet Warszawski / Centrum Nauk Biologiczno-Chemicznych)
	Abstrakt	The goal of this project is to characterize the structural dynamics of RNA, DNA, and nucleic acid–protein complexes at atomistic resolution using large-scale molecular dynamics simulations, enabling identification of functionally relevant conformational states and interaction mechanisms. Nucleic acids and their complexes exhibit highly dynamic behavior, where function is governed by transitions between multiple conformational states. Experimental approaches provide limited access to these dynamic ensembles, and computational methods are often restricted by insufficient sampling. Molecular dynamics (MD) simulations offer a rigorous framework for modeling such systems, but require extensive sampling across multiple independent trajectories and long simulation timescales to achieve statistically meaningful descriptions of conformational landscapes. This project employs large-scale GPU-accelerated MD simulations to generate converged structural ensembles of nucleic acid systems. Multiple trajectories will be initiated from diverse conformations and simulated over extended timescales reaching the microsecond regime, enabling exploration of slow conformational transitions and rare but functionally relevant states.The resulting ensembles will be analyzed to quantify flexibility, characterize interaction interfaces, and identify persistent and transient binding pockets. This ensemble-based approach enables robust identification of structural and dynamic features that are not accessible through static models or limited simulations. In addition, the generated large-scale simulation datasets will provide high-quality training data for machine learning models aimed at predicting nucleic acid structure, dynamics, and interaction properties, supporting the development of next-generation data-driven approaches.

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	Ocena	4,13
8.	Tytuł projektu	***Efficient Continual Pretraining for Multilingual Scientific Reasoning Models on Permissive Data***
	Wnioskodawca	Wojciech Kusa (Naukowa i Akademicka Sieć Komputerowa - Państwowy Instytut Badawczy)
	Abstrakt	The project aims to develop an efficient methodology for continual pretraining of compact multilingual language models specialized in scientific reasoning. Building on the Aurora-M paradigm of continual pretraining and the MixtureVitae dataset design, we focus on improving reasoning capabilities using high-quality, permissively licensed data. The planned work includes: (i) constructing a curated multilingual scientific reasoning corpus based on permissive sources, (ii) adapting continual pretraining strategies to avoid catastrophic forgetting while enhancing reasoning skills, and (iii) evaluating performance on scientific QA, mathematical reasoning, and code-related benchmarks. Unlike large-scale foundation model training, this project targets models in the 1B–7B parameter range, enabling efficient use of LUMI resources while still requiring substantial GPU compute due to long training sequences and multilingual data. The emphasis is on reasoning density rather than raw scale. The expected outcome is a reproducible training pipeline and a set of open models demonstrating strong reasoning performance under strict data governance constraints. This will contribute to transparent and legally compliant AI development in Europe.
	Ocena	4,0
9.	Tytuł projektu	***Explainable and adversarial analysis of AI models***
	Wnioskodawca	Przemysław Biecek (Politechnika Warszawska / Wydział Matematyki i Nauk Informacyjnych)
	Abstrakt	The aim of our research is to explain the decision-making process of deep learning models used in computer vision. We

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		focus on developing synthetic explanation techniques, such as counterfactual visual explanations, and on devising new example-based explanation methods. Synthetic methods offer broad possibilities but require the use of computationally expensive generative models. We also investigate the application of game theory to the interpretation of language-visual models, such as CLIP and SigLIP. We pay particular attention to the efficient approximation of Shapley values and feature interactions in high-dimensional spaces. Additionally, we are developing concept-based explanations using sparse autoencoders (SAEs), which allow complex representations to be decomposed into more unambiguous ones. Thanks to a self-supervised approach, we avoid the need for labelled data. All elements of the project are heavily dependent on access to substantial computational resources (GPUs) and storage space necessary for working with large datasets and models.
	Ocena	3,75

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