LUMI

Rozstrzygnięcie konkursu PLL/2025/09 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	***Towards resolution of the puzzling discrepancy between reference electronic structure methods in calculation of interaction energies between large molecular systems***
	Wnioskodawca	dr hab. inż. Michał Lesiuk, Uniwersytet Warszawski
	Ocena	4,79
	Streszczenie projektu	*A few years ago a puzzling discrepancy [Nature Communications 12, 3927 (2021)] has been discovered between two reference quantum-chemical methods: (i) local-orbitals CCSD(T) theory and (ii) diffusion Monte Carlo method, when both were applied to interaction energies between large molecular systems. This discrepancy is a cause for a major concern because both methods were seen as a source of benchmark-quality theoretical data and were expected to agree to within chemical accuracy (kcal/mol) when interaction energies are considered. Even more importantly, both methods are used as a source of reference data for other theoretical models, such as density functional theory or force fields, which are routinely applied to a plethora of systems of chemical and biological relevance. Therefore, if any (or both) of these methods provide results which are not as accurate as believed, this problem will propagate to a multitude of other fields. Moreover, domain based variants of local-orbital DLPNO-CCSD(T) have become a de facto tool for accuracy in industrial computational chemistry research. As explained in detail in the next section of the proposal, the objective of the current research is to investigate the sources of the found*

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		discrepancy by using a new and emerging family of electronic structure methods which are developed within our group: rank-reduced coupled cluster methods based on tensor decomposition techniques [J. Chem. Phys. 156, 064103 (2022)]. By comparing our results with the published data we plan to shed new light on the origins of the discrepancy and hope to provide a definitive answer to this puzzling situation.
2.	Tytuł projektu	***Dynamics and non-equilibrium properties of inhomogeneous Fermi superfluids***
	Wnioskodawca	dr inż Bugra Tuzemen, Instytut Fizyki PAN
	Suma punktów	4,75
	Streszczenie projektu	*This project investigates vortex dynamics and persistent currents in inhomogeneous Fermi superfluids using time-dependent density functional theory. Spatial variations in the pairing field arising from spin imbalance in ultracold gases or nuclear lattice structures in neutron stars can fundamentally alter vortex motion and dissipation mechanisms.* *In spin-imbalanced ultracold Fermi gases, population imbalance disrupts standard Cooper pairing and can generate spatially modulated order parameters or localized polarized structures. A key question is whether transverse forces, such as the debated Iordanskii force [Iordanskii1966], play a measurable role in vortex dynamics. Persistent currents in ring geometries provide a complementary probe, with preliminary results indicating that spin imbalance introduces novel vortex nucleation patterns that are sensitive to pairing field inhomogeneities.* *In neutron star crusts, vortices interact with a crystalline lattice of nuclei immersed in a neutron superfluid. We will conduct systematic studies of vortex-nucleus pinning forces for different layers of the star using state-of-the-art 3D time-dependent approaches. We aim to compare the Brussels–Montreal density functional, which is specifically designed for astrophysical applications [BSk], with others that are widely used by the community, such as SLy4 and SkM*, to see how the pinning force depends on the model.* *Both systems require fully microscopic 3D simulations without geometric restrictions, demanding top-tier supercomputers like LUMI. This research will be conducted in collaboration with experimentalists at LENS for ultracold gases and with the Brussels group for neutron star physics.*

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3.	Tytuł projektu	***Modelling spin-split antiferromagnets at high pressure***
	Wnioskodawca	dr hab. Dominik Kurzydłowski, Uniwersytet Kardynała Stefana Wyszyńskiego w Warszawie
	Ocena	4,70
	Streszczenie projektu	*Unconventional magnetism, such as altermagnetism and spin-split antiferromagnetism, has attracted considerable attention due to its fundamental scientific relevance and promising potential for spintronic applications [Q. Liu, X. Dai, and S. Blügel, Nat. Phys. **21**, 329 (2025)]. These magnetic phases challenge the traditional dichotomy of ferromagnets and antiferromagnets by introducing symmetry-driven spin textures, that enable novel transport properties without the need for net magnetization.* *Recently, direct spectroscopic evidence of spin splitting has been provided in the antiferromagnet MnTe2 [Y. Zhu et al., Nature 626.7999 (2024)]. It was shown that in this pyrite-type compound the in-plane components of spin are antisymmetric about the high-symmetry planes of the Brillouin zone, comprising a plaid-like spin texture in the antiferromagnetic ground state. This finding comprised an important step in the development of AFM spintronics and opened the possibility for studying similar exotic quantum phenomena in related materials.* *The current project aims at modelling the influence of hydrostatic compression on the structural, electronic and magnetic properties of MnTe2 and related compounds, i.e. MnX2, where X is a chalcogenide (S, Se, Te) or a halogen (F, Cl, Br). Our research will be concerned with pressures exceeding 1 GPa (=10 kbar) and reaching 100 GPa, as such compression offers means for inducing a controlled and continuous perturbation of materials properties [see for example Y. Yang et al., Nat. Commun. 14, 2260 (2023)]. Our aim is to understand the mechanism responsible for the appearance of unconventional magnetism by studying its evolution with compression, and predict the emergence of novel pressure-induced phenomena. Importantly, the results of modelling will in parallel be validated by experimental measurements performed on selected compounds by means of the diamond anvil cell (DAC).*

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4.	Tytuł projektu	***Lattice dynamics and thermal conductivity of a novel Cu-based thermoelectric chalcogenide Cu6+yTe3-xS1+x***
	Wnioskodawca	dr hab. inż. Bartłomiej Wiendlocha, Akademia Górniczo-Hutnicza w Krakowie
	Ocena	4,70
	Streszczenie projektu	*The rising global demand for energy is intensifying the search for new and more efficient energy sources.In this context, the thermoelectric (TE) effect has gained renewed attention amid the challenges of global warming and the current energy crisis. TE materials offer possibilities for renewable energy technologies, enabling the direct conversion of waste heat into electricity or the construction of solid-state heat pumps.However, the low efficiency of existing TE materials continues to be a major challenge in the field.* *Our group has joined this project to clarify the microscopic origins of these exceptional properties. In collaboration with the AGH team and Dr M. Koza (ILL Grenoble), where neutron-scattering studies of lattice dynamics will be done, we aim to understand how electronic structure, phonon spectra, disorder, and lattice anharmonicity govern the thermal and electronic transport in this materials family. Advanced DFT calculations, combined with experimental insights, will enable quantitative evaluation of phonon thermal conductivity and its key controlling factors. This understanding will guide further optimization of thermoelectric performance through targeted alloying or chemical doping, ultimately supporting the development of novel efficient, cost-effective TE materials.*
5.	Tytuł projektu	***Chemical evolution in collapsing stars***
	Wnioskodawca	prof. Agnieszka Janiuk, Centrum Fizyki Teoretycznej PAN
	Ocena	4,67
	Streszczenie projektu	*The project aims to explore the process of massive star collapse leading to formation of a black hole and accretion inflow/outflow phenomena. The astrophysical appearance manifests as bright transients in a broad energy range. Electromagnetic gamma ray bursts prompt and afterglow emission in Optical/Infrared is expected, as well as a kilonova transient driven by radioactive decay of elements synthesized in*

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		the outflowing ejecta. To simulate collapsing stars and their remnants., we use numerical scheme HARM (High Accuracy Relativistic MHD). The recently developed code branches used our team, HARM-EOS, with tabulated equation of state, and HARM-SELFG, with evolving Kerr metric and self-gravity modules, have been integrated. The code HARM-COMBO accounts for bot chemical evolution of collapsing star as well as for the spacetime evolution. We focus on powering electromagnetic signals observable as kilonova transients, possibly related to collapsars and accompanied by a long-living GRB jet driven by the central engine. We also explore the role of magnetic fields in driving these outflow ejecta and calculate the mass and velocity of the magnetically-accelerated winds that are needed to provide enough abundances of the nucleosynthetic yields. Code performance and grid settlements have been already tested and optimized on LUMI during our previous grant, and first results obtained to proof the role of disk winds in kilonova engine and their chemical enrichments. Now our HARM-COMBO code is ready to be launched in collapsar setups, where the jet and winds are embedded in dense stellar material. These endeavors require substantial resources, available at the powerful LUMI supercomputer.
6.	Tytuł projektu	***Improving the precision of predictions for EIC physics***
	Wnioskodawca	dr hab. Piotr Korcyl, Uniwersytet Jagielloński w Krakowie
	Ocena	4,63
	Streszczenie projektu	*The project is devoted to the numerical calculations of cross-section in high-energy nuclear scattering experiments. The experimental measurements of such cross-sections are being performed at LHC, both with protons and heavy ions, and will be expanded in the upcoming Electron-Ion Collider, a facility that is being built at the Brookhaven National Laboratory in the US. The theory which describes the internal structure of hadrons and heavy ions is Quantum Chromodynamics (QCD). It is a complicated theory of interacting quarks and gluons and can be studied analytically only in specific conditions. One of such interesting regime is the high energy limit. Although this makes it possible to derive analytically the formulae for the cross-sections, their numerical evaluation is a very non-trivial and complex problem. In view of the new experimental data, the purpose of this project is to develop further the numerical*

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		techniques, and provide beyond-the-state-of-the-art predictions for various cross-sections. Very recently a new, more precise evolution equation (NLO Balitsky-Kovchegov equation) was derived. We implemented and tested its stability. This project is parallel to the work that is being performed within the plleicphysics grant. Within that allocation we already developed a framework which provides a unified description of several collision processes which has never been achieved within frameworks with saturation included. We also studied various algorithms for Bayesian inference from the posterior distribution of the model parameters. We are now able to combine the various elements together with the new equation and significantly improve on previous works. Within this new allocation we will prepare theoretical estimates for various cross-sections with the improved precision (NLO) and perform comparisons with various experimental data simultaneously.
7.	Tytuł projektu	***Hard carbon electrode materials for Na-ion batteries***
	Wnioskodawca	dr Oleksandr Malyi, ENSEMBLE3 spółka z ograniczoną odpowiedzialnością
	Ocena	4,58
	Streszczenie projektu	*The project aims to accelerate the development of low-cost, high-energy-density, and long-cycle-life sodium-ion batteries by creating a comprehensive and predictive model of hard carbon anodes. Our goal is to uncover the fundamental mechanisms that control sodium storage, transport, and capacity in both pristine and doped hard carbon, and to use this understanding to guide the design and optimization of next-generation anode materials. To achieve this, we will construct realistic structural models of hard carbon that capture its multiscale features, including turbostratic domains, pore networks, defects, and heteroatom dopants. We will combine density functional theory with machine learning interatomic potentials and molecular dynamics to simulate sodium adsorption, insertion, diffusion, and clustering across a wide range of conditions. This multilevel approach will allow us to predict voltage profiles, identify the role of structural motifs in capacity contributions, and determine how doping strategies can enhance performance. The modelling insights will directly support our experimental partners, who will synthesize and test the most promising hard carbon compositions. By linking theory with experiment, the*

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		project aims to deliver design principles that enable the fabrication of low-cost hard carbon anodes with improved initial Coulombic efficiency, higher plateau capacity, and superior rate performance. The overall outcome will be a validated computational framework and clear materials guidelines that advance sodium ion battery technology toward practical and scalable energy storage solutions.
8.	Tytuł projektu	***Computational modeling of structural dynamics in potassium and sodium channels with focus on disordered domains***
	Wnioskodawca	dr Katarzyna Walczewska-Szewc, Uniwersytet Mikołaja Kopernika w Toruniu
	Ocena	4,46
	Streszczenie projektu	*This project aims to resolve a critical gap in structural biology: the functional role of intrinsically disordered regions (IDRs) in ion channel gating. While high-resolution structures provide static snapshots, the mechanism by which dynamic, flexible IDRs allosterically control the opening of the structured channel pore remains unknown. This is a fundamental problem as these disordered regions are key to the regulation of crucial potassium (e.g., KATP) and sodium (e.g., Nav1.5) channels, with mutations linked to severe channelopathies.* *Our goal is to use advanced molecular dynamics simulations to bridge this knowledge gap. We will model the full-length structures of selected channels, explicitly including their N- and C-terminal IDRs. Using both standard and enhanced sampling molecular dynamics, we will simulate the transition from closed to open states and characterize the allosteric network connecting the disordered domains to the pore. This approach allows us to capture the conformational ensemble and dynamics that are invisible to crystallography.* *The significance of this research is twofold. First, it will provide a novel, dynamic model of ion channel regulation, moving beyond static structures. Second, by elucidating these mechanisms, our work will identify potential new allosteric sites for therapeutic intervention, offering a pathway for developing drugs targeting previously "undruggable" disordered regions.*
9.	Tytuł projektu	***Resonance Raman Spectroscopy of Large Molecular Systems***

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	Wnioskodawca	dr Emilia Brumboiu, Uniwersytet Mikołaja Kopernika w Toruniu
	Ocena	4,46
	Streszczenie projektu	*The aim of this project is to showcase a recent implementation of resonance Raman spectroscopy in VeloxChem by determining resonance Raman spectra of large molecular systems and revealing size-dependent spectral trends in increasingly large fullerenes, going from C60 and C70 to C240 and possibly beyond. Raman spectroscopy measures the change of the static polarizability with respect to nuclear displacements when a molecule absorbs a visible photon and relaxes by emitting a photon with a different photon energy. Resonance Raman (RR) scattering occurs when the incoming photon energy coincides with the excitation energy of an electronic excited state and the signal intensity is increased significantly (usually three to six oredrs of magnitude). RR selectively enhances vibrational modes coupled to the resonant electronic transition and is therefore sensitive to pi-electron delocalization, subtle topology differences, and local strain. However, there are very few implementations of RR spectroscopy and most are limited medium-sized molecules (around 50 atoms). Our recent MPI + OpenMP parallel implementation of the molecular Hessian and complex polarizability gradient in VeloxChem [1, 3] enables the computation of RR spectra of large molecules, as C60 and beyond, allowing to determine size-dependent trends. The goal of the current project is to compute RR spectra for molecules of unprecendented size for this spectroscopy, determine their size-dependent optical properties, and correlate these properties to RR spectral features.*

Projekty niezakwalifikowane do realizacji:

Lp.	Projekt	
1.	Tytuł projektu	***How Glycan influence thermal stability ?***
	Wnioskodawca	dr Alexis Descamps, Uniwersytet Jagielloński w Krakowie
	Ocena	4,33

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	Streszczenie projektu	*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.* *Task 1 focuses on the effect of glycosylation on local protein stability, particularly for the Spike RBD domain. This study, part of an ongoing collaboration with experimental partners (i.e Danny Hsu from Academia Sinica), will reproduce experimental melting curves for 4 systems as show in Figure 1 using computationally demanding HREX simulations. The results will provide molecular-level insights essential for selecting the next systems for experimental comparison.* *Task 2 investigates the influence of glycosylation sites and glycan–glycan interactions. Though still poorly explored, these interactions are crucial for understanding how glycans stabilize or destabilize protein active regions. This work represents a first step toward integrating glycans into docking method development. To evaluate these effects, 2D umbrella-sampling simulations will be performed between six glycans of varied structures as show in the Figure 2.*
2.	Tytuł projektu	***Stripes in the t-J model at finite temperature***
	Wnioskodawca	prof. Jacek Dziarmaga, Uniwersytet Jagielloński w Krakowie
	Ocena	4,21
	Streszczenie projektu	*In our recent work (arXiv:2510.04756, supported by ACK Cyfronet AGH), we used the iPEPS tensor network to explore the t-J model at high and medium temperature (including the controversial pseudogap phase), where the state of the system remains translationally invariant. In order to push our exploration to lower temperatures, we have to assume a more general tensor network that allows for breaking the translational symmetry. With the symmetry breaking, it should*

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		be possible to represent the hypothetical low-temperature stripe phases efficiently. The stripe order was demonstrated in the ground state at zero temperature. Our aim is to estimate the transition/crossover temperature to the low-temperature striped phase. Unlike other methods suffering from finite size effects, our infinite tensor network will adddress this question directly in the limit of infinite system size. We want to answer the long standing question if the striped phases in the t-J/Hubbard model exist at finite temperature or only in the ground state at zero temperature. We are encouraged by the results in the attached file that shows a tendency towards stripe formation at finite temperature obtained by a different method in arXiv:2510.04756. As the method is a simulation on a 32x4 cylinder, it has strong finite size effects and is not quite conclusive. We hope to reach a clear-cut conclusion with our infinite PEPS.
3.	Tytuł projektu	***High-Resolution Spatiotemporal Modelling of Large-Scale Low-Carbon Power Systems Using State-of-the-Art GPU and CPU Solvers***
	Wnioskodawca	dr inż. Pablo Benalcazar, Instytut Gospodarki Surowcami Mineralnymi i Energią PAN
	Ocena	4,04
	Streszczenie projektu	*The project focuses on tackling the computational challenges posed by large-scale, long-horizon power system optimization using advanced HPC resources on LUMI. The central modelling framework to be tested is a large-scale mixed-integer linear programming model developed at the Mineral and Energy Economy Research Institute of the Polish Academy of Sciences. The model integrates GIS-based spatial information and employs specialized temporal and spatial reduction techniques, such as representative periods and clustering, to mitigate dimensionality. Despite these improvements, the resulting model remains computationally intensive as it generates very large search trees that cannot be solved efficiently on standard workstation hardware.* *A key objective of the project is to evaluate how state-of-the-art optimization technologies perform on such large-scale problems. We will systematically compare traditional multi-core CPU-based MILP solvers with next-generation GPU-accelerated optimization approaches, including massively parallel*

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		branch-and-bound methods and GPU-based linear algebra engines designed for large integer programming. This will involve running several hundred scenarios under varying temporal and spatial settings to assess scalability, robustness, and sensitivity to modeling choices, while identifying critical computational bottlenecks in long-term planning workflows. *The expected outcomes include: (1) quantitative performance benchmarks documenting solve times, memory consumption, and parallel scaling efficiency for CPU-based versus GPU-accelerated MILP solvers across energy system scenarios on LUMI infrastructure and identifying problem characteristics favoring GPU acceleration; (2) methodological best-practice guidelines for formulation strategies, solver configuration, and hardware selection tailored to large-scale, multi-decade capacity expansion problems, including optimal temporal/spatial resolution trade-offs and memory management.*
4.	Tytuł projektu	***Prolonging Receptor Residence via Binding Isotope Effects: High-Performance ONIOM Calculations of Diazepam at the GABA-A Benzodiazepine Site***
	Wnioskodawca	dr Mateusz Nowicki, Politechnika Łódzka
	Ocena	4,00
	Streszczenie projektu	*We will develop and validate a rigorous, structure-based workflow that predicts position-specific binding isotope effects (BIEs) for diazepam bound at the benzodiazepine site of the human GABA-A receptor (PDB 6X3X). BIEs quantify how isotopic substitution shifts the binding equilibrium; positions with inverse BIE (<1) are expected to enhance affinity and extend receptor residence of the deuterated isotopologue. We will compute a full "BIE map" over all non-exchangeable hydrogens and relevant microstates (protonation/rotamers), quantify uncertainties, and rank deuteration proposals (single positions and minimal sets) for follow-up. This directly operationalizes the BIE-guided paradigm that favors selective labeling to prolong the active bound form while avoiding deuterium release characteristic of metabolism-driven (KIE) approaches.*
5.	Tytuł projektu	***Gravitational Waves and Dark Matter studies***

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	Wnioskodawca	dr Syed Naqvi, Instytut Fizyki Jądrowej PAN
	Ocena	3,83
	Streszczenie projektu	*We aim to probe dark-matter (DM) effects on the neutron-star equation of state (EOS) using gravitational-wave (GW) signatures in binary neutron star (BNS) inspirals and mergers. DM-modified EOS stiffens/suppresses tidal deformability Λ and induces spin-induced quadrupole moments (SIQM), altering both inspiral phase (spin-precession) and post-merger ringdown. This project will:* *1. compute matched-filter signal-to-noise ratios (SNR) and Fisher-matrix forecasts for O4/O5 BNS events using IMRPhenomD_NRTidalv2 waveforms augmented with DM-dependent SIQM (κ_s) and Λ(m,ρ_DM) from microphysical EOS (SLy+DM, APR+DM);* *2. perform population-level inference on 50–100 mock O4 BNS detections to constrain DM fraction in NS cores (f_DM < 5%);* *3. generate Einstein Telescope (ET) mock data (10^6 BNS events, 2035 sensitivity) and conduct full Bayesian parameter estimation + hierarchical modeling with Bilby/GWPop to recover joint (Λ, κ_s, f_DM) posteriors via trans-dimensional RJMCMC;*
6.	Tytuł projektu	***Impact of molecular shape and charge distribution on stability of the ferroelectric nematic phase ferroelectric nematic liquid crystals***
	Wnioskodawca	prof. Antoni Kocot, Uniwersytet Śląski w Katowicach
	Ocena	3,58
	Streszczenie projektu	*Over the past two years, thermotropic polar nematic phases, including splay antiferroelectric (NS) and ferroelectric nematic (NF) phases, have been experimentally discovered in wedge-shaped mesogens with large dipole moments (~11 D for RM734). Although the existence of ferroelectric nematics was predicted by Born in 1916, achieving long-range polar order has proven challenging due to weak dipolar interactions and strong thermal motion. Recent findings indicate that molecular shape and short-range interactions are crucial for stabilizing polar nematic order. The primary goal of this project is to elucidate the relationship between molecular structure and the macroscopic properties of polar nematic materials. This will be*

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		achieved by analyzing the orientation and polar order of a series of molecules with varying structures. The project combines the synthesis of new materials promoting polar nematic phases with density functional theory (DFT) modeling, focusing on short-range intermolecular interactions that influence molecular conformations. The expected outcomes include a deeper understanding of the mechanisms driving ferroelectric nematic ordering and predictive insights into designing new materials with tailored properties for advanced technological applications.
7.	Tytuł projektu	***Localization properties of many-body disordered systems studied by spectral and time-dynamics methods***
	Wnioskodawca	prof. Jakub Zakrzewski, Uniwersytet Jagielloński w Krakowie
	Ocena	3,25
	Streszczenie projektu	*The understanding of ergodicity-breaking transitions in quantum systems is incomplete. Recent results indicate that very strong disorder may be required to sustain localization. This is attributed to rare, long-range correlated events that destabilize localization, with the most correlated states forming cat-state pairs absent in noninteracting systems. Presently, no microscopic explanation of this effect is known. One of the objectives is to uncover the physical mechanism behind cat-state formation in Anderson insulators upon adding interactions, through combined analytical and numerical analysis of different interaction types, offering a new understanding of localization in the thermodynamic limit. Another proposed study concerns spin systems with off-diagonal disorder representing a new class of models revealing the ergodicity breaking. They display unconventional localization properties, as shown by us. 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. In addition, the presence of disorder requires averaging over many realizations, further amplifying the computational demands. We will also continue our studies of the interplay between interactions and disorder effects, investigating the generation of non-stabilizerness (a measure of quantum complexity of states). We will show how disorder affects the propagation of this resource to different initial states*

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		and establish its connection to quantum entanglement. In this project, we aim to investigate how interactions added to the Anderson model lead to the emergence of non-Gaussian resources, investigate its capability to distinguish the ergodic-MBL regime, and study their time dynamics using exact diagonalizations as well as state-of-the-art time evolution codes.
8.	Tytuł projektu	***Structural, electronic, and transport properties of 2D borophene, MBenes, and Au-nanoparticle/2D-layer systems***
	Wnioskodawca	dr hab. Nevill Gonzalez Szwacki, Uniwersytet Warszawski
	Ocena	2,83
	Streszczenie projektu	*The scientific objective of the project is to conduct a systematic, high-accuracy theoretical study of low-dimensional boron-based materials and their hybrids. The project will address several interconnected problems: the stability and electronic topology of borophene nanoribbons; interlayer coupling and stacking behavior in bilayer borophene; chemical reactivity and catalytic enhancement induced by Au nanoparticles; and the evolution of reaction intermediates associated with Li–CO_2 battery chemistry. Understanding these mechanisms requires consistent, cross-validated first-principles simulations. The project aims to develop a full microscopic description of the interplay between structure, charge redistribution, magnetism, and transport. These insights will contribute to identifying promising candidate materials for next-generation electronic, spintronic, and catalytic devices, with emphasis on tunability, chemical sensitivity, and energy-conversion efficiency.*
9.	Tytuł projektu	***Neutron star theoretical inputs for the gravitational waves to be detected with the future Einstein Telescope***
	Wnioskodawca	dr hab. David Alvarez Castillo, Instytut Fizyki Jądrowej PAN
	Ocena	2,46
	Streszczenie projektu	*The equation of state (EoS) of strongly interacting nuclear matter plays a central role in understanding the structure and evolution of neutron stars, which are unique astrophysical laboratories for probing dense nuclear matter. Multimessenger astronomy is combining electromagnetic observations,*

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gravitational-wave signals, and, potentially, neutrino detections. It provides complementary and unprecedented constraints on the EoS. Investigating the EoS with multimessenger data is essential not only for understanding the phases of strongly interacting matter, including the possible appearance of deconfined quark matter, but also for testing fundamental physics such as QCD in its nonperturbative regime.

These studies require extensive computational resources because modern EOS inference relies on large-scale parameter scans, Bayesian sampling, and repeated numerical solutions of the Tolman-Oppenheimer-Volkoff (TOV) equations for millions of parameter combinations. As a result, reliable EOS constraints require many CPU hours on high-performance computing clusters to explore the parameter space with sufficient resolution and statistical robustness.

Our work for GW parameter estimation involves performing large-scale Fisher matrix analyses using Mathematica, where we compute parameter uncertainties and correlations for waveform models that include spin-induced quadrupole moments and eccentricity effects. In parallel, we employ Bayesian inference frameworks in Python, such as PyCBC Inference and dynesty, to validate Fisher-based predictions and to explore the full posterior structure of parameters for both black hole and neutron star binaries. The computing resources from this grant will enable high-precision numerical evaluations, extensive parameter-space scans across mass ratios and spins, and population-level analyses. Moreover, gravitational waves from oscillating compact stars will also be computed following a well established numerical scheme.

EuroHPC Joint Undertaking

The acquisition and operation of the EuroHPC supercomputer is funded jointly by the EuroHPC Joint Undertaking, through the European Union's Connecting Europe Facility and the Horizon 2020 research and innovation programme, as well as the of Participating States FI, BE, CH, CZ, DK, EE, IS, NO, PL, SE.

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