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Rozstrzygnięcie konkursu PLL/2023/04 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* (zasoby CPU i GPU) na podstawie przedstawionych recenzji Panel Ekspertów zakwalifikował do realizacji następujące projekty:

Lp.	Projekt	
1.	Tytuł projektu	***Physics of quantum materials: gapped metals***
	Wnioskodawca	dr Oleksandr Malyi, ENSEMBLE3
	Suma punktów	114
	Streszczenie projektu	*Our research focuses on a deep dive into the study of gapped metals - a class of quantum materials with distinctive electronic properties. Exhibiting a unique combination of an internal band gap with a high free carrier concentration, these materials present a diverse range of applications from photocatalysis to transparent conductors and thermoelectrics. Despite their high potential, the discovery and understanding of gapped metals have primarily been achieved through trial and error. Our research aims to provide a more systematic understanding, contributing to their more efficient and effective use in technology.*
2.	Tytuł projektu	***The study of protein dynamics important in neurobiology***
	Wnioskodawca	dr Katarzyna Walczewska-Szewc, UMK/WFAIS
	Suma punktów	108
	Streszczenie projektu	*With increasing life expectancy, our society is ageing. This process increases the incidence of neurodegenerative diseases, such as Alzheimer's disease (AD) and Parkinson's disease (PD). These are the two most common causes of dementia among older people. They*

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affect 10% and 2-3% of people over 65, respectively, although they also occur in younger people. Since the exact cause of these disorders is still not fully understood, available therapies only help alleviate the symptoms of the disease without slowing its progression. The common factor between the two diseases is the progressive accumulation of misfolded protein aggregates in well-ordered structures, usually referred to as amyloid. Although the protein aggregates involved in distinct neurodegenerative disorders are different, the process of protein misfolding, its intermediates, end-products, and primary features are remarkably similar.

However, there is another common feature of the two diseases. In pathological protein deposits formed by alpha-synuclein (αSyn) in PD and Tau protein in AD, there is an increased concentration of a particular enzyme, prolyl oligopeptidase (PREP).

PREP was discovered 50 years ago and classified as a peptidase relevant to neuropeptide metabolism. It was quickly recognized as an excellent target for treating neurological disorders, especially as evidence emerged that inhibition of PREP activity reduces cognitive decline and dementia in several animal models. Enthusiasm began to fade, however, when further research determined that PREP's role as a regulator of neuropeptide metabolism was not that clear.

Recently, interest in PREP has begun to grow again, as it has been observed that direct interaction with PREP is enough to start the process of pathological aggregation of αSyn in PD and Tau protein in AD. Data shows that small molecule inhibition of PREP leads to decreased PREP-seeded αSyn aggregation and enhanced clearing of already formed aggregates via autophagy. The most spectacular proof of this was the reversal of Parkinson's disease symptoms in mice by researchers at the University of Helsinki.

The molecular mechanisms by which PREP interacts with αSyn and Tau are still unknown. We also do not know why certain compounds cause PREP to lose its ability to trigger pathogenic aggregation since it is clearly not correlated with its enzymatic activity. Answering such questions would help us better understand the early-stage formation of amyloid fibrils. Understanding the origin of PREP-seeded aggregation at the molecular level allows for the search for novel chemical compounds that inhibit those processes and, in the future, gives us a chance for a disease-modifying therapy for several neurodegenerative diseases.

That is why I established collaboration with worldwide experts in

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		PREP experimental research. I want to answer such questions in the proposed project using state-of-the-art methods of computer modelling of bio-molecules. *The research plan is divided into two specific parts:* *1. Identification of ligand binding sites of PREP, which can modulate protein-protein interactions. In this part of the project, we want to numerically determine the structural determinants of binding different components to PREP's internal cavity. This will help to fill substantial gaps in our knowledge about PREP structure and function.* *2. Identification of molecular mechanisms of PREP - amyloid interaction. An output of this part of the project will be to explain the structural determinants of αSyn-PREP and Tau-PREP interactions on a molecular level and to determine the changes in the energy landscapes caused by the presence of PREP. Knowing particular structural stages and determining crucial amino acids in such interactions (and further amyloid aggregation induced by this interaction) will allow us to define potential targets for further research. Here we will use several state-of-art computational methods. Among all, the time-lagged independent component analysis will be used for the automatic construction of misfolding-related collective variables, and enhanced sampling of the amyloid dynamics will be performed using metadynamics simulations.*
3.	Tytuł projektu	***Persistent ferromagnetism in oxide heterostructures***
	Wnioskodawca	dr Igor di Marco, UMK/WFAIS
	Suma punktów	107
	Streszczenie projektu	*Heterostructures of transition metal oxides have been widely explored to construct novel magnetic materials to integrate in future technological applications. Following the experimental progress of the last decade, it was recently suggested that growing superlattices of LaMnO3 and SrMnO3 along the (111) direction may result into a very robust half-metallic ferromagnetism. In this project, we intend to determine the fundamental characteristics of this family of superlattices, upon variation of compositional parameters and epitaxial strain. This analysis will be based on a multi-scale approach where electronic structure calculations via density-functional theory (DFT) will be used to extract parameters for simulations of atomistic spin dynamics. Our fundamental goal is the determination of the magnetic phase diagram, to be used as a guideline for future*

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		experimental studies.
4.	Tytuł projektu	***Large-scale molecular dynamics simulations of galectin-3 biomolecular condensates***
	Wnioskodawca	dr Paweł Rogowski, PAN/Instytut Fizyki
	Suma punktów	104
	Streszczenie projektu	*Biomolecular condensates (BCs) are fluid droplets that form in biological cells by liquid-liquid phase separation (LLPS). Their major components are intrinsically disordered proteins. Vast attention has been given in recent years to BCs inside the cytosol and nucleus. BCs at the cell membrane have not been studied to the same extent so far. However, recent studies provide increasingly more examples of BCs at the cell membrane that function as platforms for diverse biological processes. Galectin-3, for example, is known to mediate clathrin-independent endocytosis and has been recently shown to undergo LLPS, but the function of BCs of galectin-3 in endocytic pit formation is unknown. The purpose of our research project is to fill in this knowledge gap. Our aim is use molecular dynamics (MD) methods, firstly, to study the formation and properties of BCs of galectin-3 and, secondly, to elucidate the mechanisms of membrane deformations by BCs of galectin-3.*
5.	Tytuł projektu	***Long-time simulations of model G-quadruplex structures***
	Wnioskodawca	dr inż. Mateusz Kogut, PG/Wydział Chemii
	Suma punktów	100
	Streszczenie projektu	*G-quadruplexes (G4, see Fig. 1) are non-canonical structures formed by guanine-rich sequences of nucleic acids that have been shown to exist in living cells where they are thought to participate in regulation of gene expression and chromosome maintenance. DNA G4s are highly polymorphic and can fold into a variety of three-dimensional structures, differing in the relative orientation of the four guanine tracts and in the arrangement of loop regions, which makes them versatile and potentially programmable building blocks for bionanotechnology. An often delicate conformational equilibrium between different possible G4 structures depends on the length and composition of the oligonucleotide in a manner not yet fully understood.*

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		The goal of the current project is to advance our understanding of this sequence-structure relation so as to allow for a comprehensive model-based design of DNA G-quadruplexes with a desired folded conformation. This will involve determination of conformational landscapes of a wide range of G4-forming sequences and analysis of these landscapes for structural and energetic principles underlying the relative stability of possible G4 folds.
6.	Tytuł projektu	***Molecular dynamics simulations in studying functional selectivity of GPCR ligands***
	Wnioskodawca	dr hab. Dorota Latek, UW/Wydział Chemii
	Suma punktów	98
	Streszczenie projektu	*G protein-coupled receptors constitute targets of nearly half of the currently available drugs. The major problem in the drug discovery process is drug selectivity. Weakly selective drugs frequently cause side effects or life-threatening adverse drug reactions and demonstrate decreased efficacy caused by their low binding affinity for one molecular target. Recent advances in cryo-EM have allowed for the rapid increase in the number of GPCR structures in both, inactive and active conformational states. Although the receptor subtype selectivity of drugs can be easily assessed by comparison of structures or homology models of receptor subtypes in most cases, assessment of the functional selectivity of drugs still encounters difficulties. Assurance of functional selectivity of drugs for only one signaling pathway requires studying the full complex including ligand, receptor, and G protein/beta-arrestin in large timescales accessible only for microsecond MD simulations (see Fig. 1).*
7.	Tytuł projektu	***Large scale modelling of multiphase composites***
	Wnioskodawca	dr hab. Eligiusz Postek, PAN/IPPT
	Suma punktów	98
	Streszczenie projektu	*Modern Ceramic Matrix Composites (CMCs) are used in many strategic industrial sectors, such as aerospace, nuclear power plants, and space exploration. Following the experiments on the composites, the most important is their microstructure for the composites' loading resistance (mechanical or thermal). It has been found that the*

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		interfaces between the particular phases play significant role. The same concerns the influence of different imperfections like voids and inclusions. Employing the up-to-date CT scanning technology it appeared possible to observe the phases distinctly in high detail. The voids, initial cracks and inclusions are well visible as well. The CT scanning is done on the cylindrical samples. Using the CAD programs the CT scans were converted into the numerical models, namely, finite element method (FEM) and peridynamics (PD). The properties of the interface are evaluated using molecular dynamics and ab-initio methods at the microscale. At the end, an approach to obtain numerical model of multiphase composites that would include the described features above is expected to elaborate.
8.	Tytuł projektu	***DYNAmics of STrongly interacting nuclei in neutron stars inner crust***
	Wnioskodawca	dr Daniel Pęcak, PW/Wydział Fizyki
	Suma punktów	98
	Streszczenie projektu	*Neutron stars are compact remnants of gravitational core-collapse supernova explosions. The interior of a neutron star can be divided into an inhomogeneous crust and uniform core. The inner crust consists of a crystal lattice of nuclei immersed in a sea of superfluid neutrons in a charge neutralizing background of free electrons. The presence of a superfluid medium effectively changes the masses of the nuclei but also the interaction between them. These effective masses and interactions are crucial to study collective excitations and assess the stability of the nuclear lattice, and to determine transport properties, which in turn are key microscopic inputs for modeling the thermal evolution of neutron stars, their rotational evolution and their oscillations. In this project, we plan to determine these parameters by means of fully microscopic dynamical simulations of the inner crust of a neutron star. Only top-tier supercomputers such as LUMI are able to tackle the time evolution of three-dimensional problems at quantum level with no geometric restrictions.*
9.	Tytuł projektu	***Cold atom quantum simulation of lattice gauge theories***
	Wnioskodawca	prof. dr hab. Jakub Zakrzewski, UJ/FAIS
	Suma punktów	86

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	Streszczenie projektu	*This grant is the continuation of an extremely successful gauge1 -gauge3 grants in ACK Cyfronet. e aim to simulate latiice gauge theories in cold atom settings in optical lattices, Rydberg atoms or quantum circuits. The aim is to construct and study numerically different simple models (like Schwinger model) fong beyond one-dimensional problems, successfully studied in the previous grants. We shall study quasi 2D models, most probably in the topology of a cylinder (long one direction with open boundary conditions and short second direction with periodic boundary condition) which should be feasible to do within tensor network approaches due to recent developments also in our group. We shall study ground state phases as well as the dynamics.*
10.	Tytuł projektu	***Ab initio Molecular Dynamics Investigation of the Decomposition and Melting processes in the InN crystal***
	Wnioskodawca	dr Jacek Piechota, PAN/Instytut Wysokich Ciśnień
	Suma punktów	79
	Streszczenie projektu	*Indium nitride, InN, is of special interest due to the very important applications in solar cells and high speed electronics. However, there are still many difficulties to be overcome: doping of InN and In-rich InGaN and heteroepitaxial growth of InN with other nitrides (GaN, AlN). Also, the p-T phase diagram and melting curve of InN are completely unknown, properties crucial to obtain InN single crystals of quality and size suitable for precise measurements and studies of homoepitaxy and heteroepitaxy.* *The principal aim of this project is to describe physical phenomena occurring in the InN crystal lattice under conditions of high temperatures and pressures adequate for the construction of the phase diagram.* *The ab initio Molecular Dynamics approach we use is able for the first time to detect the formation of nitrogen molecules accompanying thermal decomposition of InN. We will make efforts to demonstrate wurtzite-to-rocksalt phase transition in InN by increasing the pressure. Our method has been validated with a good, consistent set of experimental data on GaN and can be of great use in further exploring III-V semiconductor physics.*

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Projekty niezakwalifikowane do realizacji

Lp.	Projekt	
1.	Tytuł projektu	***Hydrogen evolution reaction activity study of polymeric Carbon Nitride Nanocomposite***
	Wnioskodawca	dr Narayan Som, PAN/Instytut Wysokich Ciśnień
	Suma punktów	70
	Streszczenie projektu	*Polymeric Carbon Nitride (PCN) has gained significant attention as a photocatalyst for hydrogen evolution reactions since 2009. The properties of PCN primarily depend on the synthesis route and precursors utilized, such as urea, melamine, cyanamide, thiourea, and dicyandiamide. In this study, we investigate the synthesis route of polymeric carbon nitride (g-C_3N_4) nanocomposites with a high specific surface area and visible light semiconductor characteristics. The nanocomposites were synthesized through a series of experimental procedures, and their structural and optical properties were thoroughly characterized.* *The PCN obtained from melamine exhibited a lower band gap of 2.35 eV and a lower BET surface area of 10.46 m^2/g when subjected to thermal condensation at 550℃ for 3 hours. While PCN derived from melamine displayed a lower band gap, resulting in high solar to hydrogen efficiency, its lower surface area hindered catalytic activity, emphasizing the importance of a higher surface area. Conversely, PCN obtained from urea exhibited a higher band gap of 2.7 eV and demonstrated a higher surface area. Therefore density functional theory (DFT) calculations will be conducted to gain insights into the electronic structure and band properties of the synthesized nanocomposites. The results will provide a comprehensive understanding of the visible light semiconductor behaviour and will confirms the band tuning and high surface area of g-C_3N_4 nanocomposites.* *"Furthermore, this groundbreaking project seeks to explore and assess the remarkable computational photocatalytic properties exhibited by the cutting-edge polymeric carbon nitride nanocomposites (PCN nanocomposites). By employing advanced computational techniques, we aim to unravel the intricate*

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		mechanisms underlying the preferential charge transfer at the heterojunctions of these remarkable materials, specifically focusing on the interaction between PCN and adsorbed hydrogen. *To achieve this, we will employ state-of-the-art methodologies such as Löwdin charge analysis and charge density plot visualizations. These powerful tools will enable us to delve deep into the fascinating world of PCN nanocomposites and gain valuable insights into their charge transfer dynamics. Through a comprehensive evaluation of the obtained computational results, we will unravel the underlying principles that govern the exceptional photocatalytic performance of these nanocomposites.*
2.	Tytuł projektu	***Molecular simulation of graphene based materials***
	Wnioskodawca	dr Arun Srikanth Sridhar
	Suma punktów	0 (wniosek odrzucony na etapie oceny formalnej)
	Streszczenie projektu	*The project will explore wetting and adhesion of solvents on graphene. Large scale simulations of droplets of organic solvents on graphene will be simulated. Contact angles will be then analyzed. Work of adhesion will also be computed using advanced free energy techniques. The results will be analyzed in terms of thermodynamic quantities. These results are expected to provide guidelines for graphene exfoliation and using graphene in the manufacture of industrial coatings.*

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