LUMI

Rozstrzygnięcie konkursu PLL/2023/05 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	***PAIRS - Pairing dynAmics In nucleaR colliSions***
	Wnioskodawca	prof. dr hab. Piotr Magierski, Politechnika Warszawska
	Ocena	4,79
	Streszczenie projektu	*Collisions between atomic nuclei at low energies are stringent tests of our understanding of the quantum many-body problem. As nuclei collide with energies at the vicinity of the Coulomb barrier, they have ample time to interact and morph. This leads to an intricate interplay between their structure effects, like intrinsic deformations and neutron skins, and the dynamics of collective excitations and particle transfer. All of these phenomena will contribute to the eventual measured observables of the reaction.* ***In that sense low-energy collisions probe the underlying features of nuclear physics.*** *In order to treat these disparate effects coherently, one must use state-of-the-art theoretical methods that rely on modern high performance computing systems, like LUMI, to make principled predictions and analyze a variety of nuclear reactions.*
2.	Tytuł projektu	***Amyloid-β42 recognition by J-domain proteins***
	Wnioskodawca	dr Bartłomiej Tomiczek, Uniwersytet Gdański
	Suma punktów	4,38

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	Streszczenie projektu	*Alzheimer's disease is associated with the formation of amyloid plaques in a brain. Insoluble plaques consist of amyloid fibers that are formed by the aggregation of Amyloid-β42 (Aβ) peptide. Along with other pathological changes, aggregation of Aβ42 peptides contributes to neurodegeneration.* *The J-domain protein (JDP) family is a diverse group of proteins that play a key role in protein homeostasis. Within the JDP family, class A and B proteins, which differ from each other in domain organization and substrate specificity, have been identified as strong inhibitors of Aβ42 fibrils formation. However, the exact molecular mechanism of such activity has not been described to date.* *The aim of the project is to understand the molecular mechanism of amyloid-β42 recognition by JDPs. This will involve determination of conformational landscapes of a wide range of amyloid-β42 -JDP complexes in all-atom molecular dynamics simulations(MD) and free-energy calculations of amyloid-β42 -JDP binding for each conformer.* *This research will help us to better understand how JDPs prevent amyloid-β42 from elongation. Understanding these mechanisms may contribute to the development of new, effective therapeutic strategies for Alzheimer's disease.*
3.	Tytuł projektu	***Physical properties of vdW layered materials***
	Wnioskodawca	dr Magdalena Popielska, Uniwersytet Warszawski
	Ocena	4,21
	Streszczenie projektu	*This project is a continuation of the previous project on LUMI supercomputer (PLL/2022/03/016435), which has been completed in 50% (in 4 papers the acknowledgment of the LUMI grant is placed). In our recent papers we point out the promising 2D materials for thermoelectrics (Applied Mat.Today 34, 101902 (2023)), as well as optical properties. The 2D systems are taken from two-dimensional classes of materials such as MBenes\MXenes and MPX3 families, respectively.*

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		Thesimulations are examined within the framework of Density Functional Theory DFT with the aid of widely used software Quantum Espresso VASP. The optoelectronic properties such as exciton binding energies will be deeply discussed using BerkeleyGW software. In addition the quantities such as Seebeck coefficient electrical conductivity and thermal conductivity will be analyzed by solving the Boltzmann transport equation BTE for electrons and phonons and based on their figure of merit values for selected MXenes and MBenes materials. Our recent paper (arXiv:2308.13109v1) demonstrates that MnPSe3 and MnPS3 monolayers are promising materials for opto-spintronics applications. Next, we expect to point out the best vdW heterostructures that exhibit optically active transition working at room temperature. Additionally, we want to identify the best suitable vdW heterostructures based on MXenes and MBenes materials for thermoelectric applications. applications.
4.	Tytuł projektu	***Prediction of protein features at scale***
	Wnioskodawca	dr hab. Łukasz Kozłowski, Uniwersytet Warszawski
	Ocena	3,96
	Streszczenie projektu	*Proteins serve as the powerhouse of living organisms. The comprehensive understanding of their sequence, 3D structure, physico-chemical attributes, and function remains a primary focus for molecular biologists. This knowledge enables inquiries into biologically significant questions and facilitates drug design, among other applications. In the proposed project, I will analyse ~4 billion sequences from MGnify and few other databases. The project aims to provide an in-depth description of the physicochemical properties of proteins which will be made accessible to the scientific community through a freely available web-based database.*
5.	Tytuł projektu	***Predicting the crystal structure and studying the properties of low-dimensional materials***
	Wnioskodawca	dr hab. Nevill Gonzalez Szwacki, Uniwersytet Warszawski
	Ocena	3,67

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	Streszczenie projektu	*The aim of the present work is to perform first-principles calculations to determine the transport, dynamic, and structural properties of two-dimensional Boron sheets and MBenes. Our goal is also to explore borophenes and MBenes as possible materials to be used in the gas sensor field.*
6.	Tytuł projektu	***Rational Design of 2D materials for photo(electro)catalysis***
	Wnioskodawca	dr hab. Silvio Osella, Uniwersytet Warszawski
	Ocena	3,67
	Streszczenie projektu	*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). The peculiar electronic properties of single subunits are rationally assessed with a material-by-design approach and combined in a "bottom-up" fashion at the nanoscale to address bottlenecks of photo(electro)catalysis related to solar light harvesting, efficient charge separation and transport as well as the catalytic activity. This will be achieved by the assembly of nanomaterials with low dimensionality.* *The new concept is the use of only "green" low dimensional materials to accomplish efficient light absorption, charge separation and catalysis to obtain high valuable chemicals such as ammonia, ethylene and ethanol. The final goals are to achieve a broad light absorption and efficient photoinduced charge separation, to reduce charge recombination losses, to decrease the kinetic energy barrier for N2 and CO2 reduction reactions using low overpotential and efficient energetic (>50%), to enhance the selectivity towards highly desired products (Faradic Efficiency > 85%) and to enhance the life cycle of the entire device for at least 100 hours.* *To this end, we will use modular nanoscale building blocks (NBBs), such as graphene quantum dots (GQDs), two-dimensional materials (2DMs, including MoS2, TeS2) and 2D-MOF catalysts as functional components to pave the way toward the creation of novel inexpensive products with sets of*

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		properties that can be tailored with atomic precision. By combining the best of three worlds (e.g. strong light absorption in GQDs, excellent charge transport in 2DMs, and high catalytic activity of 2D-MOFs), the hybridization of GQDs, 2DMs, and 2D-MOFs all in one single light weight and stable unit, will enable cutting-edge, lower-cost, and sustainable photocatalysts for highly efficient NRR and CO2RR.
7.	Tytuł projektu	***Catalytic activity of Heterostructure based on Polymeric Carbon nitride***
	Wnioskodawca	dr Narayan Som, Instytut Wysokich Ciśnień Polskiej Akademii Nauk
	Ocena	3,42
	Streszczenie projektu	*The persistent challenge we face today is the energy crisis and the increasing emission of CO2 resulting from the widespread use of fossil fuels. In the era of advanced technology, computational materials design using Density Functional Theory (DFT) has emerged as a crucial tool, allowing scientists to explore and optimize materials before conducting experiments. Addressing this challenge necessitates innovative solutions, and the computational design of catalysts, pivotal components in our daily lives, offers a promising avenue. Catalysts, especially those that are earth-abundant, stable, and environmentally friendly, hold the key to resolving the energy crisis. One significant approach involves the water-splitting process, generating hydrogen gas as a clean energy source. Additionally, materials capable of adsorbing CO2 gas and catalyzing its reduction can mitigate CO2 accumulation, mitigating global warming. Our focus lies on the catalytic activity of materials like polymeric carbon nitride and metal oxides such as Transition metal doped ZnO and ZrO2.* *Polymeric carbon nitride and metal oxides like ZnO and ZrO2 are promising, although challenges exist, such as low surface area, wide band gap, and recombination rates. However, these drawbacks can be overcome through techniques like doping, strain application, and creating heterostructures. Doping alters material stability and electronic properties, while heterostructures, specifically type II, reduce recombination rates and modify surface area and electronic properties. Computational methods facilitate the formation and prediction of these heterostructures, aiding catalyst design.*

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Our research, employing Density Functional Theory, not only delves into the dynamical stability and electronic properties of materials but also investigates surface reactivity through adsorption energy calculations. In the context of the Hydrogen Evolution Reaction (HER), we explore dominant reaction paths, such as Volmer-Heyrovsky and Volmer-Tafel mechanisms. Catalyst descriptors, including Volmer-Gibbs free energy and solar-to-hydrogen efficiency, guide our studies. For instance, our findings reveal that PCN-ZnO nanocomposites exhibit higher hydrogen-to-solar efficiency than pristine PCN, following the Volmer-Heyrovsky reaction path. To further enhance catalytic activity, we will explore complex heterostructures, demanding substantial computational power. Our focus extends to designing novel heterostructures involving polymeric carbon nitride, ZrO2, or transition metal doped ZnO.

Beyond hydrogen production, our study delves into oxygen evolution, leading to hydrogen peroxide generation, a vital energy-intensive chemical. By investigating water splitting, H2O2 production, and CO2 reduction within our system, we aim to uncover fundamental aspects and catalytic phenomena enhancing the activity of new heterostructures compared to pristine PCN.

In essence, our research endeavours to unlock the potential of computational materials design, specifically focusing on catalysts, to address the energy crisis, mitigate CO2 emissions, and contribute significantly to sustainable energy solutions.

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