LUMI

Rozstrzygnięcie konkursu na granty obliczeniowe realizowane na superkomputerze LUMI (PLL/2022/03)

Zgodnie z *Regulaminem konkursu na dostęp do zasobów obliczeniowych na superkomputerze LUMI dla naukowców z Polski* na podstawie przedstawionych recenzji Panel Ekspertów zakwalifikował do realizacji następujące projekty:

Lp.	Projekt	
1.	Tytuł projektu	***2D Materials mechanical properties optimization***
	Wnioskodawca	prof. dr hab. Wacław Kuś, Politechnika Śląska
	Znormalizowana suma punktów (skala 0-5)	4,46
	Streszczenie projektu	*The aim of the work is to verify the algorithm for the optimization of two - dimensional structures on the atomic scale. Optimization of nanostructures is particularly important in attempts to create gradient materials with changing mechanical properties obtained as a result of nanosheet modification by introducing voids o r different material phases. Performing calculations with the use of Molecular Dynamics and the need to solve many problems makes it necessary to apply parallel calculations with the use of thousands of cores. The use of supercomputer is the only way to obtain new results for relatively large nanostructures. It is expected to optimize nanosheets made of two - dimensional materials such as Molybdenum Disulfide, Silicene and Germanene. The work will result in new two - dimensional materials with the required material properties. There will also be a description of the methodology for performing calculations with hierarchical parallelization of nanostructure optimization.*
2.	Tytuł projektu	***DYNAmics of STrongly interacting nuclei in neutron star's inner crust***
	Wnioskodawca	dr Daniel Pęcak, Politechnika Warszawska
	Znormalizowana suma	4,38

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.

Republic of Poland

CYFRONET

	punktów (skala 0-5)	
	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 with no geometric restrictions at quantum level.*
3.	Tytuł projektu	***Electronic, optical and thermoelectric properties of layered materials and selected heterostructures***
	Wnioskodawca	dr Magdalena Birowska, Uniwersytet Warszawski
	Znormalizowana suma punktów (skala 0-5)	4,08
	Streszczenie projektu	*Here we perform high throughput calculations of novel 2D materials and their heterostructures to point out the best candidates for designed thermoelectric and optical properties. The 2D systems will be taken from two-dimensional classes of materials such as MBenes/Menes and MPX 3 families. The simulations will be examined within the framework of Density Functional Theory (DFT) with the aid of widely used software*

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.

Republic of Poland

CYFRONET

		(Quantum Espresso, VASP). The optoelectronic properties such as absorption spectra, 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. We expect to point out the best candidates that exhibit optically active transition working at room temperature, as well as the best suitable candidates for thermoelectric applications.
4.	Tytuł projektu	***High-pressure stabilization of elusive transition-metal fluorides***
	Wnioskodawca	prof. dr hab. Dominik Kurzydłowski, Uniwersytet Kardynała Stefana Wyszyńskiego w Warszawie
	Znormalizowana suma punktów (skala 0-5)	3,58
	Streszczenie projektu	*Binary compounds are composed of only two chemical elements. A discovery of a novel binary compound nowadays represents a considerable challenge and is a scientific achievement akin to the discovery of a novel element a century ago. These simple compounds further our understanding of elements and their chemical reactivity. Prediction and synthesis o f novel binary compounds with elements in unusual oxidation states represent a major research challenge in contemporary chemistry. Fluorine is the most electronegative element and the most reactive non - metal, and it is often referred to as the tiger of the periodic table. Fluorine chemistry is usually associated with high oxidation states. As a result low - valent transition - metal fluorides have proven elusive and are hitherto unknown, even though their heavier halogen analog s are common. This project aims to explore the possibility of the synthesis of elusive low - valent transition - metal fluorides at pressures exceeding 1*

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.

Republic of Poland

CYFRONET

		GPa (10 000 bar). Chemistry under these extreme conditions is very interesting and enables the discovery of compounds with unusual compositions and stoichiometries.
5.	Tytuł projektu	***Non-covalent interactions investigations in ligand-protein complexes and molecular crystals***
	Wnioskodawca	dr hab. Aneta Jezierska, Uniwersytet Wrocławski
	Znormalizowana suma punktów (skala 0-5)	3,54
	Streszczenie projektu	*In-depth studies of non-covalent interactions (NCIs), mandatory to understand correctly phenomena at the molecular level, meet a major problem: lack of time-evolution data. Insight into NCI properties in time domain, with temperature influence accounted for, will allow to describe complex chemical systems more finely. Therefore, Car-Parrinello, Born-Oppenheimer and Path Integral molecular dynamics (MD) will be used to study time-dependent features of ligands in the binding pockets of proteins related to gout and neurodegenerative/psychiatric disorders (e.g. monoamine oxidases/transporters). Molecular crystals will be also studied in the contexts of NCI signatures. We expect the ab-initio MD studies to shed new light onto the action of the biologically relevant ligands , and on the molecular crystals properties. We provide also a novel theoretical point-of-view to investigate NCIs, leading to more rational drug design process via e.g. improved force fields for molecular docking.*

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.

Republic of Poland

CYFRONET