LUMI

Rozstrzygnięcie konkursu na pilotażowe granty obliczeniowe realizowane na superkomputerze LUMI (zasoby CPU)

Zgodnie z *Regulaminem konkursu na pilotażowe granty obliczeniowe dla naukowców z Polski realizowane na superkomputerze LUMI* (zasoby CPU) na podstawie przedstawionych recenzji Panel Ekspertów zakwalifikował do realizacji następujące projekty:

Lp.	Projekt	
1.	Tytuł projektu	***Supersolidity in ultracold Fermi gas***
	Wnioskodawca	prof. dr hab. Gabriel Wlazłowski, Politechnika Warszawska
	Suma punktów	107
	Streszczenie projektu	*Systems that exhibit at the same time properties of solids and superfluids are called supersolids. In such system particles can flow without energy losses, while at the same time the matter is organized in crystalline structure. Combining properties of two different types of material into a single one seems to be counterintuitive, however they were indeed observed in experiments involving Bose-Einstein condensates (BECs). Within this project we will test if a similar state of matter can be also created with ultracold fermionic gases, which are known to form a different type of superfluid. We will apply very accurate method of density functional theory to obtain quantitative predictions, and in particular to investigate the transition from superfluid to supersolid state. The results will provide deep insight into nature of supersolids, and will help to address the questions concerning limits of stability of such exotic structures.*
2.	Tytuł projektu	***Drugging the genomic RNA of SARS-CoV-2 with small molecules***
	Wnioskodawca	prof. dr hab. Janusz M. Bujnicki, Międzynarodowy Instytut Biologii Molekularnej i Komórkowej
	Suma punktów	87

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

	Streszczenie projektu	*ARS-CoV-2 has caused a rapidly expanding global pandemic. There is a desperate need for new medicines to treat it. The SARS-CoV-2 genome is made of RNA, and it encodes viral proteins as well as contains regulatory RNA elements, which are necessary for the virus. Consequently, these RNA elements have been proposed as useful targets for the development of new RNA-targeting antiviral drugs.* *We have determined experimentally the secondary structure of the SARS-CoV-2 genomic RNA, and identified nine conserved regions, which contain 3D pockets potentially druggable by small organic molecules (Manfredonia et al. Nucleic Acids Research 2000:v48,22,12436–12452).* *We will use our new tools including AnnapuRNA and SimRNA-Ligand to model the interactions of druggable 3D motifs in SARS-CoV-2 RNA with a library of small organic molecules. The unique ability to model the flexibility of RNA will allow us to predict the binding modes and activity of screened molecules with higher accuracy than with a conventional virtual screening. The activity of the top-scored molecules will be validated experimentally in our laboratory.*

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