Annex 3.

Form of opening (renewal) for Project / Sub-project of LRIP

APPROVED

JINR DIRECTOR

_____________/__________________

"_____" ______________________ 202 г.

PROJECT PROPOSAL FORM

Opening/renewal of a research project/subproject of the large research infrastructure project within the Topical plan of JINR

1. General information on the research project of the theme/subproject of the large research infrastructure project (hereinafter LRIP subproject)

1. **Theme code / LRIP** (for extended projects) - *the theme code includes the opening date, the closing date is not given, as it is determined by the completion dates of the projects in the topic.*

2. **Project/LRIP subproject code** (for extended projects)

Not available.

3. **Laboratory**

BLTP

4. Scientific field

Theoretical Physics

5. Title of the project/LRIP subproject

Complex materials

6. Project/LRIP subproject leader(s)

E. M. Anitas

7. **Project/LRIP subproject deputy leader(s) (scientific supervisor(s))**

Not available.

2 Scientific case and project organization
2.1 Annotation

The enormous recent progress both in the art of sample preparation and in the measurement techniques have boosted our capacity to generate high-quality and large sets of data on structural and physical properties of new complex materials. The availability of such data, together with the development of analytical and numerical methods, opens the door to significantly advance our understanding of such materials, and of how their structure and properties correlate at different scales. Indeed, such a synergetic approach is behind recent breakthroughs in various applications such as quantum computing, fusion energy, biological or composite materials.

2.2 **Scientific case** (aim, relevance and scientific novelty, methods and approaches, techniques, expected results, risks)

The overarching goal of this project will be theoretical studies of physical phenomena and processes in condensed matter, studies of properties of new advanced materials, constructing and analysis of theoretical models and development of analytical and computational methods for their solution.

Relevant complex materials that are aimed to be investigated are atomically thin semiconductors colossal magneto-resistance compounds, heavy-fermion systems, low-dimensional quantum magnets with strong spin-orbit interaction or topological insulators. They attract now considerable attention, both from the point of view of fundamental studies and as promising materials for applications, e.g., the quantum computing, will be analyzed. Similarly, smart composite materials, fractal and layered structures, and biological macromolecules will be also analyzed.

The planned studies for these types of materials are the following:

- Establishing a semi-analytical relationship between the energy and size of the excitons in atomically thin semiconductors and the average dielectric constant to its immediate dielectric surroundings.
- Deriving the long-range dipole-dipole interaction between excitons in their excited states
- Theoretical and experimental investigations of the structure of complex hierarchical systems, including fractals and biological macromolecules.
- Estimation of the exchange parameters of Kitaev materials based on transition and rare-earth metals and calculation of their spin-wave spectrum.
- Theoretical investigations of electronic properties of nanoparticles for electronics research.
- Theoretical and experimental investigations of dense random packing with a power-law size distribution at nano and micro scales.
- Application and development of quantum algorithms for computational problems in condensed matter physics and quantum chemistry.
- Development of a theory of stability for mixtures of quantum fluids.

- Numerical and experimental investigation of irradiation resistance of various compounds.
- Numerical and theoretical study of nuclear quadrupole interactions in rutile and rare-earth oxides;
- Investigation of spin waves with tensor networks and density matrix renormalization group methods
-

The main methods planned to be used are the following:

- Standard quantum mechanical and quantum chemistry methods;
- Numerical and analytical methods;
- Small-angle scattering (neutrons, X-rays);
- Neutron scattering and irradiation;
- Ab initio calculations;
- Molecular dynamics simulations, etc;

2.3 Estimated completion date

2028

4. Participating JINR laboratories

- Frank Laboratory of Neutron Physics (A. S. Doroshkevich, A. I. Kuklin).
- Meshcheryakov Laboratory of Information Technology (Z. A. Sharipov, Z. K. Tukhliev, E.P. Yukalova, P. V. Zrelov, O. V. Ivancova, L. A. Siurakshina).
- Flerov Laboratory of Nuclear Reactions (M. N. Mirzayev).
- Dzhelepov Laboratory of Nuclear Problems (E. P. Popov).

2.4.1 MICC resource requirements

Computing resources	**Distribution by year**				
	1st year	2nd year	3rd year	4th year	5th year
Data storage (TB) - EOS - Tapes	1	1	1	1	1
Tier 1 (CPU core hours)	1	1	1	1	1
Tier 2 (CPU core hours)	1	1	1	1	1
SC Govorun (CPU core hours) - CPU - GPU	1	1	1	1	1

Clouds (CPU cores)					

2.5. Participating countries, scientific and educational organizations

Organization	Country	City	Participants	Type of agreement
Institute of Solid State Physics	Bulgaria	Sofia	H. Chamati	Joint work
University of Sao Paulo	Brazil	Sao Carlos	V. S. Bagnato	Joint papers
West University of Timisoara	Romania	Timisoara	I. Bica	Joint work

2.6. Key partners *(those collaborators whose financial, infrastructural participation is substantial for the implementation of the research program. An example is JINR's participation in the LHC experiments at CERN).*

Not available.

3. Manpower
3.1. Manpower needs in the first year of implementation

№№ n/a	Category of personnel	JINR staff, amount of FTE	JINR Associated Personnel, amount of FTE
1.	research scientists	12	0
2.	engineers	0	0
3.	specialists	0	0
4.	office workers	0	0
5.	technicians	0	0
	Total:	**12**	**0**

3.2. Available manpower
3.2.1. JINR staff

No.	Category of personnel	Full name	Division	Position	Amount of FTE
1.	research scientists	E. M. Anitas	BLTP Directorate	Deputy Director BLTP	1
		A. L. Kuzemsky	Sector 1 BLTP	Leading Research Scientist	1
		H. N. Cam	Sector 1 BLTP	Leading Research Scientist	1
		V. I. Yukalov	Sector 1 BLTP	Leading Research Scientist	1
		V. Yu. Yushankhai	Sector 1 BLTP	Leading Research Scientist	1
		A. A. Donkov	Sector 1 BLTP	Senior Research Scientist	1
		P. A. Maksimov	Sector 1 BLTP	Senior Research Scientist	1

		A. Yu. Cherny	Sector 1 BLTP	Senior Research Scientist	1
		A. A. Vladimirov	Sector 1 BLTP	Research Scientist	1
		N. D. Tung	Sector 1 BLTP	Junior Research Scientist	1
		N. N. Bogoliubov	Sector 1 BLTP	Principal Research Scientist	0.1
2.	engineers				
3.	specialists				
4.	technicians				
	Total:	**11**			

3.2.2. JINR associated personnel

No.	Category of personnel	Partner organization	Amount of FTE
1.	research scientists	0	0
2.	engineers	0	0
3.	specialists	0	0
4.	technicians	0	0
	Total:	**0**	**0**

4. Financing
The project will be funded through the theme "Theory of complex systems and advanced materials"

Project (LRIP subproject) Leader __________/___________/

Date of submission of the project (LRIP subproject) to the Chief Scientific Secretary: _________
Date of decision of the laboratory's STC: 13.04.2023, document number: 14

Year of the project (LRIP subproject) start: 2024

APPROVAL SHEET FOR PROJECT / LRIP SUBPROJECT

TITLE OF THE PROJECT/LRIP SUBPROJECT

SHORT DESIGNATION OF THE PROJECT / SUBPROJECT OF THE LRIP

PROJECT/LRIP SUBPROJECT CODE

THEME / LRIP CODE

NAME OF THE PROJECT/ LRIP SUBPROJECT LEADER

AGREED

JINR VICE-DIRECTOR	SIGNATURE	NAME	DATE
CHIEF SCIENTIFIC SECRETARY	SIGNATURE	NAME	DATE
CHIEF ENGINEER	SIGNATURE	NAME	DATE
LABORATORY DIRECTOR	SIGNATURE	NAME	DATE
CHIEF LABORATORY ENGINEER	SIGNATURE	NAME	DATE
LABORATORY SCIENTIFIC SECRETARY THEME / LRIP LEADER	SIGNATURE	NAME	DATE
PROJECT / LRIP SUBPROJECT LEADER	SIGNATURE	NAME	DATE
APPROVED BY THE PAC	SIGNATURE	NAME	DATE