University	*NUST MISIS*
Level of English proficiency	*C2*
Educational program and field of the educational program for which the applicant will be accepted	*Physical and Technical Sciences*
List of research projects of the potential supervisor (participation/leadership)	- *Multiscale modeling of functional coatings using atomistic methods and machine learning techniques;* - *Study of the magnetic and electronic properties of quasi-two-dimensional magnets;* - *Spin liquid;* - *Fundamental aspects of mathematical models in physics – from the Hubbard model to the Heisenberg model.*
List of the topics offered for the prospective scientific research	*- Defects in quasi-two-dimensional magnets and their influence on electronic and magnetic properties;* *- Study of the magnetic and transport properties of semiconductor/2D magnet heterostructures;* *- Spectra of magnetic excitations in low-dimensional magnets;* *- Modeling thin films within the framework of multiscale methods;* *- Study of protective functional coatings using multiscale modeling methods;* *- Development of interatomic potential - from first-principles description to macroscopic models.*
 Research supervisor: Kartsev Alexey, PhD (Lund University, Sweden)	*Condensed matter physics* Supervisor's research interests *Solid State Physics, Electronic Theory of Solids, Scientific Programming, Lattice Dynamic, Density Functional Theory, Many-body Theory, Strongly Correlated Systems, Hubbard Model, UltraCold Atoms, Exact static and time-dependent methods, Numerical solution of model Hamiltonians, 2D materials and van der Waals crystals, Magnetism in 2D, Machine Learning* Research highlights *(при наличии)* *The research group has extensive experience in scientific programming using various mathematical methods and techniques for processing materials science big data, as well as a wealth of knowledge in quantum computing for materials science through software packages based on the density functional theory, such as VASP and Quantum Espresso. The project leader and participants possess all the necessary theoretical and analytical tools to conduct this research. The research will be conducted in close collaboration with the staff of the Laboratory of Computer Design of Materials at MIPT, the Laboratory of Atomistic Modeling at Queen's University in Belfast (UK), the University of Edinburgh (UK), and Stanford University (USA), which will provide access to additional computational resources on state-of-the-art computing clusters of world-class standards. It is also worth noting that all*

	members of the research group actively collaborate with leading international laboratories, and the publication level of the group members is on par with global standards. All of this, combined with unique experience and knowledge in the field of real materials, provides a significant foundation and great opportunities for their application in the development of advanced technologies based on solid-state physics within the framework of this project. The computational part of the project will be carried out in collaboration with JSCC RAS (the supercomputer center of the Russian Academy of Sciences) on the MVS-15000BM cluster using the MPICH software environment. *The group is already involved in the implementation of a large project supported by the Ministry of Science and Higher Education of the Russian Federation. Thus, the researchers involved in this project already have a well-coordinated team and possess more than sufficient knowledge in condensed matter theory, crystallography, programming, numerical methods of mathematical physics, and the use of UNIX OS. The team members have extensive experience in adapting quantum-mechanical computation packages for supercomputing systems aimed at computer modeling of the atomic and electronic structure of nanomaterials, significant expertise in calculating atomic and electronic structures, as well as the mechanical and energy characteristics of nanomaterials, and experience in studying the physicochemical properties of metal nanoparticles and their oxides, which is supported by a large number of publications and previously funded projects.*
	Supervisor's specific requirements: *Specialization in the field of condensed matter physics and solid-state physics;* *Knowledge of the basics of quantum mechanics.* *Experience working with numerical methods.* *Experience in performing first-principles calculations.* *Knowledge of the basics of UNIX systems; Python; Bash; Fortran; C++.*
	Supervisor's main publications *Web of Science **27**, Scopus **28**, RSCI **34*** 1. Vasilyev, D., Ikhsanov, R.S., Zheleznyi, M. and Kartsev, A., 2025. Calculations of elastic and thermal properties of the strengthening C14 Fe6Nb4Al2 Laves phase using the density functional theory. Journal of Materials Science, pp.1-15. 2. Chowde Gowda, C., Kartsev, A., Tiwari, N., Sarkar, S., Alexander, S. A., Chaudhary, V., & Tiwary, C. S. (2024). Harvesting Magneto-Acoustic Waves Using Magnetic 2D Chromium Telluride (CrTe3). Small, 2405197. 3. Zhou, D., Semenok, D. V., Xie, H., Huang, X., Duan, D., Aperis, A., Oppeneer P. M., Michele Galasso M, Kartsev

	A. ... & Cui, T. (2020). High-pressure synthesis of magnetic neodymium polyhydrides. Journal of the American Chemical Society, 142(6), 2803-2811. 4. Kartsev, A., Augustin, M., Evans, R. F., Novoselov, K. S., & Santos, E. J. (2020). Biquadratic exchange interactions in two-dimensional magnets. npj Computational Materials, 6(1), 150. 5. Cesar, D., Acharya, A., Cryan, J. P., Kartsev, A., Kling, M. F., Lindenberg, A. M., ... & Marinelli, A. (2022). Ultrafast quantum dynamics driven by the strong space-charge field of a relativistic electron beam. Optica, 10(1), 1-10.+ 6. Kushchuk LI, Kartsev AI. TMN (TM= V, Cr, Mn, Fe, Co) monolayers–a new class of non-van der Waals 2D magnets. Nanoscale. 2025;17(16):10292-302. 7. Gowda CC, Kartsev A, Tiwari N, Safronov AA, Pandey P, Roy AK, Ajayan PM, Galvão DS, Tiwary CS. Non-thermal magnetic deicing using two-dimensional chromium telluride. Journal of Materials Chemistry C. 2024;12(46):18691-703. 8. Kobernik TN, Kartsev AI. Gas Adsorption on the Co2Te3 Monolayer: Density Functional Theory Study. The Journal of Physical Chemistry Letters. 2024 Nov 29;15(49):12151-5. 9. Andrade X, Pemmaraju CD, Kartsev A, Xiao J, Lindenberg A, Rajpurohit S, Tan LZ, Ogitsu T, Correa AA. Inq, a modern GPU-accelerated computational framework for (time-dependent) density functional theory. Journal of Chemical Theory and Computation. 2021 Nov 2;17(12):7447-67. *10.* Lega P, Kartsev A, Nedospasov I, Lv S, Lv X, Tabachkova N, Irzhak A, Orlov A, Koledov V. Blocking of the martensitic transition at the nanoscale in a Ti 2 NiCu wedge. Physical Review B. 2020 Jun 1;101(21):214111.
	Results of intellectual activity *(при наличии)* *State registration of a computer program. Registration number (certificate): 2025661836.A program for calculating the structural states and lattice parameters of crystalline materials by the NEB method.*