Dr. Irina Gumarova (Piyanzina)– **Curriculum Vitæ**

Personal Information

20.09.1989 born in Almetyevsk, Tatarstan republic, Russia, female, Russian citizen, 1 child.

Current work address:

PostDoc at Yerevan State University, Institute of Physics, Center of Semiconductor Devices and Nanotechnology, Computational Materials Science Laboratory, 1 Alex Manoogian St. Yerevan

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Previous professional career

01/2022-12/2024	Researcher, Lab for Computer Design of New Materials and Machine Learning, Institute of Physics, Kazan Federal University, Kazan, Russia.
01/2019-12/2024	Researcher at Kazan Physical-Technic Institute named after E.K. Zavoiskii, Kazan, Russia.
09/2013-12/2024	Teaching Lecturer at Institute of Physics, Kazan Russia.
04/2015-08/2017	Visiting scientist at Augsburg University, Experimental Physics IV, Augsburg, Germany Advisor: Dr. Prof. T. Kopp and Dr. V. Eyert from Materials Design INC.
09/2013-10/2017	PhD student, Junior Researcher at Kazan Federal University, Lab for Physics of Complex Systems, Kazan, Russia. Advisor: Dr. Prof. D.Tayurskii.
09/2012-10/2013	Master student in Institute of Superior Institute of Materials and Advance Mechanics (ISMANS), Le Mans, France. Advisor: Dr. B. Minisini.
09/2011-06/2013	Master student in Kazan Federal University, Institute of Physics, Lab for Physics of Complex Systems, Kazan, Russia. Advisor: Dr. Prof. D. Tayurskii.
09/2007-06/2011	Student at Kazan Federal University on a radio-spectroscopy in “radiophysics”, Kazan, Russia

Education

09/2020	Kazan Federal University Degree obtained: **PhD (candidate of physical-mathematical sciences)** Qualifying dissertation: Ab-initio investigation of structural and electronic properties of surfaces and interfaces based on $LaAlO_3$ and $SrTiO_3$. Supervised by Prof. D.Tayurskii

09/2013	Superior Institute of Materials and Advance Mechanics (Institut Supérieur des Matériaux et Mécanique Avancés, ISMANS, Le Mans, France) Degree obtained: **Master of Engineering** Qualifying dissertation 1: Glass transition temperature investigation of polymers by atomistic simulation Qualifying dissertation 2: Prediction of dipole moments and polarizabilities for azobenzene derivatives using density functional theory.
06/2013	Kazan Federal University, Institute of Physics Degree obtained: **Master of Physics** Qualifying dissertation: Monte-Carlo simulations of thermodynamic properties of heavy hydrocarbons.
06/2011	Kazan State University, Institute of Physics Degree obtained: **Bachelor of Radio-physics.** Qualifying dissertation: Bose-Einstein condensation and exchange interaction in atomic hydrogen
05/2007	Physical-Mathematical Lyceum No.2, Almetyevsk

Grands and Awards

09/2012-04/2013	Scholarship of Pays de la Loire for studying at Institute of Advanced Materials, ISMANS, Le Mans, France
09/2015-06/2016	Scholarship of Government of Russian Federation
11/2015-01/2016	DAAD scholarship
02/2016-05/2016	DFG through the transregional collaborative research center TRR 80, Germany
06/2022	Award named after Kozirev in Kazan Physical-Technical Institute RAS
09/2023	Award named after E.K.Zavoiskii in Kazan Federal University

Supervision of Graduate Students

Since 2020 ~ 13 Master and Graduate students

Teaching Activities

2013-2024 Lab and Seminar Course on General physics, Kazan Federal University

2021-2024 Lecture on Computer design on new materials, Kazan Federal University

Third-party fundings

2017-2019 The leader of the project 18-32-00595 “Theoretical and experimental study of the structural, electronic and magnetic properties of heterostructures based on ferroelectric oxides.”

2018-2020 The executor of the project 18-02-00675 “Investigation of the phase transition to the polar state under the influence of an electric field and light in relaxors.”

2018-2020 The executor of the project 18-42-160005 “Investigation of new heterostructural materials using ferroelectric films to create working elements of solar cells.”

2018-2020 The executor of the project 20-02-00981 “Investigation and modification of the properties of a highly conductive region at the ferroelectric-dielectric interface by optical methods”

2020-2022 The executor of the project 20-02-00981 “Investigation of the Phenomenon of Ferromagnetism in Epitaxial Films of Palladium with an Implanted Impurity of 3d Elements”

2021-2023 The executor of the project 21-12-00179 “Investigation of the Possibility of Controlling the Electrically Conductive and Magnetic Properties of a Highly Conductive State at the Interface between a Ferroelectric and a Dielectric.”

2021-2023 The executor of the project 21-72-10178 “Investigation of the Possibility of Controlling the Superconducting Current in the Design of a Spin Valve Based on a Ferroelectric Substrate.”

Current Research Interests

Ab initio modeling of structural, electronic, and magnetic properties of heterostructures based on transition metal oxides. Giant Rashba coupling at Metal/Polar-Insulator Interfaces. Magnetoelectric coupling at heterostructures based on Ferroelectrics. Polymers characterization by means of molecular dynamics. Machine learning for materials properties prediction. Materials for batteries applications. Low-impurity magnetic alloys properties prediction. Magnetic nanoparticles design and properties prediction.

Author and Co-Author of more than 57 articles in international peer-reviewed journals.

h-Index (Scopus): 12

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Scopus (Author ID): 55587448700

Scientific and related software knowledge

VASP (including ab initio MD, Phonon, SO coupling calculations etc.), Gaussian, LAMMPS, Gibbs (Monte-Carlo calculations), Quantum Espresso, Materials Studio, and others.

Python various scientific libraries, Wolfram Mathematica, MS Office, Origin, Latex, and others

Languages

Native Russian, Fluent English (~C1), German (B1), French (basics), Armenian (basics)