RUSLAN A. MALLAEV

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Education

Moscow Institute of Physics and Technology (MIPT) September 2020 - July 2024
Landau School of Physics and Research
B.S. Degree program: Applied mathematics and physics
Basic department: Computational physics of condensed matter and living systems

General GPA: 3.83/4.0 (8.5/10 - top 10% of the course)
Final thesis: 10 (best possible)

Moscow Institute of Physics and Technology (MIPT) September 2024 - Present
Landau School of Physics and Research
M.S. Degree program: Applied mathematics and physics
Basic department: Computational physics of condensed matter and living systems

Current degree: 2nd year student
General GPA: 4.0/4.0 (9.1/10 - top 3% of the course)

Work experience

Laboratory of biomolecular modeling, Shemyakin–Ovchinnikov October 2021 - Present
Institute of bioorganic chemistry RAS
- Investigation of the role of transmembrane domains in activation of single-pass membrane receptors
- Modeling and analysis of conformational dynamics and dynamic coupling in bimolecular ensembles
- Understanding of allosteric communication in biomolecules using information theory

TerraQuantum AG April 2022 - August 2025
- Numerical solution of differential equations in scientific and industrial problems of quantum chemistry
- Multidimensional optimization in soft matter and quantum chemistry problems
- AI approaches for pharmaceuticals

Center for Pedagogical Excellence October 2020 - August 2022
- Worked as a teacher of a high-level physics course for high school students
- Worked as a methodologist in compiling a program for schoolchildren in Olympiad physics

Conference presentations

Student Biochemical Forum March 2023
– Talk presented in Moscow, Russia: **Ruslan A. Mallaev**, Anton A. Polyansky, *Studying allosteric communication of biomolecules using information theory*, Abstract link
All-Russian Scientific Conference MIPT – Best Student Report April 2023, 2024, 2025
– Talk presented in Moscow, Russia: **Ruslan A. Mallaev**, Anton A. Polyansky, *Studying the communication of biomolecules using information theory*, Abstract link
Symposium on Bioinformatics and Computer-Aided Drug Discovery (BCADD) – 2nd Degree Diploma September 2023
– Talk presented online: **Ruslan A. Mallaev**, Elena T. Aliper, Roman G. Efremov, Anton A. Polyansky, *ARTEMIS: Studying the communication of biomolecules using information theory*, Abstract link

Publications

R. A. Mallaev, B. Bernrieder, R. G. Efremov, A. A. Polyansky, "ARTEMIS: an Information-Theory Based Framework for Analysis of Communication in Biomolecular Systems" , *to be submitted*

R. A. Mallaev, D. Morozov, R. Ellerbrock, "Quantized Tensor Train Approach for Hartree-Fock method", *to be submitted*

C. Zurek, **R. A. Mallaev**, A. C. Paul, N. van Staalduinen, P. Pracht, R. Ellerbrock, C. Bannwarth, "Tensor Train Optimization for Conformational Sampling of Organic Molecules", *J. Chem. Theory Comput.* **2025**

Personal skills

Molecular modeling	MD, GROMACS, PARENT, VMD, PyMOL, OVITO, APBS
Languages	English (B1), French (A2), Russian (native)
Software	C++ (STL, GSL, Boost, etc.), Python (numpy, scipy, pytorch, etc.), Bash, Wolfram Mathematica, Git, LaTeX, SQL
Math	Numerical Linear Algebra, Tensor Networks, Information Theory, Dimensionality Reduction, Convex Optimization