Sergiy Bubin – Curriculum Vitae, February 2025

Sergiy Bubin, Professor
Department of Physics
School of Sciences and Humanities
Nazarbayev University
53 Kabanbay Batyr Ave
Astana, 010000, Kazakhstan

Office: 7E.333
+7 (7172) 69-46-63
sergiy.bubin@nu.edu.kz
www.sergiybubin.org
linkedin.com/in/sergiy-bubin
0000-0002-2783-078X

Personal data

Born: June 12, 1977 in Usharal, Kazakhstan
Nationality: dual – Ukraine & USA Marital status: married

Education

2001-2006	PhD in Physics (minor in Chemistry), University of Arizona, Tucson, USA Thesis title "Accurate Non-Born–Oppenheimer Variational Calculations of Small Molecular Systems" (advisor: Ludwik Adamowicz)
1998-1999	MSc in Physics, National Taras Shevchenko University of Kyiv, Kyiv, Ukraine Thesis title "Precise Variational Calculations of 3- and 4-Particle Quantum Mechanical Systems" (advisor: Ivan V. Simenog, Bogolyubov Institute for Theoretical Physics)
1994-1998	BSc in Physics, National Taras Shevchenko University of Kyiv, Kyiv, Ukraine Thesis title "Variational Calculations of $e^+e^-e^-$" (advisor: Ivan V. Simenog, Bogolyubov Institute for Theoretical Physics)
1992-1994	High School Diploma, Volyn Regional Natural Science Lyceum, Lutsk, Ukraine

Employment history

2014-pres.	Assistant Professor, Associate Professor, Professor – Department of Physics School of Sciences and Humanities, Nazarbayev University, Astana, Kazakhstan
2013-2014	Postdoctoral researcher – Department of Chemistry, University of Rochester, Rochester, NY, USA
2009-2012	Postdoctoral researcher – Department of Physics & Astronomy, Vanderbilt University, Nashville, TN, USA
2008-2009	Postdoctoral researcher – Quantum Chemistry Research Institute, Kyoto, Japan
2006-2008	Postdoctoral researcher – Department of Chemistry, University of Arizona, Tucson, AZ, USA

Research interests

Atomic and molecular physics; Quantum few-body systems; Quantum chemistry; Electronic structure calculations; Explicitly correlated methods; Non-Born–Oppenheimer calculations of atoms and molecules; Relativistic corrections; Fine and hyperfine structure in atoms and molecules; Wave function fitting methods; Computational nanoscience; Real-space real-time time-dependent density functional theory; Non-adiabatic molecular dynamics; Coupled electron-ion dynamics; Molecules and materials subjected to short intense laser pulses; Interaction of energetic ions with nanostructures; Modeling of atmospheric transport and dispersion; Numerical linear algebra; Numerical optimization; High performance computing; Parallel programming

Publication record

Total number of peer-reviewed journal publications: 109

	Google Scholar	Scopus	Web of Science
H-index	32	27	26
Number of citations	3268	2618	2565
User ID / Profile link	mIP9uWQAAAAJ	6507799092	AGI-3418-2022

Key Technical Accomplishments

- Development of a general theoretical framework and associated computer codes for high-precision theoretical spectroscopy of few-electron atoms and ions, incorporating finite nuclear mass as well as leading relativistic and quantum electrodynamics effects. The method has diverse applications, including accurate atomic fine structure calculations, studies of the stability of weakly bound positron–atom complexes, determination of physical constants and nuclear properties (e.g., nuclear radii), testing of fundamental laws and symmetries, and searches for new physics.
- Development of a general theoretical framework and computer codes for high-accuracy non-Born–Oppenheimer calculations of small molecules. This work lays the foundation for reexamining and potentially redefining fundamental concepts in chemistry, such as molecular structure, geometry, and chemical bonding.
- Co-development of a real-space, real-time time-dependent density functional theory (TDDFT) code for studying quantum dynamics at the nanoscale. This code enables the investigation of coupled electron-nuclear dynamics in various systems, particularly in molecules and materials exposed to strong femtosecond laser pulses.

Funding portfolio

- 01/2025–12/2027 "Precise atomic structure calculations with explicitly correlated functions" (Single Principle Investigator), \$150k. Funding Agency: Nazarbayev University Office of Provost. All proposals are peer-reviewed by ORAU (Oak Ridge Associated Universities) experts and only the top-ranked receive NU internal funding.
- 01/2021–12/2023 "Accurate theoretical spectroscopy of few-electron systems" (Single Principle Investigator), \$150k. Funding Agency: Nazarbayev University Office of Provost. All proposals are peer-reviewed by ORAU (Oak Ridge Associated Universities) experts and only the top-ranked receive NU internal funding.
- 01/2018–12/2020 "Center of Excellence for Fundamental and Applied Physics" (Co-PI, responsible for Computational Physics subprogram), \$478k total for seven subprograms. Funding agency: Ministry of Education and Science of Kazakhstan.
- 01/2018–12/2020 "Quantum-mechanical modeling of molecules beyond the Born–Oppenheimer approximation" (Single Principle Investigator), \$150k. Funding Agency: Nazarbayev University Office of Provost. All proposals are peer-reviewed by ORAU (Oak Ridge Associated Universities) experts and only the top-ranked receive NU internal funding.
- 01/2015–12/2017 "Development of computational approaches for explicitly correlated treatment of quantum-mechanical systems" (Single Principle Investigator), \$40k. Funding agency: Ministry of Education and Science of Kazakhstan.

Society memberships

American Physical Society (2007-current)

Professional service

- **Reviewer**: Physical Review A, The Journal of Chemical Physics, Physical Review Letters, Chemical Physics Letters, Chemical Physics, Applied Physics Letters, and Few-Body Systems
- **Panel Member**: National Scientific Council of Kazakhstan in the priority area "Rational use of natural resources, including water resources, geology, processing, new materials and technologies, safe devices and constructions" (2018-2020)

Teaching portfolio

- **At the level of professor**:
  Quantum Mechanics I & II, Classical Mechanics II, Classical Mechanics (graduate), Introductory Physics I & II for Physics Majors, Introductory Physics I & II for Scientists and Engineers, Computational Modeling and Simulation (graduate), Computational Physics, Statistical Mechanics

- **At the teaching assistant and postdoctoral level (before Nazarbayev University)**: Methods of Mathematical Physics, Physical Chemistry, Computational Physics, Introductory Mechanics, Introductory Electricity and Magnetism, Quantum Chemistry, Thermal and Statistical Physics, Quantum Mechanics

Student and Postdoc Supervision at Nazarbayev University

Name	Position	Years	Placement / Where went to
Saeed Nasiri	Postdoc	2020-pres.	
Pavel Rzhevskii	MSc Student	2023-pres. (MSc thesis)	
Ilyas Nagiyev	BSc Student	2024-pres. (research proj.)	
Toreniyaz Shomenov	PhD Student	2019-2024 (MSc, PhD th.)	Postdoc at Natl. Laboratory Astana
Dmitry Tumakov	Postdoc	2023	Postdoc at University of Hamburg
Yerkezhan Bolatbekova	BSc Student	2022-2023 (BSc thesis)	MSc prog. at Nazarbayev University
Aidynbek Tussipzhan	MSc Student	2021-2023 (research proj.)	IT Industry / Software Development
Abutalif Akylbekov	BSc Student	2021-2022 (research proj.)	IT Industry / Software Development
Jian Liu	Postdoc	2021-2022	Postdoc at U. of the Witwatersrand
Maxim Lagay	BSc Student	2021-2022 (research proj.)	MSc prog. at University of Bologna
Arsen Abulgazimov	BSc Student	2019-2021 (BSc thesis)	MSc prog. at Nazarbayev University
Assan Khassenov	BSc Student	2020-2021 (BSc thesis)	IT Industry / Software Development
István Hornyák	Postdoc	2018-2019	Postdoc at Eötvös Loránd U Budapest
Ayan Batyrkhanov	MSc Student	2018-2019 (MSc thesis)	PhD prog. at University of Arizona
Anvar Adylov	BSc Student	2017-2018 (research proj.)	MSc prog. at Nazarbayev University
Amir Bralin	BSc Student	2015-2018 (BSc thesis)	PhD prog. at Purdue University
Yerassyl Balkybek	BSc Student	2017-2018 (BSc thesis)	MSc prog. at Nazarbayev University
Anarzhan Abilgazy	BSc Student	2016-2017 (BSc thesis)	PhD prog. at SUNY Buffalo
Alina Umerbekova	BSc Student	2016-2017 (BSc thesis)	PhD prog. at Rutgers University
Yerbolat Dauletyarov	BSc Student	2014-2015 (BSc thesis)	PhD prog. at University of Arizona
Rustam Gatamov	BSc Student	2014-2015 (BSc thesis)	PhD prog. at Vanderbilt University

Service to Department and University

2019-pres.	Leader of NU HPC Team – overseeing the work of existing High Performance Computer systems on campus and procurement of future ones
2020-pres.	Member of NU High Performance Computing Committee
2019-pres.	Leader of HPCNC Research Cluster (High Performance Computing, Cybersecurity, and Neworking) comprised of 15+ NU faculty from SSH and SEDS
2023-pres.	Physics Department Hiring/Screening Committee Coordinator
2018-2019	Physics Colloquium Series Coordinator
2018-2019	Physics Department Scheduler
2015-2018	Member of Physics Curriculum Commitee
2015-2019	Physics Department Hiring/Screening Committee Coordinator

Conference and school organization

Organizer and Chair of Focus Session "Precision Spectroscopy of Molecules: Status and Perspectives" at APS March Meeting 2019, Boston MA

Organizer and Chair of Focus Session "Explicitly Correlated Methods and Quantum Few-Body Systems" at APS March Meeting 2017, New Orleans LA

Organizer and Chair of Focus Session "Explicitly Correlated Methods and Quantum Few-Body Systems" at APS March Meeting 2016, Baltimore MD

Organizer and Chair of Focus Session "Explicitly Correlated Methods and Quantum Few-Body Systems" at APS March Meeting 2015, San Antonio TX

Organizer and Chair of Focus Session "Explicitly Correlated Methods and Quantum Few-Body Systems" at APS March Meeting 2014, Denver CO

Organizer of Focus Session "Explicitly Correlated Methods and Quantum Few-Body Systems" at APS

March Meeting 2013, Baltimore MD

Lecturer, Vanderbilt/Columbia Molecular Modelling Cybercamp, Vanderbilt University, 2012

Co-organizer and Principal Lecturer, Computational Nanoscience Summer School, Vanderbilt University, 2011

Selected publications

S. Bubin, M. Pavanello, W.-C. Tung, K. L. Sharkey, and L. Adamowicz, Chemical Reviews **113**, 36 (2013).

J. Mitroy, S. Bubin, W. Horiuchi, Y. Suzuki, L. Adamowicz, W. Cencek, K. Szalewicz, J. Komasa, D. Blume, and K. Varga, Reviews of Modern Physics **85**, 693 (2013).

S. Bubin and O. V. Prezhdo, Physical Review Letters **111**, 193401 (2013).

S. Bubin and L. Adamowicz, Physical Review Letters **118**, 043001 (2017).

T. Shomenov and S. Bubin, Physical Review E **108**, 065308 (2023).

Volunteer service

2024 Served as a coach/mentor of a team of 8 high school students from Kazakhstan in the BL4S Beamline 4 Schools contest organized by CERN. The team's proposal was shortlisted (made it to the top 10% of the 461 participating teams from 78 countries) and received a prize.

Appearance in media

2021-2022 Took part in three short episodes of PopSci show "Science" on *Khabar 24* (a major Kazakh TV channel):

- Magic of quantum physics
- The latest computing technology and supercomputers
- What was remarkable in science in 2021 and what discoveries can we expect in 2022?