

# Sergiy Bubin – curriculum vitae, circa 2019

Associate Professor  
Department of Physics  
School of Science and Technology  
Nazarbayev University  
53 Kabanbay Batyr Ave  
Nur-Sultan, 010000, Kazakhstan

Phone: +7 (7172) 69-46-63  
Email: [sergiy.bubin@nu.edu.kz](mailto:sergiy.bubin@nu.edu.kz)  
Web: <http://sergiybubin.org>

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## EDUCATION

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| 2001-2006 | Ph.D. (Physics, minor in Chemistry), University of Arizona<br>Thesis title “Accurate Non-Born–Oppenheimer Variational Calculations of Small Molecular Systems” under supervision of Ludwik Adamowicz   |
| 1998-1999 | M.S. (Physics), National Taras Shevchenko University of Kyiv, Kyiv, Ukraine<br>Thesis title “Precise Variational Calculations of 3- and 4-Particle Quantum Mechanical Systems” under supervision of Prof. Ivan V. Simenog (Bogolyubov Institute for Theoretical Physics) |
| 1994-1998 | B.S. (Physics), National Taras Shevchenko University of Kyiv, Kyiv, Ukraine<br>Thesis title “Variational Calculations of $e^+e^-e^-$ ” under supervision of Ivan V. Simenog (Bogolyubov Institute for Theoretical Physics)   |
| 1992-1994 | High School Diploma, Volyn Regional Natural Science Lyceum, Lutsk, Ukraine   |
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## EMPLOYMENT HISTORY

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| 2016-present | Associate Professor, Department of Physics, School of Science and Technology, Nazarbayev University, Astana, Kazakhstan            |
| 2014-2016    | Assistant Professor, Department of Physics, School of Science and Technology, Nazarbayev University, Astana, Kazakhstan            |
| 2013-2014    | Postdoctoral researcher, Department of Chemistry, University of Rochester, Rochester, USA (in the group of Oleg Prezhdo)           |
| 2009-2012    | Postdoctoral researcher, Department of Physics and Astronomy, Vanderbilt University, Nashville, USA (in the group of Kalman Varga) |
| 2008-2009    | Postdoctoral researcher, Quantum Chemistry Research Institute, Kyoto, Japan (in the group of Hiroshi Nakatsuji)                    |
| 2006-2008    | Postdoctoral researcher, Department of Chemistry, University of Arizona, Tucson, USA (in the group of Ludwik Adamowicz)            |
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## RESEARCH INTERESTS

Atomic and molecular physics; Quantum chemistry; Computational nanoscience; Electronic structure calculations; Explicitly correlated methods; Non-Born–Oppenheimer calculations of atoms and molecules; Relativistic corrections; Wave function fitting methods; Variational Quantum Monte Carlo; Time-dependent density functional theory; Nonadiabatic molecular dynamics; Coupled electron-ion dynamics; Strong-field phenomena; 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; Scientific programming and numerical analysis in general; High performance computing; Parallel programming

## PUBLICATION RECORD

Total number of publications in peer-reviewed journals	88
Number of citations	1782 (Web of Science)
	1815 (Scopus)
	2157 (Google Scholar)
<i>h</i> -index	23 (Web of Science)
	23 (Scopus)
	25 (Google Scholar)

Google Scholar profile: <http://scholar.google.com/citations?user=mIP9uWQAAAAJ>

Scopus profile: <https://www.scopus.com/authid/detail.uri?authorId=6507799092>

ResearcherID profile: <http://www.researcherid.com/rid/M-2410-2013>

## KEY TECHNICAL ACCOMPLISHMENTS

- Development of a general theoretical framework and computer code for high-accuracy non-Born-Oppenheimer calculations of small molecules. This development paves a way to reexamine and even question the fundamental concepts central to chemistry – molecular structure, geometry, and chemical bonding.
- Development of a framework for predictive theoretical spectroscopy of few-electron atoms with the inclusion of finite nuclear mass, relativistic, and quantum electrodynamics effects. This framework can have many applications relevant to the determination of fundamental constants and properties (e.g. nuclear radii), as well as complement precision measurement experiments that aim to test fundamental laws and symmetries and search for new physics.
- Rigorous prediction of the existence of an electronically excited state in a positronic atom, which can be used to guide its experimental detection.
- Co-development of real-space real-time TDDFT code for studying quantum dynamics at the nanoscale. This code can be used to investigate coupled electron-nuclear dynamics in various systems, in particular molecules and materials subjected to strong femtosecond laser pulses.

## FUNDING PORTFOLIO

- 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.
- 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.
- 01/2018–12/2020 “Center of Excellence for Fundamental and Applied Physics” (Co-PI, responsible for Computational Physics subprogram), \$360k total for seven subprograms. Funding agency: Ministry of Education and Science of Kazakhstan.

## TEACHING PORTFOLIO

- *At professor level:*  
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

- ***At teaching assistant level (before Nazarbayev University):***

Methods of Mathematical Physics, Physical Chemistry, Computational Physics, Mechanics, Electricity and Magnetism, Quantum Chemistry, Thermal and Statistical Physics

### STUDENT AND POSTDOC SUPERVISION AT NAZARBAYEV UNIVERSITY

Name	Position	Years (Thesis)	Placement / Where went to
István Hornyák	Postdoc	2018-current	
Ayan Batyrkhanov	MS Student	2018-2019 (MS thesis)	PhD program at University of Arizona
Anvar Adylov	UG Student	2017,2018 (summer)	MS program at Nazarbayev U
Amir Bralin	UG Student	2015-2018 (BS thesis)	PhD program at Purdue University
Yerassyl Balkybek	UG Student	2017-2018 (BS thesis)	MS program at Nazarbayev U
Anarzhhan Abilgazy	UG Student	2016-2017 (BS thesis)	PhD program at SUNY Buffalo
Alina Umerbekova	UG Student	2016-2017 (BS thesis)	PhD program at Rutgers University
Yerbolat Dauletyarov	UG Student	2014-2015 (BS thesis)	PhD program at University of Arizona
Rustam Gatamov	UG Student	2014-2015 (BS thesis)	PhD program at Vanderbilt University

### SERVICE TO DEPARTMENT AND UNIVERSITY

2018-current Physics Colloquium Series Coordinator  
 2018-current Physics Department Scheduler  
 2015-2018 Member of Physics Curriculum Committee  
 2015-current Physics Hiring Committee Secretary

### SOCIETY MEMBERSHIPS

American Physical Society, American Chemical Society

### 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)

### 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 and K. Varga, [Applied Physics Letters](#) **98**, 154101 (2011).

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).