**CURRICULUM VITAE**

# Dmitri A. Babikov


TITLE: Professor of Chemistry

CURRENT ADDRESS:
Marquette University
Department of Chemistry
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Milwaukee, WI 53201-1881
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EDUCATION:

The Moscow Institute of Physics and Technology, Russia

- Ph.D., Nov. 1998 Plasma Physics & Chemistry
- M.S., June 1995 Applied Physics & Math
- B.S., June 1993 Natural Sciences

PROFESSIONAL EXPERIENCE:

Marquette University: Chemistry Department,

- Full Professor — Aug. 2014 – present
- Associate Professor — Aug. 2010 – Jul. 2014
- Assistant Professor — Aug. 2004 – Jul. 2010

Visiting Professor, University of Rennes, France — Sept.-Oct., 2025
University of Pierre and Marie Curie, — May-June, 2010

Postdoctoral Fellow, Theoretical Division, Los Alamos National Laboratory — Dec. 2000 – Jul. 2004

Postdoctoral Research Scientist, Chemistry Division, Argonne National Laboratory — March 2000 – Nov. 2000

Postdoctoral Fellow, Department of Chemistry, University of Illinois at Chicago — Apr. 1999 – Feb. 2000

Graduate Research Scientist, Laboratory of Atomic and Molecular Collisions, France — Nov. 1996 – Feb. 1999

MEMBERSHIPS:

American Chemical Society 2001 –present
American Physical Society 2019 –present

AWARDS:

| | |
|---|---|
| • Way Klingler Sabbatical Fellowship Award (Marquette University Graduate School) | 2025 – 2026 |
| • Faculty Professional Mentor Award (Marquette University) | 2025 – 2026 |
| • NERSC CPU Time Awards (National Energy Research Scientific Computing Center at LBNL) | 2002 – 2026 |
| • Haberman-Pfletschinger Distinguished Chair (Marquette University) | 2022 – 2025 |
| • Way Klingler Research Fellowship Award (Marquette University) | 2020 – 2023 |
| • Full-Year Sabbatical Fellowship (Marquette University) | 2018 – 2019 |
| • Emerson Center for Scientific Computation Visiting Fellowship Award (Emory University) | 2009 – 2010 |
| • Way Klingler Young Scholar Award (Marquette University) | 2008 – 2009 |
| • Prestigious Postdoctoral Fellowship from Director of Los Alamos National Laboratory | 2000 – 2003 |
| • Scholarship for Doctoral Research from the International Student Exchange Program in France (CIES) | 1996 – 1999 |

GRANTS: EXTERNAL FUNDED (over $4.4 M total)

| Agency | Title | Dates | Amount |
|---|---|---|---|
| • IBM Quantum Credits | "Simulating Quantum Molecular Dynamics on Quantum Computers" | 06/25-05/26 | $10,000 |
| • Northwestern Mutual Data Science Initiative | "Parallel Implementation of Neural Networks for The Prediction of Molecular Collision Cross Sections" | 09/25-12/25 | $5,000 |
| • Northwestern Mutual Data Science Initiative | "Implementation of Neural Networks for The Prediction of Molecular Collision Cross Sections" | 09/24-12/24 | $5,000 |
| • IonQ Research Credits | "Simulating Quantum Molecular Dynamics on Quantum Computers" | 01/25-06/26 | $30,000 |
| • NASA, APRA | "One database of collisional energy transfer for all water isotopologues" | 07/23-06/26 | $470,000 |
| • NSF, ExpandQISE | "ExpandQISE: Quantum Molecular Dynamics on Quantum Computers" Role: PI, collaborative at 70/30 | 07/23-06/26 | $800,000 |
| • NSF, Chemical Theory and Modeling | A supplement to the existing grant to implement quantum computing | 09/22-08/23 | $50,000 |
| • NSF, Chemical Theory and Modeling | "Mixed Quantum Classical Theory for the Collisional Quenching of iCOMs" | 07/21-06/24 | $398,200 |
| • NSF, Atmospheric | "Computational Study of Symmetry- | 09/19-08/22 | $404,000 |

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|---|---|---|---|
| Chemistry Program | Driven Isotope Effects and O-MIF" | | |
| • NASA, Astrophysics | "Computational Studies of Collisional Energy Transfer using MQC Theory" | 01/17-12/19 | $332,700 |
| • NASA, Exobiology | "Revealing the role of recombination reactions in S-MIF" | 06/15-05/18 | $273,000 |
| • NSF, Catalyzing New Intern. Collaborations | "Benchmark Studies of Collisional Energy Transfer using MQCT" | 11/13-01/15 | $40,000 |
| • NSF, Atmospheric Chemistry Program | "Modeling Ozone MIF in Gas Phase and on Surfaces" | 07/13-06/16 | $305,100 |
| • NSF, Chemical Theory and Modeling | "Manipulating Quantum Information with Vibrational Qubits". Role: PI, collaborative at 50/50 | 09/10-08/13 | $480,500 |
| • AFOSR, Molecular Dynamics | "Non-Born-Oppenheimer Spectroscopy of Energetic Triatomics" | 07/09-06/10 | $93,500 |
| • NSF, Atmospheric Chemistry Program | "Quantum Origin of Anomalous Isotope Effects" | 06/09-05/12 | $285,000 |
| • Petroleum Research Fund, ACS | "Quantum Origin of Anomalous Isotope Effect in Ozone Formation" | 09/05-08/07 | $35,000 |
| • NSF, Atomic and Molecular Physics | "Vibrational State Approach to Quantum Computation" | 05/05-04/08 | $150,000 |

GRANTS: INTERNAL FUNDED

| **Program** | **Title** | **Dates** | **Amount** |
|---|---|---|---|
| Way Klingler Sabbatical | Research on Quant. Comp. | 2025-2026 | $5,000 |
| Haberman Chair Fund | Research, MQCT | 2022-2025 | $30,000 |
| Way Klingler Fellowship | Research, iCOMs | 2020-2023 | $150,000 |
| Faculty Development Award | Travel to TCRC | 01/14 | $600 |
| Faculty Development Award | Travel to MOLEC XVII | 03/08 | $700 |
| Summer Faculty Fellowship | "Anomalous Isotope Effect in Ozone Formation" | 06/08-07/08 | $5,500 |
| Faculty Development Award | "Anomalous Isotope Effect in Ozone Formation" | 06/08-07/08 | $3,000 |
| Summer Faculty Fellowship | "Anomalous Isotope Effect in Ozone Formation" | (2005, *declined by PI due to other funding*) | $5,500 |
| Faculty Development Award | "Anomalous Isotope Effect in Ozone Formation" | (2005, *declined by PI due to other funding*) | $4,500 |
| Start-Up Package | Assistant Professor | 2004-2006 | $130,000 |

SERVICE TO

| | | |
|---|---|---|
| University: | HPC Committee | 2026 |
| | Jury for Faculty Mentor Awards | 2026 |
| | Promotion and Tenure Committee | 2024 – present |
| | Sabbatical Review Committee | 2022 – 2024 |
| | Mellon Fund Proposal Review Committee | 2019 – 2020 |
| | Core Curriculum Review Committee | 2013 – 2015 |
| Department: | Advisor for Student Associates of ACS | 2004 – 2005 |
| | Physical Chemistry Committee | 2004 – 2012 |
| | Undergraduate Committee | 2006 – 2010 |
| | | 2013 – 2018 |
| | chaired in | 2014 – 2018 |
| | Graduate Committee | 2004 – 2006 |
| | | 2010 – 2012 |
| | chaired in | 2012 – 2013 |
| | | 2019 – 2023 |
| | Search Committee | 2007 – 2011 |
| | Research Advancement Committee | 2010 – 2011 |
| | Graduate Recruiting Committee | 2019 – 2020 |
| | chaired in | 2023 – 2025 |
| | Chem Major Advisors Committee: | 2015 – present |
| | Committee on Teaching | 2015 – present |
| | Advisory Committee | 2023 – present |

Profession: Organized Symposium on *"Quantum and Semi Classical approaches to Molecular Dynamics"* at the GLRM of ACS, May 31, 2006, Milwaukee.

Organized a series of *Quantum Information/Quantum Computing Seminars*, jointly with Debbie Perouli (Department of Computer Science at Marquette), as a part of seminar programs at both departments, with several world-recognized lecturers delivering talks at either Chemistry or Computer Science departments, which included:

- 2019S: Yuri Alekseev, Argonne National Laboratory;
- 2019S: Artur Izmaylov, University of Toronto;
- 2019F: Sabre Kais, Purdue University;
- 2020S: Hannes Bernien, University of Chicago;
- 2021S: Joseph Lukens, Oak Ridge National Lab (COVID, postponed);
- 2022F: George Schatz, Northwestern University
- 2024S: Michael R. Wasielewski, Northwestern
- 2024S: Micheline Soley, UW-Madison
- 2024F: Timur Tsherbul, University of Nevada
- 2024F: Bill Poirier, Texas Tech University

COURSES TAUGHT:

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|---|---|
| Chem 1001: | General Chemistry 1 (often taught two sections, ~270 students per section) |
| Chem 4433: | Physical Chemistry 1 |
| Chem 4434: | Physical Chemistry 2 |
| Chem 5431: | Physical Chemistry: Fundamentals with Applications in Bio-Sciences |
| Chem 6401: | Research Tools in Physical Chemistry (graduate, computational quantum chemistry) |

## THESES/DISSERTATIONS DIRECTED:

| | |
|---|---|
| 1) Leidi Jiang, | graduated, 2009 with M.S. |
| 2) Yingying Gu, | graduated, 2011 with M.S. |
| 3) Xiang Sheng, | graduated, 2011 with M.S. |
| 4) Lei Wang, | graduated, 2012 with Ph.D. |
| 5) Dmytro Shyshlov | graduated, 2015 with Ph.D. |
| 6) Alexander Teplukhin | graduated, 2017 with Ph.D. |
| 7) Alexander Semenov | graduated, 2017 with Ph.D. |
| 8) Bikram Mandal | graduated, 2021 with Ph.D. |
| 9) Igor Gayday | graduated, 2021 with Ph.D. |
| 10) Lisa Grushnikova | graduated, 2022 with Ph.D. |
| 11) Sahad Nikzat | graduate student in Spring 2022 (dropped) |
| 12) Adil Yermek | graduated, 2024, with M.S. |
| 13) Ramin Salehi | graduate student 2023-2024 (dropped) |
| 14) Sohrab Salimibani | graduate student 2023-2024 (dropped) |
| 15) Carolin Joy | graduated, 2025 with Ph.D. |
| 16) Dulat Bostan | graduated, 2025 with Ph.D. |
| 17) Nandu Krishna | graduate student since Aug. 2023 (Ph.D. program) |
| 18) Tamila Kunyasheva | graduate student since Aug. 2023 (Ph.D. program) |
| 19) Vivek Vijay | graduate student since Jan. 2025 (Ph.D. program) |

## OTHER SERVICE ON DISSERTATION COMMITTEES:

| | | | |
|---|---|---|---|
| 1) Calvin Mukarakate, | Marquette University | Ph.D. | 2008 |
| 2) Juan Blandon, | U. of Central Florida | Ph.D. | 2009 |
| 3) Stephen Majoni, | Marquette University | Ph.D. | 2011 |
| 4) Ryan Zaari, | University of Alberta | Ph.D. | 2012 |
| 5) Maxim Ivanov | Marquette, Chemistry | Ph.D. | 2016 |
| 7) Brian Pattengale | Marquette, Chemistry | Ph.D. | 2018 |
| 6) Longhao Huang | Marquette, Engineering | Ph.D. | 2020 |
| 8) Niloufar Hendinejad | Marquette, Chemistry | Ph.D. | 2020 |
| 9) Mark Mitmoen | Marquette, Chemistry | M.S. | 2022 |
| 10) Nick Langer | Marquette, Chemistry | Ph.D. | 2024 |
| 11) Rustam Sabitov | Marquette, Chemistry | Ph.D. | 2024 |
| 12) Ronald Mutete | Marquette, Chemistry | Ph.D. | in progress |

## SUPERVISION OF POSTDOCTORAL RESEARCHERS:

| | |
|---|---|
| 1) Evgeny Vetoshkin | May. 2005 – Apr. 2007 |
| 2) Meiuy Zhao | Sept. 2005 – Aug. 2007 |
| 3) Mehdi Ayous | Nov. 2010 – Aug. 2011 |
| 4) Mikhail Ivanov | Oct. 2009 – Apr. 2014 |
| 5) Alexander Teplukhin | May 2017 – May 2018 |
| 6) Bikram Mandal | June 2021 – Dec. 2022 |
| 7) Igor Gaidai | June 2021 – Jan. 2023 |
| 8) Jayakrushna Sahoo | Jan. 2025 – present |
| 9) Dulat Bostan | Aug. 2025 – present |
| 10) Carolin Joy | Aug. 2025 – present |

## SUPERVISION OF UNDERGRADUATE STUDENTS:

| | | |
|---|---|---|
| 1) Leo Nugraha (undergrad at Marquette) | Dec. 2010 – | May 2011 |
| 2) Sara Russell (summer intern, Alverno College) | June 2011 – | Aug. 2011 |
| 3) Andrew Kreatsoulas (undergraduate research) | Jan. 2013 – | May 2013 |
| 4) Sarah Huber (undergraduate research) | Jan. 2015 – | May 2015 |
| 5) Nicholas Wrasman (undergraduate research) | Jan. 2015 – | May 2015 |
| 6) Gavin Johnson (summer research) | May 2021 – | Aug. 2021 |
| 7) Andrew Antoine (undergraduate research) | Jan. 2022 – | May 2022 |
| 8) Alex Eng (summer research) | May 2022 – | Aug. 2022 |
| 9) Kayla Imanzi (summer research) | May 2023 – | Aug. 2024 |
| 10) Jonathan Andrade-Plascencia (undergraduate research) | Aug. 2024 – | Aug. 2025 |
| 11) Greg Occhiogrosso (undergraduate research) | Aug. 2024 – | in progress |

PEER REVIEWD RESEARCH PUBLICATIONS (125 TOTAL)

( * - corresponding author):

*IN PREPARATION*

1. Nandu Krishna, Igor Gaidai, Adil Yermek, Ahren Jasper, and Dmitri Babikov, "Master-Equation Simulations of Ozone Formation Kinetics with Accurate Quantum Mechanical Input Data", in progress.
2. J. Sahoo, B. K. Kendrick, and D. Babikov, "Mixed Quantum/Classical Theory for Fine-Structure Inelastic Transitions in the Scattering of $^2\Pi$ Molecule with Structureless Target" in progress.
3. F. Tonolo, V. Vijay, E. Quintas-Sánchez, C. Joy, R. Dawes, D. Babikov and F. Lique, "Collisional rate coefficients for rotational state-to-state transitions in ethanimine molecule", in progress, 2026.
4. C. Joy, G. Occhiogrosso, B. Mandal, and D. Babikov "A Machine Learning Approach for Computationally Efficient Prediction of State-to-State Transition Cross Sections for Molecular Collision Processes", in progress.

*SUBMITTED / PUBLISHED AS FULL PROFESSOR (62 papers)*

5. V. Vijay, F. Tonolo, E. Quintas-Sánchez, A.B. Planas, C. Joy, R. Dawes, F. Lique and D. Babikov, "Collisional energy transfer in ethanimine + He system", submitted, 2026. https://doi.org/10.48550/arXiv.2606.08846
6. T. Kuanysheva, J. Andrade-Plascencia, J. Sahoo, B. Kendrick, and D. Babikov, "On Performance and Limitations of NISQ Hardware for Simulations of Quantum Wave Packet Dynamics", *J. Phys. Chem. Lett.*, re-submitted with corrections, 2026. https://arxiv.org/abs/2605.20078
7. D. Bostan, C. Joy, V. Vijay and **D. Babikov*** "MQCT 2026: A Program for Calculations of Inelastic Scattering of Two Molecules" *Comput. Phys. Commun.* 324, 110153, 2026.
8. C. Joy, I. Gaidai, A. Faure and **D. Babikov***, "Mixed quantum/classical theory (MQCT) for Rotational Excitation of HDO in Collisions with $H_2$: Symmetry Breaking Effects and Time-Dependent Dynamics" *J. Chem. Theor. Comp.* 21, pp. 10669–10678, 2025.
9. B. Mandal, **D. Babikov**, P.C. Stancil, R.C. Forrey, R.V. Krems and N. Balakrishnan. "Neural network ensemble for computing cross sections for rotational transitions in $H_2O$ + $H_2O$ collisions" *Phys. Chem. Chem. Phys.* 27, pp. 23000 - 23012, 2025.
10. T. Kuanysheva, B. Kendrick, L. Cincio, and **D. Babikov***, "Quantum Simulation of Molecular Dynamics Processes – A Benchmark Study Using Classical Simulator and Present-Day Quantum Hardware", *J. Phys. Chem. A* 129, pp. 6470-6481, 2025.
11. J. Andrade-Plascencia, T. Kuanysheva, D. Bostan, B. Kendrick and **D. Babikov*** "Mixed Quantum/Classical Theory Approach to Rotationally Inelastic Molecular Collisions Implemented on a Quantum Computer", *J. Chem. Theor. Comp.* 21, pp. 6305–6314, 2025.
12. C. Joy, D. Bostan, B. Mandal and **D. Babikov*** "Rate coefficients for rotational state-to-state transitions in $H_2O$ + $H_2$ collisions as predicted by mixed quantum/classical theory" *Astronomy & Astrophysics* 692, A229, 2024.

13. D. Bostan, and **D. Babikov**[*] "Mixed Quantum/Classical Theory for Rotationally Inelastic Scattering of Identical Collision Partners Revised" *Phys. Chem. Chem. Phys.* 26, pp. 27567 - 27582, 2024.
14. **D. Babikov**, N. Balucani, A. Bergeat, M. Brouard, D. Chandler, M. L. Costen, M. Farnık, H. Guo, T. Gyori, D. Heard, D. Heathcote, N. Hertl, P. G. Jambrina, N. M. Kidwell, O. A. Krohn, V. Le Duc, J. Loreau, S. Mackenzie, M. McCrea, K. G. McKendrick, J. Meyer, D. Moon, A. S. Mullin, G. S. Nathanson, D. M. Neumark, K.-K. Ni, M. J. Paterson, E. Pluharova, P. Robertson, C. Reilly, G. C. Schatz, C. Sparling, A. G. Suits, P. Watson, R. Wester, S. Willitsch and A. M. Wodtke "Scattering of larger molecules" in *"New Directions in Molecular Scattering"*, *Faraday Discussions* 251, pp. 313-341, 2024.
15. B. Mandal, M. Zoltowski, M. Cordiner, F. Lique and **D. Babikov**[*], "Rotational state-to-state transition rate coefficients for $H_2O$ + $H_2O$ collisions at non-equilibrium conditions", *Astronomy & Astrophysics* 688, A208, 2024.
16. C. Joy, B. Mandal, D. Bostan, M.-L. Dubernet and **D. Babikov**[*], "Mixed Quantum/Classical Theory (MQCT) Approach to the Dynamics of Molecule-Molecule Collisions in Complex Systems", *Faraday Discussions* 251, pp. 225-248, 2024.
17. M.L. Dubernet, C. Boursier, O. Denis-Alpizar, Y.A. Ba, N. Moreau, C.M. Zwölf, M.A. Amor, **D. Babikov**, N. Balakrishnan, C. Balança, M. Ben Khalifa, A. Bergeat, C.T. Bop, L. Cabrera-González, C. Cárdenas, A. Chefai, P. J. Dagdigian, F. Dayou, S. Demes, B. Desrousseaux, F. Dumouchel, A. Faure, R.C. Forrey, J. Franz, R.M. García-Vázquez, F. Gianturco, A. Godard Palluet, L. González-Sánchez, G.C. Groenenboom, P. Halvick, K. Hammami, F. Khadri, Y. Kalugina, I. Kleiner, J. Kłos, F. Lique, J. Loreau, B. Mandal, B. Mant, S. Marinakis, D. Ndaw, P. Pirlot Jankowiak, T. Price, E. Quintas-Sánchez, R. Ramachandran, E. Sahnoun, C. Santander, P.C. Stancil, T. Stoecklin, J. Tennyson, F. Tonolo, R. Urzúa-Leiva, B. Yang, E. Yurtsever, and M. Zóltowski, "BASECOL2023 scientific content", *Astronomy & Astrophysics* 683, A41 (31 pages), 2024.
18. D. Bostan, B. Mandal, C. Joy, M. Żółtowski, J. Loreau, F. Lique, E. L. Quintas Sanchez, A. Batista-Planas, R. Dawes and **D. Babikov**[*], "Mixed Quantum/Classical Calculations of Rotationally Inelastic Scattering in the CO + CO System: A Comparison with Fully Quantum Results", *Phys. Chem. Chem. Phys.* 26, pp. 6627 – 6637, 2024. (journal cover)
19. B. Mandal, D. Bostan, C. Joy and **D. Babikov**[*], "MQCT 2024: A Program for Calculations of Inelastic Scattering of Two Molecules", *Comput. Phys. Commun.* 294, 108938, 2024.
20. K. Imanzi, D. Bostan, M. McCrea, M. Brouard, and **D. Babikov**[*], "Symmetry Breaking – A Classic Example of Quantum Interference Captured by Mixed Quantum/Classical Theory", *J. Phys. Chem. Lett.* 14, pp. 10617–10623, 2023.
21. B. Mandal, and **D. Babikov**[*], "Improved temperature dependence of $H_2O$ + $H_2O$ rotational state-to-state transition rate coefficients for cometary and planetary applications" *Astronomy & Astrophysics* 678, A51, 2023.
22. C. Joy, B. Mandal, D. Bostan and **D. Babikov**[*] "Mixed Quantum/Classical Theory for Rotational Energy Exchange in Symmetric-Top-Rotor + Linear-Rotor Collisions and a Case Study of $ND_3$ + $D_2$ System" *Phys. Chem. Chem. Phys.* **25**, pp. 17287 – 17299, 2023.

23. D. Bostan, B. Mandal, C. Joy and **D. Babikov**[*] "Description of Quantum Interference Using Mixed Quantum/Classical Theory of Inelastic Scattering" *Phys. Chem. Chem. Phys.* 25, pp. 15683 - 15692, 2023.
24. B. Mandal, and **D. Babikov**[*], "Rate coefficients for rotational state-to-state transitions in $H_2O$ + $H_2O$ collisions for cometary and planetary applications, as predicted by mixed quantum/classical theory" *Astronomy & Astrophysics* 671, A51, 2023.
25. B. Mandal, C. Joy, D. Bostan, A. Eng and **D. Babikov**[*], "Adiabatic trajectory approximation – New general method in the toolbox of mixed quantum/classical theory for collisional energy transfer", cover art, *J. Phys. Chem. Lett.* 14, 817−824, 2023.
26. B. Mandal, C. Joy, D. Bostan and **D. Babikov**[*], "MQCT 2022 – A program for calculations of inelastic scattering of two molecules", VIRT&L-COMM, Vol. 24, 2022. ISSN: 2279-8773. Web: VIRT&L-COMM (unipg.it)
27. **D. Babikov**, M. P. Burke, P. Casavecchia, W. H. Green, A. G. Dana, H. Guo, D. Heard, D. Heathcote, M. Hochlaf, A. W. Jasper, S. J. Klippenstein, M. I. Lester, C. Marti, A. M. Mebel, A. S. Mullin, T. L. Nguyen, M. Olzmann, A. Orr-Ewing, D. L. Osborn, P. A. Robertson, M. Robinson, R. Shannon, O. J. Shiels, A. G. Suits, C. Taatjes, J. Troe, "Collisional energy transfer: General discussion" in "Unimolecular Reactions", *Faraday Discussions* 238, 121-143, 2022.
28. I. Gayday, **D. Babikov**[*], A. Teplukhin, B. K. Kendrick, S. M. Mniszewski, Y. Zhang, S. Tretiak, P. A. Dub[*], "Molecular dynamics on quantum annealers" *Sci. Reports* 12, 16824 (10 pages), 2022. Open access: Molecular dynamics on quantum annealers | Scientific Reports (nature.com)
29. B. Mandal, C. Joy, A. Semenov and **D. Babikov**[*], "Mixed quantum/classical theory for collisional quenching of PAHs in the interstellar media" *ACS Journal of Earth and Space Chemistry* 6, 521-529, 2022.
30. P. Liu, J. Liu, A. Ji, C. T. Reinhard, N. J. Planavsky, **D. Babikov**, R. G. Najjar and J. F. Kasting, "Triple oxygen isotope constraints on atmospheric $O_2$ and biological productivity during the Mid-Proterozoic" *Proc. Nat. Acad. Sci.* 118, e2105074118, 2021.
31. I. Gayday and **D. Babikov**[*], "Efficient method for an approximate treatment of Coriolis effect in the calculations of quantum dynamics and spectroscopy, with application to scattering resonances in ozone", *J. Phys. Chem. A* 125, 5661–5669, 2021.
32. I. Gayday, A. Teplukhin, J. Moussa and **D. Babikov**[*], "SpectrumSDT: a program for parallel calculation of coupled rotational-vibrational energies and lifetimes of bound states and scattering resonances in triatomic systems", *Comp. Phys. Com.* 267, 108084 (9 Pages), 2021.
33. **D. Babikov**[*], E. Grushnikova, I. Gayday and A. Teplukhin, "Four isotope-labeled recombination pathways of ozone formation", *Molecules* 26, 1289 (21 pages), 2021.
34. B. Mandal, A. Semenov and **D. Babikov**[*], "Adiabatic trajectory approximation within the framework of mixed quantum/classical theory" *J. Phys. Chem. A* 124, 9877-9888, 2020.
35. I. Gayday, E. Grushnikova and **D. Babikov**[*], "Influence of the Coriolis effect on the properties of scattering resonances in symmetric and asymmetric isotopomers of ozone", *Phys. Chem. Chem. Phys.* 22, 27560 - 27571, 2020.

36. A. Teplukhin, B. Kendrick and **D. Babikov**, "Solving complex eigenvalue problems on a quantum annealer with applications to quantum scattering resonances", *Phys. Chem. Chem. Phys.* 22, 26136-26144, 2020.
37. C. Boursier, B. Mandal, **D. Babikov** and M. L. Dubernet, "New $H_2O$-$H_2O$ collisional rate coefficients for cometary applications", *Monthly Notices of Royal Astronomical Society* 498, 5489–5497, 2020.
38. I. Gayday, A. Teplukhin, B. Kendrick and **D. Babikov***, "On the role of rotation-vibration coupling in the spectra of ozone isotopomers" *J. Chem. Phys.* 152, 144104 (16 pages), 2020.
39. I. Gayday, A. Teplukhin, B. Kendrick and **D. Babikov***, "Theoretical treatment of Coriolis effect using hyper-spherical coordinates, with application to the ro-vibrational spectrum of ozone" *J. Phys. Chem. A* 124, 2808–2819, 2020.
40. A. Semenov, B. Mandal and **D. Babikov***, "MQCT: A user-ready program for calculations of inelastic scattering", *Comp. Phys. Com.* 252, 107155 (13 pages), 2020.
41. A. Teplukhin, B. Kendrick and **D. Babikov**, "Calculation of molecular vibrational spectra on a quantum annealer", *J. Chem. Theory Comput.* 15, 4555-4563, 2019.
42. I. Gayday, A. Teplukhin and **D. Babikov***, "Communication: The ratio of the number of states in asymmetric and symmetric ozone molecules deviates from the statistical value of 2" *J. Chem. Phys.* 150, 101104 (6 pages, communication), 2019.
43. I. Gayday, A. Teplukhin and **D. Babikov***, "Computational analysis of vibrational modes in tetra-sulfur using dimensionally reduced potential energy surface", *Mol. Phys.* 117, 2546-2558, 2019.
44. D. Shyshlov and **D. Babikov***, "Computational study of cold ions trapped in a double-well potential", *Mol. Phys.* 117, 1912-1925, 2019.
45. A. Teplukhin, I. Gayday and **D. Babikov***, "Erratum: Several levels of theory for description of isotope effects in ozone: Effect of resonance lifetimes and channel coupling", *J. Chem. Phys.* 149, 209901, 2018.
46. D. Babikov, D. Benoit, J. Bowman, T. Burd, D. Clary, R. Donovan, I. Fischer, F. Gianturco, M. Hochlaf, S. Kar, A. Kirrander, S. Leone, T. Malcomson, U. Manthe, A. McCoy, J. Petersen, J. Richardson, P. Slavicek, T. Stoecklin, K. Szalewicz, A. van der Avoird, R. Wester, G. Worth and A. Zehnacker-Rentien, "Quantum dynamics of isolated molecules: General discussion" *Faraday Discussions* 212, 281-306, 2018.
47. A. Teplukhin and **D. Babikov***, "Several levels of theory for description of isotope effects in ozone: Symmetry effect and Mass effect", *J. Phys. Chem. A* 122, pp. 9177-9190, 2018.
48. A. Teplukhin, I. Gayday and **D. Babikov***, "Several levels of theory for description of isotope effects in ozone: Effect of resonance lifetimes and channel coupling", *J. Chem. Phys.* 149, 164302 (13 pages), 2018.
49. A. Teplukhin and **D. Babikov***, "Properties of Feshbach and shape resonances in ozone-forming reaction and their influence on mass-independent isotope effect", *Faraday Discuss.* 212, 259-280, 2018.

50. B. Mandal, A. Semenov and **D. Babikov**[*], "Calculations of Differential Cross Sections Using Mixed Quantum/Classical Theory of Inelastic Scattering", *J. Phys. Chem. A* 122, 6157-6168, 2018.
51. C. E. Harman, A. A. Pavlov, **D. Babikov**, and J. F. Kasting, "Chain Formation as a Mechanism for Mass-Independent Fractionation of Sulfur Isotopes in the Anoxic Archean Atmosphere", *Geophys. Res. Let.* 496, 238-247, 2018.
52. A. Semenov and **D. Babikov**[*], "MQCT. I. Inelastic Scattering of Two Asymmetric-Top Rotors with Application to $H_2O$ + $H_2O$", *J. Phys. Chem. A* 121, 4855-4867, 2017.
53. A. Semenov and **D. Babikov**[*], "Three Sources of Errors in the Ehrenfest Treatment of Inelastic Scattering and Possible Ways of Resolving them", *J. Chem. Phys.* 146, 224107 (14 pages), 2017.
54. **D. Babikov**[*], "Recombination Reactions as Possible Mechanism of Mass-Independent Fractionation of Sulfur Isotopes in the Archean Atmosphere of Earth", *PNAS* 114, 3062-3067, 2017.
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59. M. Ivanov, **D. Babikov**[*], "On stabilization of scattering resonances in recombination reaction that forms ozone", *J. Chem. Phys.* 144, 154301 (9 pages), 2016.
60. **D. Babikov**[*] and A. Semenov, "Recent Advances in Development and applications of Mixed Quantum/Classical Theory for Inelastic Scattering", feature article (invited), *J. Phys. Chem. A* 120, pp. 319-331, cover art, 2016.
61. A. Semenov and **D. Babikov**[*], "Mixed Quantum/Classical Theory for Molecule-Molecule Inelastic Scattering: Derivations of Equations and Application to $N_2$ + $H_2$ System", invited paper for special issue "50 Years of Chemical Reaction Dynamics", *J. Phys. Chem. A* 119*,* pp. 12329-2338, 2015.
62. A. Semenov and **D. Babikov**[*], "Mixed quantum/classical approach for description of molecular collisions in astrophysical environments", *J. Phys. Chem. Lett.* 6, 1854 (5 pages), 2015.
63. A. Teplukhin and **D. Babikov**[*], "Visualization of Potential Energy Function using Isoenergy Approach and 3D Prototyping" *J. Chem. Educ.* 92, 305 (5 pages), 2015.

64. D. Shyshlov, E. Berrios, M. Gruebele and **D. Babikov**[*], "On Readout of Vibrational Qubits using Quantum Beats", *J. Chem. Phys.* 141, 224306 (7 pages), 2014.

65. A. Teplukhin and **D. Babikov**[*], "Interactive tool for visualization of adiabatic adjustment in APH coordinates for computational studies of vibrational motion and chemical reactions" *Chem. Phys. Let.* 614, 99 (5 pages), 2014.

66. A. Semenov, M.-L. Dubernet and **D. Babikov**[*], "Mixed Quantum/Classical Theory for Inelastic Scattering of Asymmetric-Top-Rotor + Atom in the Body-Fixed Reference Frame and Application to the $H_2O$ + He System", *J. Chem. Phys.* 141, 114304 (9 pages), 2014.

*PUBLISHED AS ASSOCIATE PROFESSOR (25 papers)*

67. M. Ivanov, M.-L. Dubernet and **D. Babikov**[*], "Rotational Quenching of $H_2O$ by He: Mixed Quantum/Classical Theory and Comparison with Quantum Results", *J. Chem. Phys.* 140, 134301 (7 pages), 2014.

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69. A. Semenov and **D. Babikov**[*], "Accurate calculations of rotationally inelastic scattering cross sections using mixed quantum/classical theory", *J. Phys. Chem. Lett.* 5, 275 (4 pages), 2014.

70. A. Semenov and **D. Babikov**[*], "Mixed quantum/classical theory of inelastic scattering in space-fixed and body-fixed reference frames", *J. Chem. Phys.* 139, 174108 (15 pages), 2013.

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76. D. Shyshlov and **D. Babikov**[*], "Complexity and simplicity of OCT pulses shaped for controlling vibrational qubits", *J. Chem. Phys.* 137, 194318 (8 pages), 2012.

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88. X. Cheng, **D. Babikov** and D. M. Schrader, "Binding energy predictions of positrons and atoms", *Phys. Rev. A* 83, 032504 (7 pages), 2011.
89. L. Wang and **D. Babikov**[*], "Adiabatic coherent control in the anharmonic ion trap: Numerical analysis of anharmonicities", *Phys. Rev. A.* 83, 022305 (16 pages), 2011.
90. B. Sivaraman, A. M. Mebel, **D. Babikov**, N. J. Mason[*], and R. I. Kaiser[*], "On the Electron-Induced Isotope Fractionation in Low Temperature $^{32}O_2/^{36}O_2$ Ices – Ozone as a Case Study", *Phys. Chem. Chem. Phys.* 13, pp. 421-427, 2011.
91. **D. Babikov**[*] and B. Kendrick, "The Infrared Spectrum of Cyclic-$N_3$: Theoretical Prediction", *J. Chem. Phys.* 133, 174310 (9 pages), 2010.

*PUBLISHED AS ASSISTANT PROFESSOR (15 papers)*

92. Y. Gu and **D. Babikov**[*], "On the role of vibrational anharmonicities in a two-qubit system", *J. Chem. Phys.* 131, 034306 (11 pages), 2009.

93. L. Jiang and **D. Babikov**[*], "A reduced dimensionality model of ozone: Semi-classical treatment of van der Waals states", *Chem. Phys. Lett.* 474, pp. 273-277, 2009.

94. **D. Babikov**[*] and M. Zhao, Response to Comment on "Anharmonic properties of the vibrational quantum computer", *J. Chem. Phys.* 128, 167102 (3 pages), 2008.

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104. **D. Babikov**[*], B. Kendrick, P. Zhang, and K. Morokuma, "Cyclic-$N_3$: II. Large geometric phase effects in the vibrational spectra", *J. Chem. Phys.* 122, pp. 44315-44335, 2005.

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*PUBLISHED DURING POSTDOCTORAL YEARS (13 papers)*

107. **D. Babikov**, B. K. Kendrick, R. B. Walker and R. T Pack, "Quantum origin of anomalous isotope effect in ozone formation", in *Scientific Reports*, pp. 44-51, edited by C. Guillou and J. Ryder, issued by the *Publication Service of the European Commission*, 2004, Ispra, Italy (EUR 21199 EN).

108. **D. Babikov**[*], "Entrance channel localized states in ozone: possible application to helium nanodroplet isolation spectroscopy", *J. Chem. Phys.* 119, pp. 6554-6559, 2003.

109. **D. Babikov**[*], B. Kendrick, R. B. Walker, and R. T Pack, "Formation of ozone: scattering resonances and anomalous isotope effect", *J. Chem. Phys.*119, pp. 2577-2589, 2003.

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111. **D. Babikov**[*], B. Kendrick, R. B. Walker, R. T Pack, P. Fleurat-Lesard and R. Schinke, "Metastable states of ozone calculated on an accurate potential energy surface", *J. Chem. Phys.* 118, pp. 6298-6308, 2003.

112. V. Sidis, M. Sizun, F. Aguillon, **D. Babikov** and E. A. Gislason, "Theory of collision-induced multi-fragmentation of metal cluster ions", in "*Recent Research Developments in Chemical Physics*" Vol. 3 (2002), pp. 315-350, published by Transworld Research Network, ISBN: 81-7895-066-9.

113. **D. Babikov**[*], R. B. Walker, and R. T Pack, "A quantum symmetry preserving semiclassical method", *J. Chem. Phys*. 117, pp. 8613-8622, 2002.

114. **D. Babikov**[*], E. A. Gislason, M. Sizun, F. Aguillon, V. Sidis, M. Barat, J. C. Brenot, J. A. Fayeton and Y. J. Picard, "Dalitz plot analysis of three-body fragmentation of $Na_3^+$ excited by He impact", *J. Chem. Phys.* 116, pp. 4871-4876, 2002.

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116. E. A. Gislason, **D. Babikov**[*], M. Sizun, F. Aguillon, V. Sidis, M. Barat, J. C. Brenot, J. A. Fayeton and Y. J. Picard, "Distribution of final electronic states following three-body fragmentation of $Na_3^+$ excited by He impact", *Chem. Phys. Let.* 341, pp. 568-574, 2001.

117. **D. Babikov**[*], E. Gislason, M. Sizun, F. Aguillon and V. Sidis, "Fragmentation of $Na_3^+$ clusters by He impact: theoretical analysis of fragmentation mechanisms", *J. Chem. Phys.* 112, pp. 9417-9426, 2000.

118. **D. Babikov**[*], E. Gislason, M. Sizun, F. Aguillon and V. Sidis, "Theory for non-adiabatic multi-channel fragmentation of the $Na_3^+$ cluster ion following a collision with a He atom", *J. Chem. Phys.* 112, pp. 7032-7041, 2000.

119. **D. Babikov**[*], E. Gislason, M. Sizun, F. Aguillon and V. Sidis, "Fragmentation of $Na_3^+$ clusters by He impact: effect of initial cluster temperature on non-adiabatic phenomena", *Chem. Phys. Let.* 316, pp. 129-134, 2000.

*PUBLISHED DURING GRADUATE STUDENT YEARS (6 papers)*

120. **D. Babikov**[*], M. Sizun, F. Aguillon and V. Sidis, "A theoretical description of multi-channel fragmentation of the $Na_3^+$ cluster-ion in collision with a He target", *Chem. Phys. Lett.* 306, pp. 226-232, 1999.

121. M. Barat, J.C. Brenot, H. Dunet, J.A. Fayeton, Y. J. Picard, **D. Babikov**, M. Sizun[*], "Complete analysis of the $Na_3^+$ fragmentation in collision with He atoms", *Chem. Phys. Let.* 306, pp. 233-238, 1999.

122. **D. Babikov***, F. Aguillon, M. Sizun and V. Sidis, "Fragmentation of $Na_2^+$ dimer ion in keV collisions with He: a coupled wave packet study", *Phys. Rev. A* 59, pp. 330-341, 1999.

123. **D. Babikov***, E. E. Son, "Electron emission in glow discharge with liquid electrolytic cathode", *Surface Investigation: X-Ray, Synchrotron and Neutron Techniques*; v.13, no. 9, pp.1127-1133, 1998.

124. **D. Babikov***, E. E. Son, "Electron emission in glow discharge with liquid electrolytic cathode", in Russian, *Poverhnost*, No. 9, p. 47, 1997.

125. **D. Babikov***, "Physical model of cathode region of glow discharge with liquid electrolyte cathode", in Russian, *Fizicheskaya Mysl Rossii*, No. 1, p. 38, 1996.

M.Sc. THESIS: **D. Babikov**, "Electron emission in glow discharge with liquid electrolytic cathode", in Russian, *Thesis*, Moscow Institute of Physics and Technology, June 1995, Moscow, Russia.

DISSERTATION: **Babikov**, "Semi-classical coupled wave packet study of fragmentation of $Na_2^+$ dimer in collision with He atom", in Russian, *Ph.D. Dissertation*, Moscow Institute of Physics and Technology, November 27, 1998, Moscow, Russia.

PATENT: SU 1704059 (M 1283644, G 01 N 27/90, 1987), "Electromagnetic transducer for monitoring conductive products", by Potapova N. F., Kalika B. A., Babikov D. A., Chaplygin V. I. and Babikov A. D.

INVITED TALKS AT CONFERENCES (35 TOTAL):

1. V. Vijay, J. Sahoo, C. Joy, D. Bostan and **D. Babikov** "Physical insight from the mixed quantum/classical simulations of collisional energy transfer" invited talk at the *Quantum Reactive Scattering Conference*, June 22-26, 2026, Gdansk, Poland.
2. **D. Babikov** "Mixed quantum classical theory for rotational state-to-state transitions in $H_2O$ + $H_2$, $H_2O$ + $H_2O$ and $H_2O$ + HCN collisions" Invited talk at the international workshop "*Water in the Universe*", Oléron Island, France, 1-3 October 2025.
3. **D. Babikov** and C. Joy, "Mixed Quantum Classical Theory of Collisional Energy Transfer", invited talk at the *XXIX Dynamics of Molecular Collisions Conference*, July 6–11, 2025, Snowbird, UT.
4. **D. Babikov** "Rigorous testing of mixed quantum/classical theory against full-quantum benchmarks", invited talk at the international workshop "*Physical and Chemical processes of astrophysical interest: Astrochemistry in the JWST era*", Saint Florent, Corsica, June 5-12, 2025.
5. **D. Babikov**, "Quantum Molecular Dynamics on Quantum Computers", invited talk at the *1st Annual NSF ExpandQISE workshop*, Jan. 16-18, 2025, Little Rock, Arkansas.
6. **D. Babikov**, "Recent Progress in Development and Applications of Mixed Quantum/Classical Theory of Molecular Collisions", invited talk at the *Quantum Reactive Scattering Conference*, June 20-24, 2024, Istanbul, Turkey.

7. **D. Babikov**, “Mixed Quantum/Classical Theory Approach to the Dynamics of Molecule-Molecule Collisions in Complex Systems”, *Faraday Discussions, New Direction in Molecular Scattering*, May 8-10, 2024, Edinburgh, UK.
8. **D. Babikov**, “MQCT 2024 – A program for calculations of inelastic scattering of two molecules”, invited talk at *Laboratory Astrophysics: EXPLORE Solar System and Beyond*, Annual NASA Lab Astro, Nov. 30-Dec. 1, 2023, NASA Headquarters, Washington DC.
9. **D. Babikov**, “MQCT – A program for calculations of inelastic scattering of two molecules”, invited talk at the *XXVIII Dynamics of Molecular Collisions Conference*, July 9–14, 2023, Snowbird, Utah.
10. **D. Babikov**, “MQCT – A program for calculations of inelastic scattering of two molecules”, invited talk at the workshop *Chemical Physics Processes of Astrophysical Interest: Towards Detection of New Species*, June 12-15, 2023, Saint Florent, Corsica, France.
11. **D. Babikov**, “MQCT – A program for calculations of inelastic scattering of two molecules”, invited talk at the *Quantum Reactive Scattering Conference*, Aug 4-9, 2022, Balaton, Hungary.
12. **D. Babikov**, “Several levels of theory for description of anomalous isotope effect in ozone”, *ACS 2020 Spring National Meeting*, Apr. 6 (virtual).
13. **D. Babikov**, “MQCT -- A User Ready Program for Calculations of Inelastic Scattering of Two Molecules”, lightning talk at the MolSSI workshop on *Rovibrational Molecular Spectroscopy*, Nov. 14-15, 2019, Blacksburg, Virginia.
14. **D. Babikov**, “Computational Studies of Inelastic Scattering Using Mixed Quantum/Classical Theory”, PI’s talk at the *Annual NASA/NSF Lab-Astro PI Program Review*, Oct. 2, 2019, Washington DC.
15. **D. Babikov**, “Several Levels of Theory for the Description of the Mass-Independent Fractionation of Oxygen Isotopes in the Ozone-Forming Reaction”, invited talk at the *Quantum Reactive Scattering Conference*, July 1-5, 2019, Saitama, Japan.
16. **D. Babikov**, “Several Levels of Theory for Description of Mass-Independent Fractionation of Oxygen Isotopes in the Ozone-Forming Reaction”, *International Symposium on Isotopomers*, March 25-28, 2018, Baton Rouge, LA.
17. **D. Babikov**, “Quantum Reaction Dynamics and Mass-Independent Fractionation in Ozone and Sulfur”, a keynote lecture at the *TSRC workshop on Mass-Independent Fractionation of Sulfur Isotopes -- Possible Molecular Origins*, June 5-10, 2016, Telluride, CO.
18. **D. Babikov**, “Recent Advances in Development and Applications of the Mixed Quantum/Classical Theory”, workshop on *Alternative Methods for Quantum Chemical Dynamics*, May 20-21, 2016, Athens, GA.
19. **D. Babikov**, “Mixed quantum/classical theory for rotationally and vibrationally inelastic scattering”, conference and workshop on *Theory of Gas-Phase Scattering for Astrophysics*, Nov. 23 - Dec. 8, 2015, Garching, Germany.
20. **D. Babikov**, “Mixed quantum/classical theory for rotationally and vibrationally inelastic scattering”, *Computational Chemical Dynamics* (a symposium in honor of Donald Truhlar), ACS National Meeting, March 21-26, 2015, Denver, CO.

21. **D. Babikov**, “Mixed quantum/classical theory for inelastic scattering and collisional energy transfer”, TSRC workshop on *New Challenges for Theory and Chemical Dynamics*, January 13-17, 2014, Telluride, CO.
22. **D. Babikov**, "Mixed quantum/classical theory for collisional energy transfer and ro-vibrational energy flow", hot-topic talk presented at Gordon research conference on “*Molecular Energy Transfer*”, Jan. 13-18, 2013, Ventura, CA, USA.
23. **D. Babikov**, “Mixed quantum/classical theory for the ozone isotope effect*”, International Symposium on Isotopomers*, June 18-22, 2012, Washington, DC.
24. **D. Babikov**, “Mixed quantum-classical theory for the collisional energy transfer and the ro-vibrational energy flow: Application to ozone stabilization”, conference on *Quantum Reactive Scattering* (QRS XI), July 17-21, 2011, Santa Fe, New Mexico.
25. **D. Babikov**, “Quantum theory for description of mass-independent isotope effects in oxygen and sulfur”, a keynote lecture at the conference “*Origins, Carriers, and Implications of Mass-Independent Fractionation of Sulfur Isotopes*” sponsored by NSF and NASA, June 12-14, 2011, Alexandria, Virginia.
26. **D. Babikov**, “Coherent and Optimal Control of Adiabatic Motion of Ions in a Trap”, Symposium at the *PACIFICHEM* meeting, Dec. 15 - 20, 2010, Honolulu, Hawaii, USA.
27. **D. Babikov**, “Quantum origin of anomalous isotope effect in ozone formation”, invited presentation at the *31st Annual Combustion Research Meeting*, US Department of Energy, Office of Basic Energy Sciences, June 1-4, 2010, Warrenton, VA.
28. **D. Babikov**, “Parallelization problem in quantum dynamics”, discussion lead at the *IMA workshop on Chemical Dynamics: Challenges and Approaches*, Jan. 12-16, 2009, Minneapolis, Minnesota.
29. **D. Babikov**, “Anomalous isotope effect in the ozone forming reaction”, *European Conference on Dynamics of Molecular Systems* (MOLEC XVII), August 23-28, 2008, St. Petersburg, Russia.
30. **D. Babikov**, “Quantum origin of anomalous isotope effect in ozone formation”, *symposium on "Quantum and Semi-Classical approaches to Molecular Dynamics*", Great Lakes Regional Meeting of the American Chemical Society, May 31 – June 2, 2006, Milwaukee WI, USA.
31. **D. Babikov**, B. Kendrick, R. B. Walker and R. T Pack, “Anomalous isotope effect in ozone formation: Discovery, hypotheses, explanation”, symposium on "*Chemical Physics in Atmospheric Science*", Fall Meeting of the ACS, August 22-26, 2004, Philadelphia, USA.
32. **D. Babikov**, B. Kendrick, R. B. Walker and R. T Pack, “Quantum origin of anomalous isotope effect in ozone formation”, *The XXth Southwest Theoretical Chemistry Conference*, November 13-15, 2003, Texas Tech University, Lubbock, Texas, USA.
33. **D. Babikov**, B. Kendrick, R. B. Walker and R. T Pack, “Quantum origin of anomalous isotope effect in ozone formation”, plenary lecture at *The Second International Symposium on Isotopomers* (ISI-2003), Nov. 3 - 7, 2003, Stresa, Italy.
34. **D. Babikov**, R. T Pack and R. B. Walker, “Anomalous isotope effects in recombination reactions: a theoretical study with semi-classical Gaussian wave-packets”, invited talk at *The*

*Second Conference on Reaction Kinetics and Atmospheric Chemistry*, June 8-10, 2001, LO-Skolen, Helsingør, Denmark.

35. **D. Babikov**, Y. J. Picard, F. Aguillon, M. Barat, J. C. Brenot, H. Dunet, J. A. Fayeton, V. Sidis and M. Sizun, "Fragmentation of the $Na_3^+$ clusters by He impact: non-adiabatic aspects", *218th ACS National Meeting, Division of Physical Chemistry*, August 22-26, 1999, New Orleans, Louisiana, USA.

INVITED LECTURES AT UNIVERSITIES OR LABS (21 TOTAL):

1. **D. Babikov**, "Recent Advances in Development and Applications of Mixed Quantum Classical Theory of Molecule-Molecule Collisions", invited lecture at the Observatory of Paris-Meudon, Oct. 14, 2025, Meudon, France.
2. **D. Babikov**, "Recent Advances in Development and Applications of Mixed Quantum Classical Theory of Molecule-Molecule Collisions", invited lecture at the University of Rennes, Oct. 6, 2025, Rennes, France.
3. **D. Babikov**, "Quantum Classical Theory of Collisional Transfer of Molecular Rotational-Vibrational Energy", invited lecture at Herzen Pedagogical University, Department of Theoretical Physics and Astronomy (host: Prof Andrey Belyaev), Jan. 31, 2024, St. Petersburg, Russia.
4. **D. Babikov**, "Quantum Classical Theory of Collisional Transfer of Molecular Rotational-Vibrational Energy", invited lecture at St. Petersburg State University, Department of Fluid Dynamics (host: Prof. Elena Kustova), Jan. 24, 2024, St. Petersburg, Russia.
5. **D. Babikov**, "Making Qubits out of Molecules and Studying Molecules Using Qubits", invited lecture at Argonne National Lab, Feb. 24, 2020, Chicago, IL.
6. **D. Babikov**, "From Molecular Quantum Dynamics to Quantum Information in Molecules", invited lecture at Sandia National Lab, Oct. 14, 2019, Livermore, CA.
7. **D. Babikov**, "Quantum and Classical Methods for Molecular Dynamics", invited lecture at the University of Nevada, Nov. 3, 2017, Las Vegas, NV.
8. **D. Babikov**, "Mixed quantum/classical theory of Molecular Collisions: Applications to Ro-Vibrational Inelastic Scattering and Recombination Reactions", invited lecture at Queen's University, Apr. 8, 2016, Kingston, ON, Canada.
9. **D. Babikov**, "Mixed quantum-classical theory for the collisional energy transfer and the ro-vibrational energy flow", invited lecture at the University of Alberta, June 11, 2012, Edmonton, Alberta, Canada.
10. **D. Babikov**, "Mixed Quantum-Classical Approach for Description of Energy Transfer in Recombination Reactions", invited lecture at the Universite Paris-Sud XI, June 7, 2010, Orsay, France.
11. **D. Babikov**, "Mixed Quantum-Classical Approach for Description of Energy Transfer in Recombination Reactions", invited lecture at the Universite Pierre et Marie Curie, June 17, 2010, Paris, France.

12. **D. Babikov**, “Quantum origin of anomalous isotope effect in ozone formation”, invited lecture at University of Wisconsin, Madison, Apr. 19, 2010.
13. **D. Babikov**, “Quantum origin of anomalous isotope effect in ozone formation”, invited lecture at Emory University, Apr. 13, 2009, Atlanta, Georgia.
14. **D. Babikov**, “Quantum origin of anomalous isotope effect in ozone formation”, invited lecture in the University of New Mexico, March 13, 2009, Albuquerque, New Mexico.
15. **D. Babikov**, “Quantum origin of anomalous isotope effect in ozone formation”, invited lecture in the Wayne State University, Oct. 31, 2007, Detroit MI, USA.
16. **D. Babikov**, “Quantum origin of anomalous isotope effect in ozone formation”, invited lecture in the University of Michigan, Nov. 1, 2007, Ann Arbor MI, USA.
17. **D. Babikov**, “Quantum origin of anomalous isotope effect in ozone formation”, invited lecture in the University of Southern California, Jan. 22, 2006, Los Angeles CA, USA.
18. **D. Babikov**, “Quantum origin of anomalous isotope effect in ozone formation”, invited lecture in the Carnegie Institution of Washington, June 19, 2006, Washington DC, USA.
19. **D. Babikov**, “Quantum origin of anomalous isotope effect in ozone formation”, invited lecture in the University of Central Florida, Apr. 16, 2004, Orlando FL, USA.
20. **D. Babikov**, “Quantum origin of anomalous isotope effect in ozone formation”, lecture at the Department of Chemistry, Marquette University, January 22, 2004, Milwaukee, Wisconsin.
21. **D. Babikov**, “Anomalous isotope effect in ozone formation: Discovery, hypothesis, explanation”, invited lecture at the National Atmospheric Chemistry Week, Oct. 19-25, 2003, Union University, Jackson TN, USA.

CONTRIBUTED TALKS (54 TOTAL):

1. T. Kuanysheva, J. Andrade-Plascencia, J. Sahoo, B. Kendrick, and **D. Babikov**, “Grid-Based Quantum Molecular Dynamics on NISQ Quantum Hardware”, a talk presented at *Natural and Engineered Complex Quantum Systems Workshop: From Quantum Chemistry to NISQ Devices*, May 26, 2026, University of Maryland, Baltimore.
2. T. Kuanysheva**,** J. Andrade-Plascencia, J. Sahoo, B. Kendrick and **D. Babikov**, “Grid-Based Quantum Molecular Dynamics on NISQ Devices”, a talk presented at *56th Midwest Theoretical Chemistry Conference*, May 23, 2026, University of Minnesota Twin Cities, Minneapolis, MN.
3. B. Mandal, **D. Babikov**, P.C. Stancil, R.C. Forrey, R.V. Krems and N. Balakrishnan, “Neural network ensemble for computing cross sections for rotational transitions in $H_2O$+$H_2O$ collisions”, DAMOP 2026 meeting of APS, June 1-5, 2026, Providence, Rhode Island.
4. **D. Babikov** and J. Andrade-Plascencia, “Quantum computer implementation of the mixed quantum/classical method for rotationally inelastic molecular collisions”, contributed talk presented at the PACIFICHEM symposium *Fragmentation and Embedded Methods in Quantum Computing*, Honolulu, Dec. 16, 2025.
5. J. Sahoo, J. Andrade-Plascencia, T. Kuanysheva, B. Kendrick and **D. Babikov**, "Simulating electronic nonadiabatic atom-molecule collisions on a quantum computer", contributed talk presented at the *Cold Molecules and Cold Chemistry – Frontiers in Experiments and*

*Theories* workshop, August 4-8, 2025, Telluride, CO.

6. N. Krishna, and **D. Babikov**, "Master Equation Simulations of recombination Kinetics of Ozone Forming Reaction," talk presented at *13th International Conference on Chemical Kinetics*, June 8 - June 13, 2025, Granlibakken, Lake Tahoe, CA.
7. T. Kuanysheva, B. Kendrick, L. Cincio and **D. Babikov**, "Simulating quantum dynamics on classical computers, quantum simulators, and real quantum hardware: A study of free particles, harmonic oscillators, and tunneling", contributed talk presented at the *ACS Spring Meeting*, March 23-27, 2025, San Diego, CA.
8. N. Krishna and **D. Babikov**, "Quantum Mechanical Description of Ozone Formation Rate", contributed talk presented at the *ACS Spring Meeting*, March 23-27, 2025, San Diego, CA.
9. D. Bostan and **D. Babikov**, "Quantum interference effect in the total cross sections of O + $N_2$ system", contributed talk presented at the *53rd Midwest Theoretical Chemistry Conference*, June 1-3, 2023, Purdue University, West Lafayette, IN.
10. Gayday I., **Babikov D.**, Teplukhin A., Kendrick B. K., Mniszewski S., Zhang Y., Tretiak S., Dub P. A., "Classical Trajectory Simulations on Quantum Annealer", *ACS Fall Meeting*, Chicago, IL, Aug. 23, 2022.
11. Gayday I., **Babikov D.**, Teplukhin A., Kendrick B. K., Mniszewski S., Zhang Y., Tretiak S., Dub P. A., "A General Method for Solving Systems of Nonlinear Differential Equations on a Quantum Annealer with Application to Molecular Dynamics", *APS Annual Meeting*, Chicago, IL, March 15, 2022
12. **D. Babikov**, "Recent progress in the mixed quantum/classical calculations of collisional energy transfer between the molecules of astrochemical relevance", ACS 2021 Spring National Meeting, Apr. 7 (virtual).
13. **D. Babikov**, "Several levels of theory for description of anomalous isotope effect in ozone", ACS 2020 Spring National Meeting, Philadelphia, PA (presentation upload).
14. **D. Babikov**, "MQCT studies of collisional excitation and quenching of water molecules", ACS 2020 Spring National Meeting, Philadelphia, PA (presentation upload).
15. P. Liu, J. Liu, C. T. Reinhard, N. J. Planavsky, D. Babikov, K. A. Boering, and J. F. Kasting, "Mid-Proterozoic Atmospheric $O_2$ Levels Re-Calculated From $\Delta^{17}O$ Values in Sulfates Using a Detailed 1-D Photochemical Model", contributed talk at the *Goldschmidt* Conference, Geochemical Society, June 21-26, 2020, Honolulu, Hawaii (presentation upload).
16. I. Gayday and **D. Babikov**, "Analysis of the bound states reveals a possible explanation for the isotope effect in ozone"; contributed talk at the *51st Midwest Theoretical Chemistry Conference*, June 6-8, 2019, University of Notre Dame, IN.
17. **D. Babikov**, "Several Levels of Theory for the Description of Isotope Effects in Ozone", contributed talk at the *50th Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics*, May 27-31, 2019, Milwaukee, Wisconsin, USA.
18. I. Gayday and **D. Babikov**, "Construction and analysis of dimensionally reduced potential energy surface of tetrasulfur and its vibrational states"; contributed talk at the *50th Annual*

*Meeting of the APS Division of Atomic, Molecular and Optical Physics*, Milwaukee, WI, May 27-31, 2019.

19. A. Teplukhin, B. Kendrick and **D. Babikov**, "Calculation of molecular vibrational spectrum on a quantum annealer"; contributed talk at the *50th Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics*, Milwaukee, WI, May 27-31, 2019..
20. E. Grushnikova and **D. Babikov**, "Calculation of scattering resonances in ozone using stabilization method", contributed talk at *50th Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics*, Milwaukee, WI, May 27-31, 2019. Milwaukee, WI, May 27-31, 2019.
21. B. Mandal and **D. Babikov**, "Mixed quantum/classical theory (MQCT) to study inelastic scattering of molecules"; contributed talk at the *50th Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics*, May 27-31, 2019, Milwaukee, WI.
22. I. Gayday and **D. Babikov**, "Analysis of vibrational states of tetrasulfur based on dimensionally reduced potential energy surface"; contributed talk at the *ACS Great Lakes Regional Meeting*, May 1-4, 2019, Sheraton Lisle Naperville Hotel, IL.
23. E. Grushnikova and **D. Babikov**, "Calculation of scattering resonances in ozone using stabilization method (progress report)" contributed talk at *Great Lakes ACS Regional Meeting*, May 1-4, 2019, Lisle, IL.
24. B. Mandal and **D. Babikov**, "Mixed quantum/classical study of symmetry-driven isotope effects in the recombination reactions: application to $S_2^*$ + Ar energy transfer"; contributed talk at the *ACS Great Lakes Regional Meeting*, May 1-4, 2019, Sheraton Lisle Naperville Hotel, IL.
25. **D. Babikov**, "Properties of Feshbach and shape resonances in ozone-forming reaction and their influence on mass-independent isotope effect", Faraday Discussions Quantum effects in Small Molecular Systems --, Sept. 10-12, 2018, Edinburgh, UK.
26. A. Teplukhin, B. Kendrick and **D Babikov**; "Several levels of theory for description of ozone-forming reaction", contributed talk at the ACS National Meeting Aug 19-23, 2018, Boston, MA.
27. **D. Babikov**, "Mixed Quantum/Classical Theory of Molecular Collisions: Applications to Rotational-Vibrational Inelastic Scattering in Astrophysical Environments", talk at the ACS National Meeting, March 18-22, 2018, New Orleans, LA.
28. C. E. Harman, A. A. Pavlov, **D. Babikov**, J. F. Kasting, "Chain Formation as a Mechanism for Mass-Independent Fractionation of Sulfur Isotopes in the Archean Atmosphere" Goldschmidt-2017 (annual, international conference on geochemistry and related subjects), Aug. 13-18, 2017, Paris, France.
29. **D. Babikov**, "Mixed Quantum/Classical Theory of Rotationally and Vibrationally Inelastic Scattering", contributed talk at the Quantum Reactive Scattering Conference (within ICCSA), July 3-6, 2017, Trieste, Italy.
30. Teplukhin A. and **D Babikov**; "Accurate calculation and detailed analysis of highly excited vibrational states of ozone", contributed talk at the 49th Midwest Theoretical Chemistry Conference, June 1-3, 2017, Michigan State University, East Lansing, MI.

31. Teplukhin A. and **D Babikov**; “Quantum mechanical study of ozone recombination”, contributed talk at the 10th International Conference on Chemical Kinetics, May 21-25, 2017, University of Illinois at Chicago, Chicago, IL.
32. Teplukhin A. and **D Babikov**; “Full-dimensional model of ozone forming reaction: Absolute value of recombination rate coefficient, its pressure and temperature dependencies”, contributed talk at the *ACS National Meeting*, August 21-25, 2016, Philadelphia, PA.
33. A. Semenov and **D. Babikov**, "Mixed Quantum/Classical Theory (MQCT) for Rotationally and Vibrationally Inelastic Scattering", contributed talk presented at 63rd Pacific Conference on Spectroscopy and Dynamics, Jan. 2016, Asilomar Conference Grounds, Monterey, CA, USA.
34. **D. Babikov**, “Mixed quantum/classical treatment of the ozone forming reaction”, symposium on New Insights from Quantum Dynamics and ab initio Potentials in High Dimensional Systems, PACIFICHEM (international conference), Dec. 14 - 20, 2015, Honolulu, HI.
35. **D. Babikov**, “Mixed quantum/classical theory for rotationally and vibrationally inelastic scattering”, symposium on Advances in Quantum Dynamics from Spectroscopy to Reactions, PACIFICHEM (international conference), Dec. 14 - 20, 2015, Honolulu, HI.
36. A. Teplukhin and **D. Babikov**, "New software for visualization of hyper-spherical coordinates and for 3D-printing of potential energy surfaces: Application to ozone molecule". Contributed talk presented at Midwest Theoretical Chemistry Conference, June 26-28, 2015, University of Michigan, Ann Arbor, MI, USA.
37. D. Shyshlov and **D. Babikov**, "Computational study of cold ions trapped in a double-well potential", contributed talk presented at Midwest Theoretical Chemistry Conference, June 26-28, 2015, University of Michigan, Ann Arbor, MI, USA.
38. D. Shyshlov and **D. Babikov**, "On Readout of Vibrational Qubits using Quantum Beats", contributed talk presented at APS March meeting, March 2-6, 2015, San Antonio, TX, USA.
39. D. Shyshlov and **D. Babikov**, "High-fidelity transformations of the vibrational qubits in thiophosgene molecule", contributed talk presented at Midwest Theoretical Chemistry Conference, June 15-17, 2014, Evanston, IL, USA.
40. D. Shyshlov and **D. Babikov**, ″High-fidelity transformations of the vibrational qubits in thiophosgene molecule″, contributed talk at the American Physical Society meeting, March 2-7, 2014, Denver, CO, USA.
41. M. V. Ivanov and **D. Babikov**, "Collisional energy transfer in the ozone forming recombination reaction", oral presentation at the "Midwest Theoretical Chemistry Conference", June 7-9, 2012, Madison, WI, USA
42. **D. Babikov**, “Coherent and Optimal Control of Adiabatic Motion of Ions in a Trap”, oral presentation at the National ACS meeting, Mar. 28 - 31, 2011, Anaheim, California, USA.
43. M. Ivanov and **D. Babikov** "Collisional energy transfer in the ozone forming recombination reaction", oral presentation at the Workshop “Spectroscopy and Dynamics of Ozone and Related Atmospheric Species” October 3-5, 2011, Reims, France.

44. M. Ayouz and **D. Babikov**, “Improved Potential Energy Surface of Ozone Constructed Using the Fitting by Permutationally Invariant Polynomial Function”, oral presentation at workshop on "Spectroscopy and Dynamics of Ozone and Related Atmospheric Species”, October 3-5, 2011, Reims, France.

45. **D. Babikov**, “Semi-classical approach to anomalous isotope effect in ozone forming reaction”, oral presentation at the National ASC Meeting, Apr. 6-11, 2008, New Orleans, Louisiana.

46. J. Barber, R. D. Averitt, D. J. Funk, D. E. Hooks, **D. Babikov**, A. J. Taylor, “Temperature-Dependent Terahertz Spectroscopy of Single Crystals of Energetic Materials”, Gordon Research Conference on EMs.

47. V. Sidis, M. Sizun, F. Aguillon, **D. Babikov** and E. A. Gislason, “The fragmentation of $Na_n^+$ cluster ions by He impact”, invited talk at the European Conference on Dynamics of Molecular Collisions (MOLEC XIV), Aug. 31 – Sept. 6, 2002, Koç University, Istanbul, Turkey.

48. M. Barat, J. C. Brenot, J. A. Fayeton, Y. J. Picard, F. Aguillon, **D. Babikov**, E. A. Gislason, V. Sidis, M. Sizun, “Experimental and theoretical analysis of collision induced fragmentation of ionic metallic clusters“, XIX$^{th}$ International Symposium on Molecular Beams, June 2001, Rom, Italy.

49. E. A. Gislason, **D. Babikov**, M. Sizun, F. Aguillon, V. Sidis, M. Barat, J. C. Brenot, J. A. Fayeton, Y. J. Picard, “First determination of final electronic states following three-body fragmentation of $Na_3^+$ excited by He impact”, Conference on Dynamical Aspects of Atomic and Molecular Systems (DYNAM 2000), May 31 - June 3, 2000, Arcachon, France.

50. **D. Babikov**, E. A. Gislason, M. Sizun, F. Aguillon and V. Sidis, “Theoretical analysis of pathways for fragmentation of the $Na_3^+$ cluster-ion in a non-adiabatic collision with He”, XVII$^{th}$ Conference on the Dynamics of Molecular Collisions, July 18-23, 1999, Lake Harmony, Pennsylvania.

51. **D. Babikov** “Semi-classical study of dissociation of $Na_2^+$ dimer in collision with He atom”, XLI$^{th}$ Scientific Conference of Moscow Institute of Physics and Technology, November 27-28, 1998, Moscow, Russia.

52. **D. Babikov**, F. Aguillon, M. Sizun and V. Sidis, “Coupled wave packet study of collision induced fragmentation of small sodium clusters”, XII$^{th}$ European Conference on Dynamics of Molecular Collisions (MOLEC), September 6-11, 1998, Bristol, UK.

53. **D. Babikov**, F. Aguillon, M. Sizun and V. Sidis, “The collision induced fragmentation of small sodium clusters”, VI$^{th}$ EPS Conference on Atomic and Molecular Physics (ECAMP), July 14-18, 1998, Siena, Italy.

54. **D. Babikov**, “Physical model of glow discharge with liquid cathode”, talk at The 3rd World Scientific Conference “International Workshop on Advanced Electronics Technology”, November 1995, Moscow, Russia.