Neepa T. Maitra

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a. Educational and Professional Background

University of Otago, New Zealand	Physics	BSc 1993
Harvard University	Physics	Ph.D 1998
UC Berkeley	Semiclassical dynamics postdoctoral fellow	1998-1999
Rutgers University	Density functional theory postdoctoral fellow	1999-2003

b. Positions

Sep 2003-Dec 2003	Visiting Scholar, Dept. of Physics, University of Otago, New Zealand
Jan 2004-Jan 2009	Assistant Professor, Dept. of Physics and Astronomy, Hunter College Doctoral Faculty Member, Graduate Center CUNY
Jan 2009-Aug 2015	Associate Professor, Dept. of Physics and Astronomy, Hunter College CUNY Doctoral Faculty Member, Graduate Center CUNY
Aug 2015-Jun 2019	Professor, Dept. of Physics and Astronomy, Hunter College CUNY Doctoral Faculty Member, Graduate Center CUNY
Sep 2019–present	Professor, Dept. of Physics, Rutgers University at Newark
July 2021– July 2024	Chair, Dept. of Physics, Rutgers University at Newark

c. Research Interests and Publications Summary

• Time-Dependent density functional theory (TDDFT); Excitations and dynamics in molecular systems and solids; Photo-induced correlated electron-ion dynamics in molecules; Classical and quantized light-matter interactions; Semiclassical methods

• 95 papers in refereed journals, 7 invited book chapters, 1 co-edited book; Full list is in Section j.

d. Honors or Awards

• American Physical Society Fellow (2024)

• Cottrell Scholar of Research Corporation for Science Advancement (2007)

• National Science Foundation CAREER Award (2006)

e. Teaching and Educational Involvement

Since joining Rutgers Fall 2019

• Instructor for graduate course Physics 780: Quantum Mechanics 3 (Interacting Electrons), Spring 2020. Designed the course, mentored students, gave lectures, and graded homework.

• Instructor for undergraduate course Physics 404: Quantum Mechanics, Fall 2020. Designed the course, mentored students, gave lectures, and graded homework, quizzes, and exams.
• Instructor for graduate course Physics 631 (later renamed 532): Graduate Quantum Mechanics, Spring 2021, 2022, 2023, 2024, 2025. Designed the course, gave lectures, mentored students, and graded homework, quizzes, and exams.
• Instructor for graduate course Physics 611: Special Topics In Physics (Theoretical; Density Functional Theory). Co-taught with Prof. Michele Pavanello. Designed half the lectures, taught and led the discussions, mentored students.
• Instructor for undergraduate course Physics 333: Applications of Math in Physics, Fall 2024, 2025. Designed the course, gave lectures, mentored students, graded homeworks, quizzes, exams.
• Preparer and Grader of Quantum Mechanics PhD Qualifying Exam (Spring 2020 – present): write exam, help students prepare, grade exam.

• Mentor of undergraduate students:
(i) Dhyey Ray (Summer 2024 – present)
(ii)Arian Vosoughinia (Spring and Summer 2020)
(iii) Phillip Martinez (Hunter College, Spring 2019 – Spring 2021)
(iv) Bart Rosenzweig (Hunter College, Spring 2019 – Summer 2021)
(v) Thomas Pender (NJIT, Spring 2023)

• Advisor of graduate students:
(i) Osman Yigit (PhD student, Fall 2025 – present)
(ii) Lynh Belousov (PhD student, Spring 2025 – present)
(iii) Anthony deMelfi (PhD student, Summer 2025)
(iv) Anna Baranova (PhD student, Fall 2023 – present)
(v) Anton Rikus (visiting MS student from Münster, Spring 2023)
(vi) Evaristo Villaseco Arribas (PhD student, Summer 2020 – Spring 2025)
(vii) Davood Dar (PhD student, Fall 2019 – Spring 2025)
(viii) Tiffany Oliveria (PhD student, Fall 2020 – Spring 2021)
(ix) Norah Hoffmann (PhD student at MPI-Hamburg, co-advisor with Angel Rubio, Spring 2018–Summer 2020)

• Mentor of postdoctoral fellows:
(i) Dr. Jack Taylor (April 2025 – present)
(ii) Dr. Lucien Dupuy (Jan 2023 – Jan 2025)
(iii) Dr. Paul Abanador (Jan 2022 – May 2022)
(iv) Dr. Saswata Roy (Nov. 2021 – April 2023)
(v) Dr. Patricia Vindel Zandbergen (Oct. 2019 – Jun 2021)
(vi) Dr. Lionel Lacombe (Jan. 2017 – Aug. 2021)

• Organizer of Pre-Meeting Tutorial on Density Functional Theory at the 2020 and 2021 APS March Meeting, Denver, CO; Lecturer at this Pre-Meeting Tutorial at the 2025 Global Physics Summit, Anaheim, CA.

• Invited Lecturer for the 6th Virtual Winter School on Computational Chemistry, Feb 17–20, 2020.

• Lead organizer of tutoring program initiative for Newark Public High School physics students, Spring 2021.

• Co-organizer of Graduate Student Seminar Series in (TD)DFT Development, with Dr. Lionel Lacombe, Summer 2021.

• Co-organizer of and Lecturer at the 9th International School and Workshop in TDDFT in Benasque, Spain, October 2022; Lecturer (remotely) at the 10th International School and Workshop of this, April 2025.

• Co-organizer of and Lecturer at the 3rd US-based School and Workshop on TDDFT, Rutgers University at Newark, June 28-July 8, 2023.

• Mentor of summer high school students:
(i) Devin Lopez (Science Park High School, Newark), Summer 2025
(ii) Gabriella de Jesus (Science Park High School, Newark), Summer 2025
(iii) Amando Sosa (Science Park High School, Newark), Summer 2024.
(iv) Luc Reyes (Union County Magnet High school, Summer 2024
(v) Nicole Ogutu (Malcolm X Shabazz High School, Newark), Summer 2023.
(vi) Gali Avni (Union County Magnet High School), Summer 2023.

• Organizer of activities for 2023 and 2024 summer high school cohort in Physics Department (about 9 students each year from Newark Public Schools and Union County Magnet High).

• External Ph.D. committee member for: Yorick Schmerwitz (and opponent, University of Iceland, Reykjavik, Iceland, Sep. 2024), Filip Cernatic (and rapporteur, Strasbourg, France, Sep 2023), Sajanthan Sekaran (Strasboug, France, Sep. 2022), Ayoub Aouina (and rapporteur, Ecole Polytechnique, France, Feb. 2022), Nian Liu (NJIT, Aug. 2022), Nengyi Huang (NJIT, Aug. 2020).

• Local PhD committee or candidacy member for Rutgers-Newark students: Shuo Tao, Valeria Rios-Vargas, Jessica Martinez, Tim Nguyen, Rishi Rao, Guanghui Su

Prior to joining Rutgers Fall 2019

• Instructor for undergraduate courses in physics at Hunter College of CUNY. Designed each course, gave lectures, graded homework, quizzes, and exams:
(i) Physics 111 (Mechanics, Heat and Sound), Spring 2004, Spring 2005, Spring 2017.

(ii) Physics 121 (Electricity, Magnetism, Light and Quantum Physics), Fall 2004.

(iii) Physics 101/100 (Basic Concepts of Physics), Fall 2005, 2006, and 2008, Spring 2009, Fall 2009 and 2011, Spring 2012, 2013, 2014, and 2015, Fall 2015 and 2016

(iv) Physics 425/625 (Quantum Theory), Spring 2007.

(v) Physics 415 (Introduction to Electromagnetic Theory I), Fall 2007.

(vi) Physics 416 (Introduction to Electromagnetic Theory II), Spring 2008.

(vii) Physics 445/645 (Introduction to Solid State Physics), Fall 2014.

(viii) Physics 342 (Optics), Spring 2016.

(ix) Physics 330 (Atomic and Nuclear Physics), Fall 2018

• Instructor for doctoral courses at the Graduate Center CUNY. Designed the course, gave lectures and graded homework:
(i) Physics 852 (Density Functional Theory and Applications), Spring 2010.

(ii) Physics 845 (Quantum Theory of Solids I), Fall 2012, Fall 2013, and Spring 2019.

• Implemented Eric Mazur's "Peer Instruction" methods in undergraduate course "Basic Concepts of Physics" at Hunter College, via clickers.

• Gave college-wide presentations in 2010 and 2012 on enhancing engagement and learning in large undergraduate science classes.

• Mentored undergraduate students (positions afterwards indicated): Izabela Raczkowska (PhD student at NYU from Fall 10), Gabriella Mullady (MA student in math from Fall09, Hunter), Sharma Goldson (MA student in math from Fall 10), Chris Canahui (continuing Hunter physics major), Allen Kamal (MA student in physics from Fall 09), David Tempel (PhD student at Harvard from Fall 07), August Krueger (PhD student at Rutgers from Fall 08), Matt Olim (software programmer), Samuel Schiffman-Ackerman (PhD student in math Penn State U), Greg Dreifus (PhD program in mechanical engineering at MIT), Maria Williams (current physics undergraduate), Gui Zhen Lu (current physics BA/MA), Stephen Crisostomo (current physics and math BA), Bart Rosenzweig (current physics), Phillip Martinez (current physics), Panagiotis Anastasiou (current physics) Nine of these students are from ethnic and gender groups that are underrepresented in science.

• Advised graduate students:
(i) Dr. Arun Rajam, PhD student, Fall 2006 – Spring 2010; thesis title "Phase-Space Explorations in Time-Dependent Density Functional Theory"; now assistant professor of physics at St John's University, New York.
(ii) Kai Luo, PhD student, Fall 2012 – Spring 2015; thesis title "Exploring Non-Equilibrium Dynamics in Time Dependent Density Functional Theory"; now postdoctoral fellow in Sam Trickey's

group at University of Florida.
(iii) Enxi Yu, PhD student, Fall 2017 – Spring 2018; on leave of absence
(iv) Norah Hoffmann, PhD student, co-advising with Angel Rubio MPI-Hamburg, May 2017 – present;
(v) Christian Gaun, MA student, Spring 2007 – Fall 2009, now in finance; studied numerical methods to propagate Schrödinger's equation for electrons in strong-fields.
(vi) Ernesto Sandoval, MA student, Jan 2013 – Spring 2015; thesis "Studies in Time-Dependent Density Functional Theory"; now in physics PhD program SUNY Binghamton.

• Advised postdoctoral scholars:
(i) Dr. Harshani Wijewardane, Aug 2007 – Jul 2009, now professor at Rajarata University, Sri Lanka
(ii) Dr. Zenaida Shields, Jun 2009 – Oct 2009, now independent consultant and researcher, Connecticut
(iii) Dr. Peter Elliott, Jan 2010 – Oct 2012, now postdoc at MPI-Halle, Germany
(iv) Dr. Johanna Fuks, Mar 2013 – April 2017, now Investigator at Dept of Physics University of Buenos Aires, Argentina
(v) Dr. Ali Abedi, Oct 2014–Jan 2015, now postdoc at DIPC San Sebastian
(vi) Dr. Elham Khosravi, Oct 2014–Jan 2015, now postdoc at DIPC San Sebastian
(vii) Dr. Graeme Gossel, Oct 2016 – Sep 2018
(viii) Dr. Lionel Lacombe, Jan. 2017 – Sep. 2021

• Regular (annual) speaker at the SCI-200 class for MARC program (Maximizing Access to Research Careers) for groups under-represented in the sciences.

• Developed CUNY Pathways Common Core Courses, PHYS 100 and 101, Spring 2012.

• Advised Hunter College Physics Club (organized alumni visits, visits to nearby graduate schools, mentoring), 2007–2010.

• Presented Pre-Meeting Tutorial on TDDFT at American Physical Society March Meeting 2008, 2010, 2012, 2016, and 2018, and organized this at the 2014 meeting

• Presented two Lectures on "Advanced TDDFT" at the 3rd, 4th, 5th, and 6th International School in TDDFT, Benasque, Spain in 2008, 2010, 2012, 2014, and 2016. These were for an audience largely of graduate students and postdoctoral fellows.

• Presented three Lectures and Re-work Sessions on TDDFT at the 3rd Cold Collisions IRTG School in Brand, Austria, in 2018.

• Co-organized and presented lectures at 1st and 2nd US-based TDDFT School in Telluride, CO, July 2017, and Rutgers University, NJ, Aug 2019; audience of graduate students and postdoctoral fellows.

• External PhD. committee member for David Tempel (PhD Harvard, April 2012), Klaas Giesbertz (PhD Vreie Universiteit Amsterdam, November 2010), Martins Brics (Rostock, Germany, November 2016), Daniel Kidd (PhD Vanderbilt University 2018), Alessandro Genova (PhD Rutgers University, 2018)

f. Grant Support for Research

Current

• *Moving Electrons through Space and Time: Enabling the Quantum Dynamics of Chirality-Induced Spin Selection Through Novel and Scalable Computational Methods*, co-PI with PI Christine Isborn (U.C. Merced), U.S. Department of Energy, 09/01/2025 - 08/31/2029, $856,995 (amount for Rutgers-Newark)

• *Dynamics of Coupled Electrons, Nuclei, and Photons from First Principles: Electronic Embedding, Exact Factorization Couplings, and Efficient Software Development*, with co-PI Michele Pavanello, U.S. Department of Energy, 08/01/2023 – 07/31/2026, $1,048,212 (total).

• *Molecules in Classical and Quantized Fields: Developing Time-dependent Density Functional and Exact Factorization Methods for Electrons, Ions, and Photons*, U.S. National Science Foundation, 05/01/2022 – 04/30/2025, $460,884.

Past

• *Chemistry at Solutions and Interfaces Center Grant*, multi-PI grant with Head PI Roberto Car, U.S. Department of Energy, 09/30/2022 – 09/29/2025, $297,000.

• *Electron-Ion Dynamics with Time-Dependent Density Functional Theory: Towards Predictive Solar Cell Modeling*, US Department of Energy, 06/01/2019 – 05/31/2022, with NEC till 05/31/2023 $376,716

• *Chemistry at Solutions and Interfaces Center Grant*, multi-PI grant with Head PI Roberto Car, US Department of Energy, 09/30/2018 – 09/29/2022, $297,500.

• *Molecules in Classical and Quantized Fields: Improving Time-Dependent Density Functional Approximations and Electron-Ion Correlation Methods* , US National Science Foundation, 09/01/2019 – 08/31/2022, $434,389.

Prior to joining Rutgers

• *Building a New Paradigm for Coupled Electron-ÂIon Dynamics via the Exact-Factorization Approach*, Research Corporation Cottrell Scholar Seed Award, 01/11/2017–31/10/2019, $50,000.

• *Electron-Ion Dynamics with Time-Dependent Density Functional Theory: Towards Predictive Solar Cell Modeling*, US Department of Energy, 02/01/2016 – 01/31/2019, $377,000.

• *Molecules in Non-Perturbative Fields: Improving Time-Dependent Density Functional Approximations and Electron-Ion Correlation Methods* , US National Science Foundation, 04/01/2016 – 03/31/2019, $417,412.

• *Support of Summer School and Workshop Focused on Theory and Applications of Time-Dependent Density Functional Theory*, Research Corporation for Science Advancement, 09/01/2016 – 08/31/2017, $5,000; 07/01/2019 – 09/01/2019 $2,500.

• *Support of a Summer School and Workshop Focused on Theory and Applications of Time-Dependent Density Functional Theory*, US Department of Energy, 09/01/2016 – 08/31/2017, $10,500.

• *Electron-Ion Dynamics with Time-Dependent Density Functional Theory: Towards Predictive Solar Cell Modeling*, US Department of Energy, 10/01/2012 – 01/31/2016, $358,953.

• *Extending the Usefulness of Time-Dependent Density Functional Theory: Dynamics, Excitations, and*

Coupling to Ions, U.S. National Science Foundation, 02/01/2012 – 01/31/2016, $411,981.

• *2013 Time-Dependent Density-Functional Theory Gordon Research Conference and Gordon Research Seminar, August 10-16, 2013.*, 06/01/2013 –05/31/2014, $8000.

• *Strong-Field Dynamics of Atoms and Molecules in Time-Dependent Density Functional Theory: A Phase-Space Exploration*, Research Foundation Cottrell Scholar Award, 07/01/2007–06/30/2010, $100,000.

• *Time-Dependent Density Functional Theory of Atoms, Molecules, and Quantum Dots*, US National Science Foundation CAREER Award, 05/01/2006 – 04/30/2011, $536,584.

• *Excitations and Response Properties in Time-Dependent Current-Density Functional Theory*, Petroleum Research Foundation (Type G), 09/01/2004 – 08/31/2006, $35,000.

• *Studies in Time-Dependent Density Functional Theory*, Hunter College Gender Equity Program, Fellow 06/2005 – 05/2007, $17,050.

• *Double Excitations in Time-Dependent Density Functional Theory*, Research Foundation of CUNY, 06/2004– 05/2005, $4,500.

g. Invited Talks

• Over 50 invited talks at workshops, conferences, or universities since joining Rutgers-Newark in Fall 2019. Please see list appended in Section k.

h. Conferences and Symposia Organized

Since joining Rutgers Fall 2019

• Co-organizer of national and international Graduate Student Seminar Series in (TD)DFT Development, with Dr. Lionel Lacombe, weekly online zoom series, Summer 2021.

• Co-organizer of Focus Session Symposium "Density Functional Theory and Beyond" at the American Physical Society March Meeting, with Kieron Burke, in Chicago IL, March 2020 (covid-cancelled) and 2022.

• Co-organizer of the 9th International School and Workshop in TDDFT in Benasque, with Alberto Castro, Hardy Gross, Angel Rubio, in Benasque, Spain, October 2022.

• Co-organizer of 3rd US-based School and Workshop on TDDFT, with Michele Pavanello, Christine Isborn, Adam Wasserman, Andre Schleife, and Carsten Ullrich, at Rutgers University at Newark, June 28-July 8, 2023.

• Organizer of Mini-Workshop on Photo-Induced Molecular Dynamics: Experiment, Theory, and Computational Modeling; with speakers from Stony Brook, U. Conn, Temple, Haverford, and Rutgers, at Rutgers-Newark, May 16, 2025.

Prior to joining Rutgers Fall 2019

• Co-organizer of 1st US-based School and Workshop on TDDFT with Christine Isborn and Andre Schleife, Telluride CO, July 2017; and 2nd iteration together with Michele Pavanello, Rutgers University Inn, August 2019.

• Co-organizer of Telluride Science Research Center workshop on Excited States and Dynamics, with Christine Isborn, at Telluride CO, July 2015.

• Organizer of CUNY-wide mini-workshops at the Graduate Center, every year since 2012, with internationally recognized scientists. The most recent include *A Celebration of the Works of Mel Levy* (May 2017) with 16 leaders in DFT speaking, and *Quantum and Classical Light-Matter Interactions* Nov 2018.

• Co-organizer of Focus Session on "Recent Advances in Density Functional Theory and Applications in Chemical Physics" at the American Physical Society March Meeting 2016, with Don Truhlar and John Perdew, Baltimore MD, Mar 2016.

• Chair of the 2013 Gordon Research Conference on TDDFT, with co-Chair Hardy Gross, at University of Biddeford, Maine, August 2013.

• Co-organizer of CECAM workshop "Density Functional Theory: Learning from the past, looking to the future", with Stefan Kurth, Sangeeta Sharma, Carsten Ullrich, Antonio Sanna, and Attila Cangi, Berlin, July 2013.

• Co-organizer of "Density Functional Theory for Chemical Physics" Symposium at the American Physical Society Meeting, with Kieron Burke, Boston, Feb 26–Mar 1, 2012.

• Co-organizer of CECAM workshop "How to Reduce Empiricism and Speed Up Accuracy in Density Functional Theory", with Kieron Burke, Adam Wasserman, Hardy Gross, Dublin, June 20–25, 2011.

• Co-organizer of a Symposium on Density Functional Theory at the American Physical Society Meeting, New Orleans, LA, March 2008.

i. Service to the University

Since joining Rutgers Fall 2019

• Member of:

- Arts and Sciences Promotions Committee, Spring 2020 – Spring 2021, Spring 2024 – present.

- General Education Committee, Fall 2022 – present

- LSC II Space Renovation Committee, representing Makerspace, Fall 2023 – present

- Department Search Committee for the experimental physics hire, Fall 2019 – Spring 2020

- Department Reappointment Committee for Teaching Laboratory Instructor Muhammed Acikgoz, Spring 2020; Teaching Professor Diane Jammula, Spring 2020; Assistant Professor Claudiu Stan Spring 2021

• Chair, Department of Physics, July 2021 – present; Major activities included:

- Managed the faculty reappointments, tenure & promotion, as listed below

- Mentored tenure-track assistant professors Claudiu Stan, Li Zhu, Xuejian Wu (met to discuss progress towards tenure and any concerns regarding teaching and research, advised strategies for applying/securing grants and visibility); and non-tenure faculty Diane Jammula and her teaching team (met to discuss and advise how department could best support her pedagogical research

and writing, such as with summer funding, and feedback on internal and external funding applications)

- Hired and helped train department administrative coordinator

- Made efforts to collaborate with RU-New Brunswick for quantum information science strategic hire

- Helped build department community through events such as undergraduate research day and end-of-semester get-togethers.

• Graduate Advisor, Department of Physics July 2021 – August 2022; met with incoming and present graduate students each year to discuss their course plan for the year and any concerns.

• Chair of Department Committees for:

- Reappointment of Associate Teaching Professor Diane Jammula Spring 2022; Assistant Teaching Professor Sheehan Ahmed Spring 2022; Teaching Instructor Joshua Rutberg Spring 2022

- Tenure and Promotion Committee for: Assistant Professor Claudiu Stan Fall 2023

- Lecturer Advancement for Dr. Estelle Epstein Fall 2023.

- Reappointment for Tenure-Track Assistant Professor Li Zhu Spring 2024

• Coordinator of the High School Summer Research Program in Physics at RU-N, with particular outreach to Newark Public Schools, Summer 2023 and 2024, and co-coordinator with Diane Jammula, Devin Mejias, Jeannette Ng, for Summer 2025

• Reviewer of 2025 Packard Fellowships for Science and Engineering for RU Internal Selection

Prior to joining Rutgers Fall 2019

• Department Undergraduate Advisor Fall 2018–Summer 2019.

• Member of Search Committee for Doctoral Lecturer position and experimental physics positions, 2015–2017

• Department Seminar Organizer Fall 2004–Spring 2007

• Department Graduate Advisor (MA and PhD programs), Fall 2008–Fall 2016

• Member of Hunter College's Pre-Professional Committee, Spring 2005

• Member of Hunter College's Curriculum Committee, Fall 2005 – Fall 2006

• Member of Senate Committee on General Education Requirements, Fall 2011–present.

• Member of Committee on Hunter College School of Arts and Sciences Strategic Plan Implementation, Fall 2013 – Spring 2014.

j. Professional Service outside the College

• Member of Award Committee for Psi-k Collaborating Early-Career Investigators (CECI) Award, 2025.

• Associate Editor: Nature Partner Journal Computational Materials, 2020 – present

• Specialist Editor: Computer Physics Communications, 2018 – present

• Editorial Advisory Board of Journal of Chemical Physics, 2021– 2024.

• Top Reviewer for Journal of Chemical Physics 2019.

• Member-at-Large (elected) of the APS DCOMP (Division of Computational Physics), 2025 – present

• Member of Scientific Advisory Board of Trieste series of meetings on Total Energies and Forces, Feb. 2023 – present.

• Member of Scientific Advisory Committee for the XV Conference for Young Researchers in Atomic and Molecular Physics, Valencia Spain, Spring 2024.

• Member of International Advisory Board of Psi-K 2020.

• Member of Scientific Advisory Board for the DOE-funded FLOSIC Center 2017 – 2021

• Advisory Panel for US-Africa Initiative for Electronic Structure, and host of scientist Steve Ndengué, Summer 2022

• Referee for journals: Physical Review (Letters, A, B, X), Journal of Chemical Physics, Physical Chemistry Chemical Physics, Journal of Chemical Theory and Computation, ACS Nano, NanoLetters, Journal of Physical Chemistry Letters, Journal of Computational Physics, Chemical Physics, International Journal of Modern Physics, International Journal of Quantum Chemistry, European Physical Journal, Molecular Physics, New Journal of Physics, Proceedings of the National Academy of Sciences.

• Referee and panel member for Funding Agencies: National Science Foundation, U.S. Department of Energy, American Chemical Society Petroleum Research Fund, Israel Science Foundation, Natural Sciences and Engineering Research Council of Canada, Ikerbasque Researchers' Assessment (Spain), Swiss National Foundation, Netherlands Organisation for Scientific Research, Leibniz Programme for Women Professors

• Organizer of several national and international research workshops and conferences, as listed in section g.

• Coordinator of Host Institute role for Rutgers-Newark for the Research Corporation for Science Advancement Fellows Program, 2025-2026, to help postdoctoral fellows prepare for faculty interviews through mock interviews, feedback on research statements, mentoring.

k. Full List of Publications

Co-edited book

Fundamentals of Time-Dependent Density Functional Theory, (Lecture Notes in Physics vol. 837), eds. M. A. L. Marques, N. T. Maitra, F. M. S. Nogueira, E. K. U. Gross, A. Rubio (Springer-Verlag, Berlin Heidelberg, 2012).

Peer-Reviewed Publications

An asterix * indicates Maitra and her research group as lead authors.

In reverse chronological order:

(95 *Excited State Densities from Time-Dependent Density Functional Response Theory**, A. Baranova and N. T. Maitra, J. Chem. Theory and Comput. **21**, 10437 (2025)

(94) *A Perspective on Many-Body Methods for Molecular Polaritonic Systems*, N. Baumann et al., J. Chem. Theory and Comput. **21**, 10035 (2025).

(93) *Roadmap for Molecular Benchmarks in Nonadiabatic Dynamics*, L.E. Cigrang et al., J. Phys. Chem. A **129**, 7023 (2025).

(92) *Capturing the elusive curve-crossing in low-lying states of butadiene with dressed TDDFT**, D.B. Dar, and N. T. Maitra, J. Phys. Chem. Lett. **16**, 703 (2025).

(91) *Electronic Coherences in Molecules: The Projected Nuclear Quantum Momentum as a Hidden Agent*, E. Villaseco Arribas and N. T. Maitra, Phys. Rev. Lett. **133**, 233201 (2024).

(90) *Exciting DeePMD: Learning excited-state energies, forces, and non-adiabatic couplings**, L. Dupuy and N. T. Maitra, J. Chem. Phys. **161**, 134103 (2024).

(89) *Reformulation of Time-Dependent Density Functional Theory for Non-Perturbative Dynamics: The Rabi Oscillation Problem Resolved**, (Editors' Suggestion) D. B. Dar, A. Baranova, and N. T. Maitra, Phys. Rev. Lett. 133, 096401 (2024)

(88) *Exact-Factorization-Based Surface Hopping without Velocity Adjustment**, L. Dupuy, A. Rikus, N. T. Maitra, J. Phys. Chem. Lett. **15**, 2643 (2024).

(87) *Nonadiabatic dynamics with classical trajectories: The problem of an initial coherent superposition of electronic states**, E. Villaseco Arribas, N. T. Maitra, F. Agostini, J. Chem. Phys. **160**, 054102 (2023).

(86) *Oscillator strengths and excited-state couplings for double excitations in time-dependent density functional theory**, D.B. Dar and N.T. Maitra, J. Chem. Phys. (Communication) **159**, 211104 (2023).

(85) *Significance of Energy Conservation in Coupled-Trajectory Approaches to Nonadiabatic Dynamics*, E. Villaseco Arribas, L.M. Ibele, D. Lauvergnat, N.T. Maitra, F. Agostini, J. Chem. Theory and Comput. **19**, 7787 (2023).

(84) *Different flavors of exact-factorization-based mixed quantum-classical methods for multistate dynamics**, E.Villaseco Arribas, P. Vindel-Zandbergen, S. Roy, N.T. Maitra, Phys. Chem. Chem. Phys. **25**, 26380 (2023).

(83) *Non-Adiabatic Approximations in Time-Dependent Density Functional Theory: Progress and Prospects**, L. Lacombe and N. T. Maitra, NPJ Comput. Mat., **9**, 124 (2023).

(82) *Energy-conserving coupled trajectory mixed quantum–classical dynamics**, E. Villaseco Arribas and N. T. Maitra, J. Chem. Phys. (Communication) **158**, 161105 (2023).

(81) *Curing the divergence in time-dependent density functional quadratic response theory*, D. Dar, S. Roy, N. T. Maitra, J. Phys. Chem. Lett. **14**, 3186 (2023).

(80) *DFT Exchange: Sharing Perspectives on the Workhorse of Quantum Chemistry and Materials Science*, Andrew Teale, Trygve Helgaker, Andreas Savin, Carlo Adamo, Balint Aradi , Alexei Arbuznikov, et al., Phys. Chem. Chem. Phys. **24**, 28700 (2022).

(79) *Exact Factorization Adventures: A Promising Approach for Non-Bound States**, E. Villaseco Arribas, F. Agostini, N. T. Maitra, Molecules **27**, 4002 (2022).

(78) *The Exact Exchange-Correlation Potential in Time-Dependent Density Functional Theory: Choreographing Electrons with Steps and Peaks**, D. Dar, L. Lacombe, N. T. Maitra, Chemical Physics Reviews **3**, 031307 (2022)

(77) *Exact-Factorization-Based Surface-Hopping for Multi-State Dynamics**, P. Vindel Zandbergen, S. Matsika, N. T. Maitra, J. Phys. Chem. Lett. **13**, 1785 (2022).

(76) *Analysis of the Classical Trajectory Treatment of Photon Dynamics for Polaritonic Phenomena**, B. Rosenzweig, N. M. Hoffmann, L. Lacombe, and N. T. Maitra, J. Chem. Phys. **156**, 054101 (2022).

(75) *Double and Charge-Transfer Excitations in Time-Dependent Density Functional Theory**, N. T. Maitra, Annu. Rev. Phys. Chem. **73**, 117 (2022).

(74) *Minimizing the time-dependent density functional error in Ehrenfest dynamics**, L. Lacombe, N. T. Maitra, J. Phys. Chem. Lett. **12**, 8554 (2021).

(73) *Exact time-dependent density functional theory for non-perturbative dynamics of helium atom**, D. Dar, L. Lacombe, J. Feist, N.T. Maitra, Phys, Rev. A, **104** 032821 (2021).

(72) *A study of the decoherence correction derived from the exact factorization approach for non-adiabatic dynamics**, P. Vindel Zandbergen, L. M. Ibele, J-K. Ha, S-K. Min, B. E. Curchod, N.T Maitra, J. Chem. Theory Comput. **17**, 3852 (2021).

(71) *Case studies of the time-dependent potential energy surface for dynamics in cavities**, P. Martinez, B. Rosenzweig, N. M Hoffmann, L. Lacombe, N.T Maitra, J. Chem. Phys. **154**, 014102 (2021).

(70) *New approaches to study excited states in density functional theory: general discussion*, J. G. Brandenberg et al. Faraday Discussions **224**, 483 (2020).

(69) *New density functional approximations and beyond: general discussion*, J.G. Brandenberg et al., Faraday Discussions **224**, 166 (2020).

(68) *Developing new and understanding old approximations in TDDFT**, L. Lacombe, and N. T. Maitra, Faraday Discussions **224**, 382 (2020).

(67) *Effect of Many Modes on Self-Polarization and Photochemical Suppression in Cavities**, N. M. Hoffmann, L. Lacombe, A. Rubio, N. T. Maitra, J. Chem. Phys. **153**, 104103 (2020).

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(51) *Density-matrix propagation driven by semiclassical correlation**, P. Elliott and N. T. Maitra, Int. J. Quant. Chem. **116**, 772 (2016).

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(18) *Undoing Static Correlation: Long-Range Charge Transfer in Time-Dependent Fensity Functional Theory**, N. T. Maitra, J. Chem. Phys. **122**, 234104 (2005).

(17) *Continuum States from Time-Dependent Density Functional Theory*, A. Wasserman, N.T. Maitra, and K. Burke, J. Chem. Phys. **122**, 133103 (2005).

(16) *Memory Formula for Perturbations in Time-Dependent Density Functional Theory**, N.T. Maitra, Int. J. Quant. Chem. **102**, 573 (2005).

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(8) *Demonstration of Initial-State Dependence in Density Functional Theory**, N.T. Maitra and K. Burke, Phys. Rev. A. **63** 042501 (2001); erratum **64** 039901 (E) (2001).

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(4) *Quantizing Constrained Systems*, L. Kaplan, N.T. Maitra and E. J. Heller, Phys. Rev. A **56**, 2592 (1997).

(3) *Barrier Tunneling and Reflection in the Time and Energy Domains: The Battle of the Exponentials**, N.T. Maitra and E. J. Heller, Phys. Rev. Lett. **78**, 3035 (1997).

(2) *Ergodic Properties of Quantized Toral Automorphisms*, S. Klimek, A. Lesniewski, N. Maitra, R. Rubin, J. Math. Phys. **38**, 67 (1997).

(1) *Semiclassical Perturbation Approach to Quantum Reflection**, N.T. Maitra and E. J. Heller, Phys. Rev. A **54**, 4763 (1996).

Invited Book Chapters

(7) *Memory: History, Initial-State Dependence, and Double-Excitations**, N.T. Maitra, in Fundamentals of Time-Dependent Density Functional Theory, eds. M. A. L. Marques, N.T. Maitra, F. Nogueira, E. K. U. Gross, and A. Rubio (Springer-Verlag, Berlin-Heidelberg, 2012).

(6) *Introduction to TDDFT**, E.K. U. Gross and N.T. Maitra, in Fundamentals of Time-Dependent Density Functional Theory, eds. M. A. L. Marques, N.T. Maitra, F. Nogueira, E. K. U. Gross, and A. Rubio (Springer-Verlag, Berlin-Heidelberg, 2012).

(5) *Initial-state dependence and memory**, N. T. Maitra, in Time-Dependent Density Functional Theory, eds. M.A.L. Marques et al. (Springer, Berlin 2006).

(4) *What is time-dependent density functional theory? Successes and Challenges**, N.T. Maitra, A. Wasserman, and K. Burke, in Proceedings of the Rodes conference in DFT , ed. A. Gonis (Kluwer) (2001).

(3) *Ten topical questions in time-dependent density functional theory**, N.T. Maitra, K. Burke, H. Appel, E.K.U. Gross and R. van Leeuwen, in Reviews of Modern Quantum Chemistry: A Celebration of the Contributions of R.G. Parr , ed. K.D. Sen (World-Scientific) (2002).

(2) *The pair density in approximate density functionals: the hidden agent**, N.T. Maitra and K. Burke, in Many-Electron Densities and Reduced Density Matrices , ed. J. Cioslowski (Kluwer, New York) (2000).

(1) *Tunneling and the semiclassical propagator: a new perspective**, N.T. Maitra and E. J. Heller, in Classical, Semiclassical and Quantum Dynamics in Atoms, Springer Lecture Notes in Physics, Ed. by H. Friedrich and B. Eckhardt, Berlin, pp. 94 - 111 (1997).

l. List of Invited or Plenary/Keynote Talks Fall 2019 – Fall 2025

(in reverse chronological order)

• *TDDFT for Molecules Driven Far from Equilibrium: Reformulating it to be as Reliable as for Response* , Workshop on "At the Frontier of Light-Matter Interaction: Visions of Future Directions", Flatiron Institute, New York, September 24–26, 2025.

• *The Projected Quantum Momentum:The Hidden Agent for Electron-Nuclear Correlation*, Psi-k Workshop Lausanne, Switzerland, August 25–28, 2025.

• *Electronic (de- and re-) coherences: the projected nuclear quantum momenta as a key hidden agent*, Canadian Society for Chemistry, Ottawa, Canada Jun 15-17, 2025.

• *Electronic (de- and re-) coherences: the projected nuclear quantum momenta as a key hidden agent*, American Chemical Society Mid-Atlantic Regional Meeting, Seton Hall University, May 29, 2025.

• *Coupled Electron-Nuclear Dynamics: The Projected Quantum Momentum as Hidden Agent*, Initative for Theoretical Sciences at CUNY, New York, May 16, 2025.

• *Electron-Nuclear Interactions in Chirality-Induced Spin-Selectivity*, Discussion Leader at the NREL/DOE Meeting, Golden CO, May 12-14, 2025.

• *The Projected Quantum Momentum: A Key Agent for Electron-Nuclear Correlation*, remotely given at the COSMOS Workshop on Early Career Development and Science,, London May 1, 2025.

• *The Projected Quantum Momentum: The Hidden Agent for Electron-Nuclear Correlation*, Princeton Center for Theoretical Sciences Workshop on Nonadiabatic dynamics, electron-phonon interactions, and spin-phonon couplings, April 30-May 2, 2025.

• *Memory-Dependence in Real-Time and Linear-Response TDDFT*, two remotely given Lectures at the Tenth International School and Workshop on TDDFT in Benasque, Spain, April 9-10, 2025.

• *Electronic (De- and Re-) Coherences: Projected Nuclear Quantum Momenta as Key Hidden Agents*,American Chemical Society Spring Meeting, San Diego, March 21-25, 2025

• *Time-Dependent Density Functional Theory: An Introduction, Global Physics Summit Pre-Meeting Tutorial on Density Functional Theory*, Anaheim, March 17, 2025

• *Electronic (De- and Re-) Coherences: Projected Nuclear Quantum Momenta as Key Hidden Agents*, Atomic and Molecular Optics Seminar, Stonybrook University, Dec 4, 2024.

• *Coupled Quantum Subsystems via the Exact Factorization Approach*, Department of Chemistry and Biochemistry, University of Iceland, Sep 20, 2024.

• *Electron-Nuclear Correlation via the Exact Factorization Approach* at the 30th Canadian Symposium on Theoretical and Computational Chemistry, Halifax, Canada, July 21–25, 2024

• *Electron-Nuclear Correlation via the Exact Factorization Approach* at the 36th Electronic Structure Workshop, Boston, June 1–4, 2024.

• *Coupled Quantum Subsystems via the Exact Factorization Approach* at the Physics Department Colloquium, Delaware University, May 8 2024.

• *Electron-Electron and Electron-Nuclear Correlations with TDDFT and the Exact Factorization Approach: Aiming for Accuracy and Efficiency!* at the international online Psi-K workshop on "Shared inter-

ests and challenges for the simulation of transport processes, out-of-equilibrium dynamics, spectroscopy, and nonadiabatic dynamics", April 24–25, 2024.

• *Coupled Quantum Systems via the Exact Factorization Approach* at the American Chemical Society Meeting, New Orleans, March 16–20 2024. (could not attend because I got covid but PhD student Arribas and postdoc Dupuy gave my prepared talk)

• *Non-perturbative dynamics with TDDFT: How to make best use of the adiabatic approximation - and go beyond* at the American Physical Society March Meeting, Minnesota, March 4 – 8, 2024.

• *Time-dependent density functional theory: Simulating dynamics far from the ground state with the adiabatic approximation*, at "Progress in Non-Equilibrium Green's Functions 8", Örebro, Sweden (remote participation) Aug 8 –11, 2023.

• *HJK Couplings in TDDFT*, 3rd US-based TDDFT Workshop, Newark, NJ, July 5 – 8, 2023.

• *Memory in TDDFT*, lectures at the 3rd US-based TDDFT School, Newark NJ, June 28–July 3, 2023.

• *Mixed quantum-classical methods based on the exact factorization approach and TDDFT for correlated electrons, nuclei, and photons*, CECAM workshop on "Triggering out-of-equilibrium dynamics in molecular systems", (remote participation) Mar 28-31, 2023

• *Exact Factorization Approach for Coupled Electrons, Nuclei, and Photons*, Department of Chemistry Seminar, University of South Carolina, (remote) Feb 7, 2023

• *Memory in TDDFT*, Two lectures at the 9th International School on "TDDFT: Prospects and Applications", Benasque, Spain, Oct 18-28, 2022

• *Quantum Dynamics via the Exact Factorization Approach*, Northeast Regional Meeting of the American Chemical Society, Rochester, NY, October 4–8, 2022.

• *Exact Factorization Approach for Coupled Electrons, Nuclei, and Photons*, Simons Center for Computational Physical Chemistry, New York University, September 19, 2022.

• *Exact Factorization Approach to Molecular Polaritonics*, Molecular Polaritonics Workshop, Straubing, Germany, September 11-15, 2022

• *Making the best of the adiabatic approximation in time-dependent density functional theory*, École Polytechnique, Paris, France, September 8, 2022

• *Making the best of the adiabatic approximation in time-dependent density functional theory*, **Plenary** talk at DFT 2022, Brussels, Belgium August 31-September 4, 2022

• *Recent Developments in the Exact Factorization Approach to Coupled Dynamics*, American Conference for Theoretical Chemistry, Palisades Tahoe, July 24–28, 2022

• *Exact-Factorization-Based Methods for Coupled Electrons, Ions, and Photons*, American Physical Society March Meeting, March 2022.

• *Exact Factorization Approach to Coupled Electrons, Ions, and Photons*, ICTP-EAIFR, Kigali, February 2022.

• *Exact Factorization Approach to Coupled Electrons, Ions, and Photons*, Pacifichem Hybrid Zoom-Hawaii conference, December 18, 2021.

• *TDDFT for Photo-Excited Dynamics: Formulations to By-Pass Memory-Dependence*, Thomas Young

Center, London UK via Zoom, December 2, 2021.

• *How to Best Use TDDFT for Ehrenfest Dynamics*, Lennard Jones Center, Cambridge UK via Zoom, November 22, 2021

• *Exact Factorization Approach to Coupled Electron, Ion, and Photon Dynamics*, Department of Physics Seminar, University of Texas El Paso, November 2, 2021.

• *Exact Factorization Adventures for Electrons, Nuclei, and Photons*, Virtual International Seminar on Theoretical Advancements Seminar Series, November 11, 2021.

• *A Tale of Two Studies: (i) Exact-factorization-derived decoherence correctionsÂ and (ii) Minimizing TDDFT errors in Ehrenfest dynamicsÂ* , Telluride Research Workshop on Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy, July 2021.

• *Time-Dependent Density Functional Theory: An Introduction*, African School on Electronic Structure Methods and Applications, via Zoom, June 2021.

• *Exact Factorization Approach to Coupled Electron, Ion, and Photon Dynamics*, Chemistry Department Seminar, University of Wisconsin, via Zoom, April 20, 2021

• *Exact Factorization Approach to Polaritonic Chemistry*, American Chemical Society Symposium in Honor of Donald Kouri, via Zoom, March 2021.

• *Exact Factorization Approach to Molecules in Classical and Quantized Fields*, Molecular Quantum Dynamics Beyond Bound States, via Zoom, March 2021.

• *Polaritonic Chemistry via the Exact Factorization Approach*, Theory and Simulation of Electronic and Optical Processes in Molecules and Materials, Zoom Seminar Series, November 18, 2020.

• *Exact Factorization Approach to Coupled Electron, Ion, and Photon Dynamics*, Berkeley Pitzer Seminar Series, November 11, 2020.

• *Exact Factorization Approach to Coupled Electron, Ion, and Photon Dynamics*, William Paterson University of New Jersey, October 8, 2020.

• *Developing New and Understanding Old Approximations in TDDFT*, Faraday Discussions, Oxford UK via Zoom, September 2020.

• *Time-Dependent Potential Energy Surfaces for Polaritonic Phenomena*, Polaritonics Zoom Seminar Series, June 2020.

• *Charge-Transfer Dynamics in TDDFT*, Virtual Winter School on Computational Chemistry, Feb 17–20, 2020.

• *Exact Factorization Approach to Coupled Electron, Ion, and Photon Dynamics*, Chemistry Department Seminar, Case Western Reserve University, Cleveland OH, Oct. 17, 2019.

• *Introduction to TDDFT and Memory*, DFT Workshop at Institute of Mathematical Sciences, Singapore, Sep 2-27, 2019.

• *Going Beyond the Adiabatic Approximation in TDDFT – And Coming Back Again*, 2nd US Workshop on Time-Dependent Density Functional Theory, Rutgers University, NJ, Aug 10–14, 2019.

• *Memory in TDDFT*, Two Lectures at the 2nd US School on Time-Dependent Density Functional

Theory, Rutgers University, NJ, Aug 4-9, 2019.