

Curriculum Vitae of Prof. Dr. Robin Santra



Contact Information:

Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY
Notkestraße 85, 22607 Hamburg, Germany

Department of Physics, Universität Hamburg
Notkestraße 9-11, 22607 Hamburg, Germany

Phone: +49-(0)40-8998-6300. Fax: +49-(0)40-8994-6300. Email: robin.santra@cfel.de

Research Interests:

- Theoretical Atomic, Molecular, and Optical Physics.
- Theoretical Chemical Physics.
- Computational Physics.
- X-ray-induced processes.
- Ultrafast laser-driven phenomena.
- Applications of short-wavelength free-electron lasers.
- Electronic-structure theory.
- Non-hermiticity in quantum mechanics.

Publications:

Author or co-author of 250 scientific publications and author of 2 textbooks.

h-index: 56 (Web of Science, <https://www.webofscience.com/wos/author/record/192744>)

Researcher ID: E-8332-2014

ORCID: <http://orcid.org/0000-0002-1442-9815>

Membership in Professional Societies:

American Physical Society

German Physical Society

American Association for the Advancement of Science

Professional Experience:

April 2015 – present: Joint appointment with the Department of Chemistry, Universität Hamburg, Germany.

July 2010 – present: Professor W 3 “Head of Theory Group”, Center for Free-Electron Laser Science, DESY and Department of Physics, Universität Hamburg, Germany.

January 2010 – June 2010: Physicist, Atomic, Molecular, and Optical Physics Group, X-ray Science Division, Argonne National Laboratory, USA.

April 2008 – June 2010: Associate Professor Part-time, Department of Physics, University of Chicago, USA.

June 2007 – December 2009: Physicist, Atomic, Molecular, and Optical Physics Group, Chemical Sciences and Engineering Division, Argonne National Laboratory, USA.

August 2005 – May 2007: Assistant Physicist, Atomic, Molecular, and Optical Physics Group, Chemistry Division, Argonne National Laboratory, USA.

September 2004 – August 2005: Postdoctoral research associate, Institute for Theoretical Atomic, Molecular and Optical Physics, Harvard-Smithsonian Center for Astrophysics, Harvard University, USA.

September 2002 – August 2004: Postdoctoral research associate with Prof. C. H. Greene, JILA, University of Colorado, USA.

December 2001 – August 2002: Postdoctoral research associate with Prof. L. S. Cederbaum, Department of Chemistry, University of Heidelberg, Germany.

Higher Education:

April 1998 – November 2001: Dr. rer. nat. (degree is comparable to a Ph.D.), *summa cum laude*, University of Heidelberg, Germany. Advisor of Doctoral Thesis: Prof. L. S. Cederbaum. Title of Doctoral Thesis: Non-hermitian many-particle theory for investigating electronic decay of valence holes in clusters.

October 1992 – February 1998: Diploma in Physics (degree is comparable to a Master’s), with distinction, University of Heidelberg, Germany. Advisor of Diploma Thesis: Prof. K. P. Jungmann. Title of Diploma Thesis: Resonant three-photon ionization of the muonium atom in intense pulsed laser fields.

Scholarships and Awards:

November 2014: Fellow of the American Physical Society (“for the theoretical description of light-matter interactions, especially for processes involving X-rays and inner-shell electrons in atoms and molecules”).

December 2008: Presidential Early Career Award for Scientists and Engineers (“for innovative research at the frontiers of science and technology, and for exceptional potential to shape the future through intellectual and inspired leadership”).

Department of Energy Office of Science Early Career Scientist and Engineer Award (“for theoretical contributions to the field of atomic, molecular, and optical science in the areas of high-order harmonic generation and strong-field absorption and ionization; and for scientific mentoring of students and the public.”).

July 2007: IUPAP Young Scientist Prize in Atomic, Molecular, and Optical Physics, International Union of Pure and Applied Physics (“in recognition for his pioneering theoretical contributions in the field of atomic, molecular, and optical physics, in particular to the phenomenon of interatomic Coulombic decay”).

September 2004 – August 2005: ITAMP Postdoctoral Fellowship, Institute for Theoretical Atomic, Molecular and Optical Physics, Harvard-Smithsonian Center for Astrophysics, Harvard University, USA.

September 2002 – August 2003: Emmy Noether Postdoctoral Fellowship, German Research Foundation (DFG).

2002: Sophie Bernthsén Award, University of Heidelberg, Germany.

May 1998 – April 2001: Ph.D. Scholarship, Graduate Research Program at the Interdisciplinary Center for Scientific Computing (IWR), University of Heidelberg, Germany.

September 1995 – March 1998: Undergraduate Scholarship, German National Academic Foundation (Studienstiftung).

Service:

- Referee for American Journal of Physics, Applied Physics Letters, Canadian Journal of Physics, Chemical Physics, European Physical Journal D, Journal of Chemical Physics, Journal of Chemical Theory and Computation, Journal of Physical Chemistry A, Journal of Physical Chemistry Letters, Journal of Physics B, Journal of Physics: Conference Series, Journal of the American Chemical Society, Molecular Physics, Nature, Nature Communications, New Journal of Physics, Physical Chemistry Chemical Physics, Physical Review A, Physical Review Applied, Physical Review B, Physical Review E, Physical Review Letters, Physical Review X, Physics Letters A, Reviews of Modern Physics, Science Advances, and Structural Dynamics.
- Proposal Reviewer for German Research Foundation (DFG), European Research Council, U.S. Department of Energy, National Science Foundation, Swiss National Science Foundation, and French National Research Agency (ANR).
- Chair, XXXV International Conference on Photonic, Electronic, and Atomic Collisions (ICPEAC), Hamburg, Germany (2027).
- Member, Management Board, Cluster of Excellence, CUI: Advanced Imaging of Matter, Universität Hamburg, Hamburg, Germany (January 2019 – present).
- Principal Investigator, Cluster of Excellence, CUI: Advanced Imaging of Matter, Universität Hamburg, Hamburg, Germany (January 2019 – present).
- Member, Executive Committee, International Conference on Photonic, Electronic, and Atomic Collisions (September 2018 – present).
- Co-organizer, Wolfgang-Pauli-Centre Theory Workshop, DESY, Hamburg, Germany (2017).
- Organizer, ITAMP workshop, “The electronic-structure problem in theoretical strong-field physics”, Institute for Theoretical Atomic, Molecular and Optical Physics, Harvard-Smithsonian Center for Astrophysics, Harvard University, Cambridge, USA (2016).
- Spokesperson, Research Theme “Extreme States of Matter: From Cold Ions to Hot Plasmas”, Helmholtz Research Program “From Matter to Materials and Life” (February 2016 – December 2020).
- Member, Management Board, Collaborative Research Center SFB 925 “Light induced dynamics and control of correlated quantum systems”, Universität Hamburg, Hamburg, Germany (June 2015 – June 2018).
- Member, DAMOP 2016 Program Committee, 2016 DAMOP Meeting of the American Physical Society, Providence, Rhode Island, USA (2016).
- Member, DAMOP 2015 Program Committee, 2015 DAMOP Meeting of the American Physical Society, Columbus, Ohio, USA (2015).
- Member, International Advisory Board, XXIX ICPEAC Satellite Meeting *ISWAMP* - 3 (Intense field, Short Wavelength Atomic and Molecular Processes - 3), Hamburg, Germany (2015).

- Co-organizer, Hamburg Photon Science Colloquium, Hamburg, Germany (January 2015 – present)
- Member, Preevaluation Panel, CRC/TRR Application, German Research Foundation (DFG), Bonn, Germany (September 2014).
- Member, DAMOP 2014 Program Committee, 2014 DAMOP Meeting of the American Physical Society, Madison, Wisconsin, USA (2014)
- Co-organizer, SFB 925 Workshop on "Quantum dynamics in systems with many coupled degrees of freedom: challenges for theory", Universität Hamburg, Hamburg, Germany (2014).
- Member, International Advisory Board, XXVIII ICPEAC Satellite Meeting *ISWAMP - 2* (Intense field, Short Wavelength Atomic and Molecular Processes - 2), Xi'an, China (2013).
- Member, Habilitation committee for Dr. Peter Nalbach, Universität Hamburg, Hamburg, Germany (December 2012 – May 2013).
- Principal Investigator, Cluster of Excellence, The Hamburg Centre for Ultrafast Imaging– Structure, Dynamics and Control of Matter at the Atomic Scale, Universität Hamburg, Hamburg, Germany (November 2012 – December 2018).
- Member, Search Committee for W1 junior professors in the areas of "Ultrafast Quantum Physics with Engineered Light Fields" and "Experimental Atomic and Molecular Physics, with a Focus on Quantum Optics and Quantum Photonic Devices", Universität Hamburg, Hamburg, Germany (November 2012 – April 2013).
- Member, Executive Committee of the MIN Graduate School, Universität Hamburg, Hamburg, Germany (November 2012 – September 2017).
- Spokesperson, PIER Helmholtz Graduate School, DESY, Universität Hamburg, Hamburg, Germany (May 2012 – present).
- Organizer of the Pauli Center Blackboard Seminar, PIER (Partnership for Innovation, Education, and Research), Universität Hamburg and DESY, Hamburg, Germany (April 2011 – July 2016).
- Organizer of the CFEL Colloquium series, Center for Free-Electron Laser Science, Hamburg, Germany (October 2010 – January 2015).
- Member, Scientific Advisory Board, Linac Coherent Light Source, SLAC, Menlo Park, California, USA (December 2011 – November 2013).
- Chair, Management Board, Center for Free-Electron Laser Science, Hamburg, Germany (November 2011 – present).
- Member, External Advisory Board, PULSE Institute, SLAC, Menlo Park, California, USA (September 2011).
- Member, Executive Board, International Max Planck Research School for Ultrafast Imaging and Structural Dynamics, Hamburg, Germany (March 2011 – April 2017).
- Member, Scientific Council, International Max Planck Research School for Ultrafast Imaging and Structural Dynamics, Hamburg, Germany (March 2011 – April 2017).
- Member, Executive Board, PIER (Partnership for Innovation, Education, and Research), Universität Hamburg and DESY, Hamburg, Germany (January 2011 – December 2013).

- Principal Investigator, Collaborative Research Center SFB 925 “Light induced dynamics and control of correlated quantum systems”, Universität Hamburg, Hamburg, Germany (October 2010 – June 2019).
- Member, Scientific Advisory Board, Photon Science Division, DESY, Hamburg, Germany (July 2010 – present).
- Member, Management Board, Center for Free-Electron Laser Science, Hamburg, Germany (July 2010 – present).
- Co-organizer, Workshop on temporally and spatially resolved dynamical phenomena DESY, Hamburg, Germany (2011).
- Co-organizer, Ultrafast X-ray Summer School 2011, DESY, Hamburg, Germany (2011).
- Member, Search Committee for “Associate Professor (W2) and head of a Max Planck Research Group in Theory within the Max Planck Research Department for Structural Dynamics (MPSD),” Universität Hamburg (October 2010 – January 2011).
- Co-organizer, KITP Workshop on “X-ray Frontiers” Kavli Institute for Theoretical Physics, University of California, Santa Barbara, USA (2010).
- Co-organizer, Focus Session on “Attosecond Science” at the March 2010 Meeting of the American Physical Society, Portland, Oregon, USA (2010).
- External Reviewer, Ph.D. Thesis of Koudai Toyota, University of Electro-Communications, Tokyo, Japan (December 2009 – January 2010).
- Co-organizer, Inaugural Fall 2009 Meeting of the Prairie Section of the American Physical Society (Iowa City, Iowa, USA, 2009).
- Member, Local Organizing Committee, XXVI International Conference on Photonic, Electronic, and Atomic Collisions, Western Michigan University, USA (2009).
- Member, Ph.D. Committee for Jock McOrist, Department of Physics, University of Chicago (October 2008 – July 2009).
- Member, Advanced Photon Source Renewal Committee, AMO & Chemistry (July 2008 – May 2009).
- Chair, Prairie Section of the American Physical Society (April 2008 – December 2009).
- Member, Argonne Chemistry Colloquium Committee (January 2007 – July 2009).
- Co-organizer, ITAMP workshop, “X-ray Free-Electron Lasers: Challenges for Theory” Institute for Theoretical Atomic, Molecular and Optical Physics, Harvard-Smithsonian Center for Astrophysics, Harvard University, USA (2006).
- Co-organizer, AMO Theory Seminar, JILA, University of Colorado, USA, academic year (2003 – 2004).

Teaching:

May 2024: Lecturer, *Theory of X-ray–matter interaction*, International School on Ultrafast X-ray & Attosecond Science, Paris-Saclay University, France.

October 2023 – February 2024: Lecturer, *Einführung in die Theoretische Physik I*, Universität Hamburg, Germany.

October 2022 – January 2023: Lecturer, *Theory of photon–matter interactions*, Universität Hamburg, Germany.

June 2022: Lecturer, *Theory of X-ray–matter interaction*, Ultrafast X-ray Summer School 2022, SLAC, Menlo Park, California, USA.

October 2021 – February 2022: Lecturer, *Theoretische Physik I*, Universität Hamburg, Germany. Voted by the UHH physics students the best Bachelor’s level theory course in the winter semester 2021/2022.

November 2020 – February 2021: Lecturer, *Einführung in die Theoretische Physik I*, Universität Hamburg, Germany.

October 2019 – February 2020: Lecturer, *Einführung in die Theoretische Physik I*, Universität Hamburg, Germany.

October 2018 – January 2019: Lecturer, *Theory of photon–matter interactions*, Universität Hamburg, Germany. Voted by the UHH physics students the best Master’s level course in the winter semester 2018/2019.

September 2018: Lecturer, *Electronic Structure at High X-ray Intensity*, FEL Physics school, Physikzentrum Bad Honnef, Germany.

August 2018: Lecturer, *Processes at high radiation intensity*, DESY summer student program, Hamburg, Germany.

May 2018: Lecturer, *Electronic decoherence and correlation effects in attosecond science*, PALM International School on Attosecond Science, Gif-sur-Yvette, Paris, France.

February 2018: Lecturer, *Adiabatic and nonadiabatic dynamics in water*, XVII DESY Research Course - Trends in Water Research, DESY, Hamburg, Germany.

October 2017 – January 2018: Lecturer, *Einführung in die Theoretische Physik I*, Universität Hamburg, Germany.

August 2017: Lecturer, *Processes at high radiation intensity*, DESY summer student program, Hamburg, Germany.

June 2017: Lecturer, *Theory of X-ray–matter interaction*, Ultrafast X-ray Summer School 2017, DESY, Hamburg, Germany.

October 2016 – January 2017: Lecturer, *Theory of photon–matter interactions*, Universität Hamburg, Germany.

August 2016: Lecturer, *Processes at high radiation intensity*, DESY summer student program, Hamburg, Germany.

October 2015 – January 2016: Lecturer, *Einführung in die Theoretische Physik I*, Universität Hamburg, Germany.

October 2015: Lecturer, *Fundamental processes in photon–matter interactions*, PIER Graduate Week, DESY, Hamburg, Germany.

August 2015: Lecturer, *Processes at high radiation intensity*, DESY summer student program, Hamburg, Germany.

June 2015: Lecturer, *Fundamentals of X-ray–matter interactions*, Ultrafast X-ray Summer School 2015, DESY, Hamburg, Germany.

October 2014 – January 2015: Lecturer, *Theory of photon–matter interactions*, Universität Hamburg, Germany.

June 2014: Lecturer, *Fundamentals of X-ray–matter interactions*, Ultrafast X-ray Summer School 2014, SLAC, Menlo Park, California, USA.

April 2014: Lecturer, *Introduction to (X-ray) photon science*, Research Exchange and Discovery Workshop, DESY and Universität Hamburg, Hamburg, Germany.

April 2014: Lecturer, *Applications of free-electron lasers in physics, chemistry and biology*, Graduate Days, Heidelberg Graduate School of Fundamental Physics, University of Heidelberg, Heidelberg, Germany.

October 2013 – January 2014: Lecturer, *Theory of photon–matter interactions*, Universität Hamburg, Germany.

September 2013: Lecturer, *X-ray multiphoton ionization: theory*, DPG Physics School on Free-electron X-ray Laser Physics, Bad Honnef, Germany.

June 2013: Lecturer, *Fundamentals of X-ray–matter interactions*, Ultrafast X-ray Summer School 2013, DESY, Hamburg, Germany.

March 2013: Lecturer, *Concepts in X-ray physics*, XII. Research Course on X-ray Science Theoretical Foundations of Research with X-ray Free Electron Lasers and Synchrotron Radiation Sources, DESY, Hamburg, Germany.

January 2013: Lecturer, *Theory of interacting electrons in electromagnetic fields*, ETH-FAST Fellow Lectures, Department of Physics, Swiss Federal Institute of Technology (ETH) Zürich, Switzerland.

November 2012: Lecturer, *X-ray physics*, FANTOM International Research School, Groningen, The Netherlands.

August 2012: Organizer of Six-Day Seminar (Materie im Strahl eines Röntgen-Freie-Elektronen-Lasers), Summer Academy XV, Max Weber-Programm Bayern und Studienstiftung des deutschen Volkes, Überlingen, Germany.

April 2012 – July 2012: Lecturer, *Theory of photon–matter interactions*, Department of Physics, Universität Hamburg, Germany.

April 2011 – July 2011: Lecturer, *Quantum mechanics I*, Department of Physics, Universität Hamburg, Germany.

March 2010 – June 2010: Lecturer, *Modern atomic physics*, Department of Physics, University of Chicago, USA.

June 2009: Lecturer, *Concepts in X-ray physics*, Ultrafast X-ray Summer School, SLAC, Menlo Park, California, USA.

March 2009 – June 2009: Lecturer, *Theory of photon–atom interactions*, Department of Physics, University of Chicago, USA.

January 2009: Lecturer, *Fun with free-electron lasers*, “FRIDAY LECTURE” in the Department of Physics at the University of Chicago, USA.

July 2008: Lecturer, *Introduction to X-ray physics from a theorist’s perspective*, Summer School on time-resolved X-ray processes in atoms, molecules and solids at the Max Planck Institute for the Physics of Complex Systems, Dresden, Germany.

June 2007: Lecturer, *Strong-field control of X-ray absorption*, Ultrafast X-ray Summer School, SLAC, Menlo Park, California, USA.

January 2004 – April 2004: Substitute Lecturer, *Electromagnetic Theory 2*, Department of Physics, University of Colorado, USA.

September 2003 – December 2003: Teaching Assistant, *Honors Mechanics Course*, Department of Physics, University of Colorado, USA.

April 2001 – July 2001: Teaching Assistant, *Quantum Chemistry I*, Department of Chemistry, University of Heidelberg, Germany.

October 2000 – February 2001: Teaching Assistant, *Quantum Chemistry II*, Department of Chemistry, University of Heidelberg, Germany.

October 1998 – February 1999: Teaching Assistant, *Introduction to Quantum Theory*, Department of Chemistry, University of Heidelberg, Germany.

April 1998 – July 1998: Teaching Assistant, *Physical Chemistry II*, Department of Chemistry, University of Heidelberg, Germany.

January 1997 – December 1997: Teaching Assistant, *Introductory Laboratory Courses in Classical Mechanics and Optics*, Department of Physics, University of Heidelberg, Germany.

Supervisory Assignments:

January 2024 – present: Anthony Ferté, postdoctoral research associate, CFEL, DESY, Germany.

January 2024 – present: Nathaniel Okpara, doctoral researcher, Department of Physics, Universität Hamburg, Germany.

November 2023 – present: Seyedeh Mojgan Soltani, doctoral researcher, Department of Physics, Universität Hamburg, Germany.

December 2022 – present: Swarnendu Bhattacharyya, postdoctoral research associate, CFEL, DESY, Germany.

October 2022 – July 2023: Matthias Richter, bachelor student, Department of Physics, Universität Hamburg, Germany.

June 2022 – November 2022: Torben Hannemann, bachelor student, Department of Physics, Universität Hamburg, Germany.

May 2022 – present: Mayank Vashistha, doctoral researcher, Department of Physics, Universität Hamburg, Germany.

April 2022 – December 2023: Arturo Moros Sopena, postdoctoral research associate, CFEL, DESY, Germany.

February 2022 – July 2022: REXIATI Dilimulati, postdoctoral research associate, CFEL, DESY, Germany.

October 2021 – present: Laura Budewig, doctoral researcher, Department of Physics, Universität Hamburg, Germany.

August 2021 – present: Sourav Banerjee, postdoctoral research associate, CFEL, DESY, Germany.

August 2021 – present: Daria Kolbasova, postdoctoral research associate, CFEL, DESY, Germany.

November 2020 – July 2021: John Bekx, postdoctoral research associate, CFEL, DESY, Germany.

May 2020 – February 2021: Stanislaw Wirok-Stoletow, bachelor student, Department of Physics, Universität Hamburg, Germany.

April 2020 – present: Ludger Inhester, senior scientist, CFEL, DESY, Germany.

March 2020 – September 2021: Laura Budewig, master student, Department of Physics, Universität Hamburg, Germany.

January 2020 – February 2020: Malik Muhammad Abdullah, postdoctoral research associate, CFEL, DESY, Germany.

November 2019 – present: Benoit Richard, doctoral researcher, Department of Physics, Universität Hamburg, Germany.

November 2019 – January 2023: Arunangshu Debnath, postdoctoral research associate, CFEL, DESY, Germany.

August 2019 – July 2020: Patrick Richter, bachelor student, Department of Physics, Universität Hamburg, Germany.

June 2019 – present: Niels Breckwoldt, doctoral researcher, Department of Physics, Universität Hamburg, Germany.

May 2019 – March 2020: Caroline Arnold, postdoctoral research associate, CFEL, DESY, Germany.

October 2018 – January 2023: Yashoj Shakya, doctoral researcher, Department of Physics, Universität Hamburg, Germany.

October 2018 – September 2022: Rui Jin, postdoctoral research associate, CFEL, DESY, Germany.

July 2018 – September 2018: Vladislav Guskov, intern, CFEL, DESY, Germany

July 2018 – September 2018: Vikoriia Isaenko, intern, CFEL, DESY, Germany

July 2018 – September 2018: Tanakrit Mamee, intern, CFEL, DESY, Germany

January 2018 – May 2022: Adrien Marjollet, doctoral researcher, Department of Physics, Universität Hamburg, Germany.

December 2017 – June 2019: Malik Muhammad Abdullah, postdoctoral research associate, Department of Physics, Universität Hamburg, Germany.

October 2017 – December 2021: Julia Schäfer, doctoral researcher, Department of Chemistry, Universität Hamburg, Germany.

September 2017 – December 2018: Timo Lohrmann, master student, Department of Physics, Universität Hamburg, Germany.

August 2017 – August 2021: Daria Kolbasova, doctoral researcher, Department of Physics, Universität Hamburg, Germany.

July 2017 – September 2017: Natasha Feinstein, intern, CFEL, DESY, Germany.

July 2017 – June 2018: Rajwant Kaur, postdoctoral research associate, CFEL, DESY, Germany.

June 2017 – October 2020: Michael Obermeyer, master student, Department of Physics, Universität Hamburg, Germany.

January 2017 – September 2017: Julia Schäfer, master student, Department of Chemistry, Universität Tübingen, Germany.

January 2017 – February 2020: Ralph Welsch, senior scientist, CFEL, DESY, Germany.

January 2017 – February 2017: Marlene Heinrich, intern, CFEL, DESY, Germany.

November 2016 – November 2020: John Bekx, doctoral researcher, Department of Physics, Universität Hamburg, Germany.

July 2016 – September 2016: Daria Kolbasova, intern, CFEL, DESY, Germany.

May 2016 – July 2016: Anurag, intern, CFEL, DESY, Germany.

May 2016 – May 2017: Pankaj Kumar Mishra, postdoctoral research associate, Department of Physics, Universität Hamburg, Germany.

April 2016 – March 2017: Friethjof Theel, bachelor student, Department of Physics, Universität Hamburg, Germany.

April 2016 – March 2021: Vladimir P. Lipp, postdoctoral research associate, CFEL, DESY, Germany.

April 2016 – present: Zoltan Jurek, senior scientist, CFEL, DESY, Germany.

March 2016 – April 2018: Sevinc Kayadaleren, master student, Department of Physics, Universität Hamburg, Germany.

December 2015 – October 2017: Antonia Karamatskou, postdoctoral research associate, Department of Physics, Universität Hamburg, Germany.

November 2015 – May 2022: Murali Krishna, doctoral researcher, Department of Physics, Universität Hamburg, Germany.

November 2015 – April 2019: Caroline Arnold, doctoral researcher, Department of Physics, Universität Hamburg, Germany.

September 2015 – June 2019: Sophia Bazzi, doctoral researcher, Department of Chemistry, Universität Hamburg, Germany.

April 2015 – July 2018: Koudai Toyota, postdoctoral research associate, CFEL, DESY, Germany.

April 2015 – September 2016: Mirco Grosser, master student, Department of Physics, Universität Hamburg, Germany.

December 2014 – June 2015: Janine Franz, master student, Department of Physics, Universität Hamburg, Germany.

October 2014 – October 2019: Ludger Inhester, postdoctoral research associate, CFEL, DESY, Germany.

September 2014 – August 2017: Zheng Li, postdoctoral research associate, CFEL, DESY, Germany.

August 2014 – present: Athiya Mahmud Hanna, doctoral researcher, Department of Chemistry, Universität Hamburg, Germany.

August 2014 – April 2016: Kota Hanasaki, postdoctoral research associate, Department of Physics, University of Hamburg, Germany.

July 2014 – September 2017: Dietrich Krebs, master student, Department of Physics, Universität Hamburg, Germany.

July 2014 – September 2014: Sayat Mimar, intern, CFEL, DESY, Germany.

July 2014 – September 2014: Dmitrii Shedogubov, intern, CFEL, DESY, Germany.

July 2014 – August 2014: Daochen Wang, intern, CFEL, DESY, Germany.

June 2014 – August 2014: Matthew Tilley, intern, Department of Physics, Universität Hamburg, Germany.

June 2014 – September 2014: Fabio Zeiser, undergraduate scientific assistant, Department of Physics, Universität Hamburg, Germany.

June 2014 – September 2014: Johannes Knörzer, undergraduate scientific assistant, Department of Physics, Universität Hamburg, Germany.

May 2014 – November 2017: Malik Muhammad Abdullah, doctoral researcher, Department of Physics, Universität Hamburg, Germany.

February 2014 – August 2017: Viktor Tkachenko, doctoral researcher, Department of Physics, Universität Hamburg, Germany.

January 2014 – present: Sang-Kil Son, senior scientist, CFEL, DESY, Germany.

January 2014 – December 2014: Yajiang Hao, postdoctoral research associate, CFEL, DESY, Germany.

October 2013 – December 2016: Vikrant Saxena, postdoctoral research associate, CFEL, DESY, Germany.

July 2013 – September 2013: Jason Khadka, intern, DESY, Germany.

July 2013 – September 2013: Ekaterina Kuzmina, intern, DESY, Germany.

July 2013 – September 2013: Stanislaw Hrivnak, intern, DESY, Germany.

June 2013 – September 2013: Elisabeth Heinrich-Josties, intern, Universität Hamburg, Germany.

July 2013 – December 2019: Daria Gorelova, postdoctoral research associate, CFEL, DESY, Germany.

July 2013 – December 2013: Muhammad Saqib, doctoral researcher, Department of Physics, Universität Hamburg, Germany.

March 2013 – October 2013: Mirco Grosser, bachelor student, Department of Physics, Universität Hamburg, Germany.

January 2013 – December 2014: Stefan Pabst, postdoctoral research associate, CFEL, DESY, Germany.

August 2012 – February 2019: Yi-Jen Chen, doctoral researcher, Department of Physics, Universität Hamburg, Germany.

June 2012 – November 2015: Antonia Karamatskou, doctoral researcher, Department of Physics, Universität Hamburg, Germany.

April 2012 – September 2012: Mario Arkenberg, bachelor student, Department of Physics, Universität Hamburg, Germany.

April 2012 – June 2013: Dietrich Krebs, bachelor student, Department of Physics, Universität Hamburg, Germany.

April 2012 – August 2012: Sebastian Grell, bachelor student, Department of Physics, Universität Hamburg, Germany.

March 2012 – November 2015: Pankaj Kumar Mishra, doctoral researcher, Department of Physics, Universität Hamburg, Germany.

August 2011 – August 2014: Zheng Li, doctoral researcher, Department of Physics, Universität Hamburg, Germany.

August 2011 – March 2015: Jan Malte Slowik, doctoral researcher, Department of Physics, Universität Hamburg, Germany.

July 2011 – September 2011: Anastasia Bityutskaya, intern, CFEL, DESY, Germany.

April 2011 – September 2013: Robert Thiele, postdoctoral research associate, CFEL, DESY, Germany.

April 2011 – March 2016: Nikita Medvedev, postdoctoral research associate, CFEL, DESY, Germany.

February 2011 – March 2016: Zoltan Jurek, postdoctoral research associate, CFEL, DESY, Germany.

February 2011 – July 2013: Gopal Dixit, postdoctoral research associate, CFEL, DESY, Germany.

February 2011 – January 2014: Arina Sytcheva, postdoctoral research associate, CFEL, DESY, Germany.

January 2011 – August 2013: Mohamed El-Amine Madjet, postdoctoral research associate, CFEL, DESY, Germany.

November 2010 – November 2020: Beata Ziaja, senior scientist, CFEL, DESY, Germany.

July 2010 – June 2016: Oriol Vendrell, senior scientist, CFEL, DESY, Germany.

June 2010 – December 2013: Sang-Kil Son, postdoctoral research associate, CFEL, DESY, Germany.

April 2009 – December 2012: Stefan Pabst, doctoral researcher, Department of Physics, Universität Hamburg, Germany.

October 2008 – June 2010: Loren Greenman, doctoral researcher, Department of Chemistry, University of Chicago, USA.

June 2008 – August 2008: Michelle R. Miller, science undergraduate laboratory intern, Argonne National Laboratory, USA.

April 2008 – April 2009: Hari R. Varma, postdoctoral research associate, Argonne National Laboratory, USA.

October 2007 – June 2010: Phay Ho, postdoctoral research associate, Argonne National Laboratory, USA.

June 2007 – August 2007: Michelle R. Miller, pre-college student, Argonne National Laboratory, USA.

April 2006 – April 2008: Christian Buth, postdoctoral research associate, Argonne National Laboratory, USA.

October 2005 – September 2007: Nina Rohringer, postdoctoral research associate, Argonne National Laboratory, USA.

January 2004 – August 2004: Jeffrey Shainline, undergraduate honors student, Department of Physics and JILA, University of Colorado, USA.

September 2002 – November 2003: Kevin Christ, undergraduate honors student, Department of Physics and JILA, University of Colorado, USA.

August 2001 – August 2002: Christian Buth, diploma student, Department of Chemistry, University of Heidelberg, Germany.

April 2000 – March 2001: Imke Müller, diploma student, Department of Chemistry, University of Heidelberg, Germany.

Textbooks:

R. Santra: Einführung in die Theoretische Physik (first edition: Springer, Berlin, 2019; second edition: Springer, Berlin, 2023).

R. Santra: Einführung in den Lagrange- und Hamilton-Formalismus (Springer, Berlin, 2022).

Publications:

250. L. Budewig, S.-K. Son, Z. Jurek, M. M. Abdullah, M. Tropmann-Frick, R. Santra: *X-ray-induced atomic transitions via machine learning: A computational investigation*. Physical Review Research **5**, 023158 (2024).

249. D. Gorelova, R. Santra: *Microscopic nonlinear optical response: analysis and calculations with the Floquet-Bloch formalism*. Structural dynamics **11**, 014102 (2024).

248. S. Li, L. Lixin, S. Bhattacharyya, C. Pearce, C. K. Li, E. Nienhuis-Marcial, G. Doumy, R. D. Schaller, S. Moeller, M.-F. Lin, G. Dakovski, D. J. Hoffmann, D. J. D. Garratt, K.A. Larsen, J. Koralek, C. Hampton, D. Cesar, J. Duris, Z. Zhang, N. Sudar, J. Cryan, A. Marinelli, X. Li, L. Inhester, R. Santra, R. L. Young: *Attosecond-pump attosecond-probe x-ray spectroscopy of liquid water*. Science **383**, 1118 (2024).

247. A. Sopena Moros, S. Li, K. Li, G. Doumy, S. Southworth, C. Otolski, R. Schaller, Y. Kumagai, J.-E. Rubensson, M. Simon, G. Dakovski, K. Kunnus, J. Robinson, C. Hampton, D. Hoffman, J. Koralek, Z.-H. Loh, R. Santra, L. Inhester, L. Young: *Tracking cavity formation in electron solvation: insights from x-ray spectroscopy and theory*. Journal of the American Chemical Society **146**, 3262 (2024).

246. E. J., M. Stransky, Z. Shen, Z. Jurek, C. Fortmann-Grote, R. Bean, R. Santra, B. Ziaja, A.P. Mancuso: *Water layer and radiation damage effects on the orientation recovery of proteins in single-particle imaging at an X-ray free-electron laser*. Scientific Reports **13**, 16359 (2023).

245. A. Rörig, S.-K. Son, T. Mazza, P. Schmidt, T.M. Baumann, B. Erk, M. Ilchen, L. Laksman, V. Music, S. Pathak, D.E. Rivas, D. Rolles, S. Serkez, S. Usenko, R. Santra, M. Meyer, R. Boll: *Multiple-core-hole resonance spectroscopy with ultraintense X-ray pulses*. *Nature Communications* **14**, 5738 (2023).
244. Z. Yin, Y.-P. Chang, T. Balčiūnas, Y. Shakya, A. Djorović, G. Gaulier, G. Fazio, R. Santra, L. Inhester, J.-P. Wolf, H. J. Wörner: *Femtosecond proton transfer in urea solutions probed by X-ray spectroscopy*. *Nature* **619**, 749 (2023).
243. A. Debnath, R. Santra: *Theory of high-energy correlated multiphoton x-ray diffraction for synchrotron-radiation sources*. *Physical Review Research* **5**, 023158 (2023).
242. R. Guillemin, L. Inhester, M. Ilchen, M. T. Mazza, R. Boll, T. Weber, S. Eckart, P. Grychtol, N. Rennhack, T. Marchenko, N. Velasquez, I. Ismail, J. Niskanen, E. Kukk, F. Trinter, M. Gisselbrecht, R. Feifel, G. Sansone, D. Rolles, M. Martins, M. Simon, R. Santra, T. Pfeifer, T. Jahnke, M.N. Piancastelli: *Isotope effects in dynamics of water isotopologues induced by core ionization at an x-ray free-electron laser*. *Structural Dynamics* **10**, 054302 (2023).
241. C. M. Casadei, A. Hosseinizadeh, S. Bliven, T. Weinert, J. Standfuss, R. Fung, G.F. Schertler, R. Santra: *Low-pass spectral analysis of time-resolved serial femtosecond crystallography data*. *Structural Dynamics* **10**, 034101 (2023).
240. D. Kolbasova, R. Santra: *Laser-pulse characterization using strong-field autocorrelation patterns and random-forest-based machine learning*. *Physical Review A* **107**, 013520 (2023).
239. N. Breckwoldt, S.-K. Son, T. Mazza, A. Rörig, R. Boll, M. Meyer, A. LaForge, D. Mishra, N. Berrah, R. Santra: *Machine-learning calibration of intense x-ray free-electron-laser pulses using Bayesian optimization*. *Physical Review Research* **5**, 023114 (2023).
238. L. Budewig, S.-K. Son, R. Santra: *State-resolved ionization dynamics of a neon atom induced by x-ray free-electron-laser pulses*. *Physical Review A* **107**, 013102 (2023).
237. S. Banerjee, Z. Jurek, M. Abdullah, R. Santra: *Chemical effects on the dynamics of organic molecules irradiated with high intensity x rays*. *Structural Dynamics* **9**, 054101 (2022)
236. S. Wirok-Stoletow, R. Jin, D. Kolbasova, S.-K. Son, A. Aquila, R. Santra: *Nonsequential two-photon absorption in solid Ge irradiated by an intense x-ray free-electron-laser pulse*. *Physical Review A* **106**, 023118 (2022).
235. C. M. Casadei, A. Hosseinizadeh, G. F. X. Schertler, A. Ourmazd, R. Santra: *Dynamics retrieval from stochastically weighted incomplete data by low-pass spectral analysis*. *Structural Dynamics* **9**, 044101 (2022).
234. O. Geffert, D. Kolbasova, A. Trabattoni, F. Calegari, R. Santra: *In situ characterization of few-femtosecond laser pulses by learning from first-principles calculations*. *Optics Letters* **47**, 3992 (2022).
233. R. Jin, Z. Jurek, R. Santra, S.-K. Son: *Plasma environmental effects in the atomic structure for simulating x-ray free-electron-laser-heated solid-density matter*. *Physical Review E* **106**, 015206 (2022).
232. Y. Shakya, R. Welsch, L. Inhester, R. Santra: *Capturing electronic decoherence in quantum-classical dynamics using the ring-polymer-surface-hopping–density-matrix approach*. *Physical Review A* **107**, 062810 (2022).
231. M. Stransky, Z. Jurek, R. Santra, A. P. Mancuso, B. Ziaja: *Tree-code based improvement of computational performance of the x-ray-matter-interaction simulation tool XMDYN*. *Molecules* **27**, 4206 (2022).
230. L. Budewig, S.-K. Son, R. Santra: *Theoretical investigation of orbital alignment of x-ray-ionized atoms in exotic electronic configurations*. *Physical Review A* **105**, 033111 (2022).

229. R. Boll, J. M. Schäfer, B. Richard, K. Fehre, G. Kastirke, Z. Jurek, M. S. Schöffler, M. M. Abdullah, N. Anders, T. M. Baumann, S. Eckart, B. Erk, A. De Fanis, R. Dörner, S. Grundmann, P. Grychtol, A. Hartung, M. Hofmann, M. Ilchen, M. L. Inhester, C. Janke, C. R. Jin, M. Kircher, K. Kubicek, M. Kunitski, X. Li, T. Mazza, S. Meister, N. Melzer, J. Montano, J. V. Music, G. Nalin, Y. Ovcharenko, C. Passow, A. Pier, A. N. Rennhack, J. Rist, D. E. Rivas, D. Rolles, I. Schlichting, L. P. H. Schmidt, P. Schmidt, J. Siebert, N. Strenger, D. Trabert, F. Trinter, I. Vela-Perez, R. Wagner, P. Walter, M. Weller, P. Ziolkowski, S.-K. Son, A. Rudenko, M. Meyer, R. Santra, T. Jahnke: *X-ray multiphoton-induced Coulomb explosion images complex single molecules*. *Nature Physics* **18**, 423 (2022).
228. T. Jahnke, R. Guillemin, L. Inhester, S.-K. Son, G. Kastirke, M. Ilchen, J. Rist, D. Trabert, N. Melzer, N. Anders, T. Mazza, R. Boll, A. De Fanis, V. Music, Th. Weber, M. Weller, S. Eckart, K. Fehre, S. Grundmann, A. Hartung, M. Hofmann, C. Janke, M. Kircher, G. Nalin, A. Pier, J. Siebert, N. Strenger, I. Vela-Perez, T. M. Baumann, P. Grychtol, J. Montano, Y. Ovcharenko, N. Rennhack, D. E. Rivas, R. Wagner, P. Ziolkowski, P. Schmidt, T. Marchenko, O. Travnikova, L. Journal, I. Ismail, E. Kukk, J. Niskanen, F. Trinter, C. Vozzi, M. Devetta, S. Stagira, M. Gisselbrecht, A. L. Jäger, X. Li, Y. Malakar, M. Martins, R. Feifel, L. Ph. H. Schmidt, A. Czasch, G. Sansone, D. Rolles, A. Rudenko, R. Moshhammer, R. Dörner, M. Meyer, T. Pfeifer, M. S. Schöffler, R. Santra, M. Simon, M. N. Piancastelli: *Inner-shell-ionization-induced femtosecond structural dynamics of water molecules imaged at an x-ray free-electron laser*. *Physical Review X* **11**, 041044 (2021).
227. A. C. Laforge, S.-K. Son, D. Mishra, M. Ilchen, S. Duncanson, E. Eronen, E. Kukk, S. Wirok-Stoletow, D. Kolbasova, P. Walter, R. Boll, A. De Fanis, M. Meyer, Y. Ovcharenko, D. E. Rivas, P. Schmidt, S. Usenko, R. Santra, N. Berrah: *Resonance-enhanced multiphoton ionization in the x-ray regime*. *Physical Review Letters* **127**, 213202 (2021).
226. A. Hosseinizadeh, N. Breckwoldt, R. Fung, R. Sepehr, M. Schmidt, P. Schwander, R. Santra, A. Ourmazd: *Few-fs resolution of a photoactive protein traversing a conical intersection*. *Nature* **599**, 697 (2021).
225. B. Richard, J. M Schäfer, Z. Jurek, R. Santra, L. Inhester: *Statistical analysis of correlations in the x-ray induced Coulomb explosion of iodopyridine*. *Journal of Physics B: Atomic, Molecular and Optical Physics* **54**, 194001 (2021).
224. F. Lehmkuhler, C. Goy, R. Santra, G. Grübel: *Wasser im Licht von Röntgenlasern*. *Physik in unserer Zeit* **52**, 298 (2021).
223. J. E. M. Stransky, Z. Jurek, C. Fortmann-Grote, L. Juha, R. Santra, B. Ziaja, A. P. Mancuso: *Effects of radiation damage and inelastic scattering on single-particle imaging of hydrated proteins with an x-ray free-electron laser*. *Scientific Reports* **11**, 17976 (2021).
222. M. Obermeyer, L. Inhester, R. Santra: *Strategies for solving the excited-state self-consistent-field problem for highly excited and multiply ionized states*. *Physical Review A* **104**, 023115 (2021).
221. X. Li, S. J. Robatjazi, L. Inhester, B. Erk, R. Boll, K. Hanasaki, K. Toyota, Y. Hao, C. Bomme, B. Rudek, L. Foucar, S. H. Southworth, C. S. Lehmann, B. Kraessig, T. Marchenko, M. Simon, K. Ueda, K. R. Ferguson, M. Bucher, T. Gorkhover, S. Carron, R. Alonso-Mori, J. E. Koglin, J. Correa, G. J. Williams, S. Boutet, L. Young, C. Bostedt, S.-K. Son, R. Santra, D. Rolles, A. Rudenko: *Pulse energy and pulse duration effects in the ionization and fragmentation of iodomethane by ultraintense hard x rays*. *Physical Review Letters* **127**, 093202 (2021).
220. Y. Shakya, L. Inhester, C. Arnold, R. Welsch, R. Santra: *Ultrafast time-resolved x-ray absorption spectroscopy of ionized urea and its dimer through ab initio nonadiabatic dynamics*. *Structural Dynamics* **8**, 034102 (2021).

219. D. Kolbasova, M. Hartmann, R. Jin, A. Blättermann, C. Ott, S.-K. Son, T. Pfeifer, R. Santra: *Probing ultrafast coherent dynamics in core-excited xenon by using attosecond XUV-NIR transient absorption spectroscopy*. *Physical Review A* **103**, 043102 (2021).
218. R. Santra, M. Obermeyer: *A first encounter with the Hartree-Fock self-consistent-field method*. *American Journal of Physics* **89**, 426 (2021).
217. Y. Kumagai, Z. Jurek, W. Xu, V. Saxena, H. Fukuzawa, K. Motomura, D. Iablonskyi, K. Nagaya, S.-I. Wada, Y. Ito, T. Takanashi, S. Yamada, Y. Sakakibara, T. N. Hiraki, T. Umemoto, M. Patanen, J. D. Bozek, I. Dancus, M. Cernaianu, C. Miron, T. Bauer, M. Mucke, E. Kukk, S. Owada, T. Togashi, K. Tono, M. Yabashi, S.-K. Son, B. Ziaja, R. Santra, K. Ueda: *Suppression of thermal nanoplasma emission in clusters strongly ionized by hard x-rays*. *Journal of Physics B: Atomic, Molecular and Optical Physics* **54**, 0441001 (2021).
216. R. Jin, M. M. Abdullah, Z. Jurek, R. Santra, S.-K. Son: *Transient ionization potential depression in nonthermal dense plasmas at high x-ray intensity*. *Physical Review E* **103**, 023203 (2021).
215. X. Li, L. Inhester, T. Osipov, R. Boll, R. Coffee, J. Cryan, A. Gatton, T. Gorkhover, G. Hartman, M. Ilchen, A. Knie, M.F. Lin, M. P. Minitti, C. Weninger, T. J. A. Wolf, S.K. Son, R. Santra, D. Rolles, A. Rudenko, P. Walter: *Electron-ion coincidence measurements of molecular dynamics with intense x-ray pulses*. *Scientific Reports* **11**, 505 (2021)
214. D. Koulentianos, A. E. A. Fouda, S. H. Southworth, J. D. Bozek, J. Küpper, R. Santra, N. V. Kryzhevoi, L. S. Cederbaum, C. Bostedt, M. Messerschmidt, N. Berrah, L. Fang, B. Murphy, T. Osipov, J. P. Cryan, J. Glowina, S. Ghimire, P.J. Ho, B. Krässig, D. Ray, Y. Li, E. P. Kanter, L. Young, G. Doumy: *High intensity x-ray interaction with a model bio-molecule system: double-core-hole states and fragmentation of formamide*. *Journal of Physics B: Atomic, Molecular and Optical Physics* **53**, 244005 (2020).
213. M. K. Ganesa Subramanian, R. Brannath, R. Welsch, R. Santra, M. Drescher: *Field-enabled quantum interference in atomic Auger decay*. *Physical Review A* **102**, 022807 (2020).
212. M. K. Ganesa Subramanian, R. Santra, R. Welsch: *Choice of the electronic basis for field-induced surface hopping*. *Physical Review A* **102**, 013107 (2020).
211. J. Bekx, S.-K. Son, B. Ziaja, R. Santra: *Electronic-structure calculations for nonisothermal warm dense matter*. *Physical Review Research* **2**, 033061 (2020).
210. K. Khalili, L. Inhester, C. Arnold, A.S. Gertsen, J. W. Andreasen, R. Santra: *Simulation of time-resolved x-ray absorption spectroscopy of ultrafast dynamics in particle-hole-excited 4-(2-thienyl)-2,1,3-benzothiadiazole*. *Structural Dynamics* **7**, 044101 (2020).
209. N. Mukharamova, S. Lazarev, J.-M. Meijer, O. Y. Gorobtsov, A. Singer, M. Chollet, M. Bussmann, D. Dzhigaev, Y. Feng, M. Garten, A. Hübl, T. Kluge, R.P. Kurta, V. Lipp, R. Santra, M. Sikorski, S. Song, G. Williams, D. Zhu, B. Ziaja-Motyka, T. E. Cowan, A. V. Petukhov, I. A. Vartanyants: *Femtosecond laser produced periodic plasma in a colloidal crystal probed by XFEL radiation*. *Scientific Reports* **10**, 10780 (2020).
208. C. Arnold, C. Larivière-Loiselle, K. Khalili, L. Inhester, R. Welsch, R. Santra: *Molecular electronic decoherence following attosecond photoionization*. *Journal of Physics B: Atomic, Molecular and Optical Physics* **53**, 164006 (2020).
207. L. Kjellsson, K. D. Nanda, J.-E. Rubensson, G. Doumy, S. H. Southworth, P. J. Ho, A. M. March, A. Al Haddad, Y. Kumagai, M.-F. Tu, R. D. Schaller, T. Debnath, M. S. Bin Mohd Yusof, C. Arnold, W. F. Schlotter, S. Moeller, G. Coslovich, J. D. Koralek, M. P. Minitti, M. L. Vidal, M. Simon, R. Santra, Z.-H. Loh, S. Coriani, A. I. Krylov, L. Young: *Resonant inelastic x-ray scattering reveals hidden local transitions of the aqueous OH radical*. *Physical Review Letters* **124**, 236001 (2020).

206. S.-K. Son, R. Boll, R. Santra: *Breakdown of frustrated absorption in x-ray sequential multiphoton ionization*. *Physical Review Research* **2**, 023053 (2020).
205. K. Nass, A. Gorel, M. M. Abdullah, A. V. Martin, M. Kloos, A. Marinelli, A. Aquila, T. R. M. Barends, F.-J. Decker, R. Bruce Doak, L. Foucar, E. Hartmann, M. Hilpert, M. S. Hunter, Z. Jurek, J. E. Koglin, A. Kozlov, A. A. Lutman, G. N. Kovacs, C. M. Roome, R. L. Shoeman, R. Santra, H. M. Quiney, B. Ziaja, S. Boutet, I. Schlichting: *Structural dynamics in proteins induced by and probed with x-ray free-electron laser pulses*. *Nature Communications* **11**, 1814 (2020).
204. A. Karamatskou, R. Esteban Goetz, C. P. Koch, R. Santra: *Suppression of hole decoherence in ultrafast photoionization*. *Physical Review A* **101**, 043405 (2020).
203. Y. Kumagai, Y. Z. Jurek, W. Xu, H. Fukuzawa, K. Motomura, D. Iablonskyi, K. Nagaya, S.-i., Wada, S. Mondal, T. Tachibana, Y. Ito, T. Sakai, K. Matsunami, T. Nishiyama, T. Umemoto, C. Nicolas, C. Miron, T. Togashi, K. Ogawa, S. Owada, K. Tono, M. Yabashi, S.-K. Son, B. Ziaja, R. Santra, K. Ueda: *Real-time observation of disintegration processes within argon clusters ionized by a hard-x-ray pulse of moderate fluence*. *Physical Review A* **101**, 023412 (2020).
202. Z.-H. Loh, G. Doumy, C. Arnold, L. Kjellsson, S. H. Southworth, A. Al Haddad, Y. Kumagai, M.-F. Tu, P. J. Ho, A. M. March, R. D. Schaller, M. S. Bin Mohd Yusof, T. Debnath, M. Simon, R. Welsch, L. Inhester, K. Khalili, K. Nanda, A. I. Krylov, S. Moeller, G. Coslovich, J. Koralek, M. P. Minitti, W. F. Schlotter, J.-E. Rubensson, R. Santra, L. Young: *Observation of the fastest chemical processes in the radiolysis of water*. *Science* **367**, 179 (2020).
201. N. Berrah, A. Sanchez-Gonzalez, Z. Jurek, R. Obaid, H. Xiong, R. J. Squibb, T. Osipov, A. Lutman, L. Fang, T. Barillot, J. D. Bozek, J. Cryan, T. J. A. Wolf, D. Rolles, R. Coffee, K. Schnorr, S. Augustin, H. Fukuzawa, K. Motomura, N. Niebuhr, L. J. Frasinski, R. Feifel, C. P. Schulz, K. Toyota, S.-K. Son, K. Ueda, T. Pfeifer, J. P. Marangos, R. Santra: *Femtosecond-resolved observation of the fragmentation of buckminsterfullerene following X-ray multiphoton ionization*. *Nature Physics* **15**, 1279 (2019).
200. S. Bazzi, R. Santra: *Ultrafast charge transfer and structural dynamics following outer-valence ionization of a halogen-bonded dimer*. *Journal of Physical Chemistry A* **123**, 7351 (2019).
199. K. Ueda, E. Sokell, S. Schippers, F. Aumayr, H. Sadeghpour, J. Burgdörfer, C. Lemell, X.-M. Tong, T. Pfeifer, F. Calegari, A. Palacios, F. Martin, P. Corkum, G. Sansone, E. V. Gryzlova, A. N. Grum-Grzhimailo, M. Novella Piancastelli, P. M. Weber, T. Steinle, K. Amini, J. Biegert, N. Berrah, E. Kukk, R. Santra, A. Müller, D. Dowek, R. R. Lucchese, C. W. McCurdy, P. Bolognesi, L. Avaldi, T. Jahnke, M. S. Schöffler, R. Dörner, Y. Mairesse, L. Nahon, O. Smirnova, T. Schlathölter, E. Campbell, J.-M. Rost, M. Meyer, K. A. Tanaka: *Roadmap on photonic, electronic and atomic collision physics: I. Light-matter interaction*. *Journal of Physics B* **52**, 171001 (2019).
198. L. Inhester, L. Greenman, A. Rudenko, D. Rolles, R. Santra: *Detecting coherent core-hole wave-packet dynamics in N₂ by time- and angle-resolved inner-shell photoelectron spectroscopy*. *Journal of Chemical Physics* **151**, 054107 (2019).
197. K. Khalili, L. Inhester, C. Arnold, R. Welsch, J. Wenzel Andreasen, R. Santra: *Hole dynamics in a photovoltaic donor-acceptor couple revealed by simulated time-resolved x-ray absorption spectroscopy*. *Structural Dynamics* **6**, 044102 (2019).
196. Y. Hao, L. Inhester, S.-K. Son, R. Santra: *Theoretical evidence for the sensitivity of charge-rearrangement-enhanced x-ray ionization to molecular size*. *Physical Review A* **100**, 013402 (2019).
195. K. Toyota, Z. Jurek, S.-K. Son, H. Fukuzawa, K. Ueda, N. Berrah, B. Rudek, D. Rolles, A. Rudenko, R. Santra: *Xcalib: a focal spot calibrator for intense x-ray free-electron laser pulses*

- based on the charge state distributions of light atoms*. Journal of Synchrotron Radiation **26**, 1017 (2019).
194. D. Kolbasova, R. Santra: *Analytical theory of attosecond transient absorption spectroscopy of perturbatively dressed systems*. Applied Sciences **9**, 1350 (2019).
 193. A. M. Hanna, O. Vendrell, R. Santra: *Time-resolved x-ray/optical pump-probe simulations on N₂ molecules*. Structural Dynamics **6**, 024101 (2019).
 192. D. Krebs, D. A. Reis, R. Santra: *Time-dependent QED approach to x-ray nonlinear Compton scattering*. Physical Review A **99**, 022120 (2019).
 191. C. Arnold, L. Inhester, S. Carbajo, R. Welsch, R. Santra: *Simulated XUV photoelectron spectra of THz-pumped liquid water*. Journal of Chemical Physics **150**, 044505 (2019).
 190. M. K. Ganesa Subramanian, R. Santra, R. Welsch: *Infrared-laser-pulse-enhanced ultrafast fragmentation of N₂²⁺ following Auger decay: Mixed quantum-classical simulations*. Physical Review A **98**, 063421 (2018).
 189. D. Popova-Gorelova, D. Reis, R. Santra: *Theory of x-ray scattering from laser-driven electronic systems*. Physical Review B **98**, 224302 (2018).
 188. B. Rudek, K. Toyota, L. Foucar, B. Erk, R. Boll, C. Bomme, J. Correa, S. Carron, S. Boutet, G. J. Williams, K. R. Ferguson, R. Alonso-Mori, J. E. Koglin, T. Gorkhover, M. Bucher, C. S. Lehmann, B. Krässig, S. H. Southworth, L. Young, C. Bostedt, K. Ueda, T. Marchenko, M. Simon, Z. Jurek, R. Santra, A. Rudenko, S.-K. Son, D. Rolles: *Relativistic and resonant effects in the ionization of heavy atoms by ultra-intense hard x-rays*. Nature Communications **9**, 4200 (2018).
 187. M. M. Abdullah, S.-K. Son, Z. Jurek, R. Santra: *Towards the theoretical limitations of x-ray nanocrystallography at high intensity: the validity of the effective-form-factor description*. IUCrJ **5**, 699 (2018).
 186. J. J. Bekx, S.-K. Son, R. Santra, B. Ziaja: *Ab initio calculation of electron-impact-ionization cross sections for ions in exotic electron configurations*. Physical Review A **98**, 022701 (2018).
 185. P. K. Mishra, V. Bettaque, O. Vendrell, R. Santra, R. Welsch: *Prospects of using high-intensity THz pulses to induce ultrafast temperature-jumps in liquid water*. Journal of Physical Chemistry A **122**, 5211 (2018).
 184. Y. Kumagai, Z. Jurek, W. Xu, H. Fukuzawa, K. Motomura, D. Iablonskyi, K. Nagaya, S.-i. Wada, S. Mondal, T. Tachibana, Y. Ito, T. Sakai, K. Matsunami, T. Nishiyama, T. Umemoto, C. Nicolas, C. Miron, T. Togashi, K. Ogawa, S. Owada, K. Tono, M. Yabashi, S.-K. Son, B. Ziaja, R. Santra, K. Ueda: *Radiation-induced chemical dynamics in Ar clusters exposed to strong x-ray pulses*. Physical Review Letters **120**, 223201 (2018).
 183. P. Zalden, L. Song, X. Wu, H. Huang, F. Ahr, O. D. Mücke, J. Reichert, M. Thorwart, P. Kr. Mishra, R. Welsch, R. Santra, F. X. Kärtner, C. Bressler: *Molecular polarizability anisotropy of liquid water revealed by terahertz-induced transient orientation*. Nature Communications **9**, 2142 (2018).
 182. J. M. Schäfer, L. Inhester, S. -K. Son, R. F. Fink, R. Santra: *Electron and fluorescence spectra of a water molecule irradiated by an x-ray free-electron laser pulse*. Physical Review A **97**, 053415 (2018).
 181. Y.-J. Chen, S. Pabst, R. Santra: *Collective resonances of atomic xenon from the linear to the nonlinear regime*. Journal of Physics Communications **2**, 045024 (2018).
 180. C. Arnold, O. Vendrell, R. Welsch, R. Santra: *Control of nuclear dynamics through conical intersections and electronic coherences*. Physical Review Letters **120**, 123001 (2018).

179. L. Inhester, B. Oostenrijk, M. Patanen, E. Kokkonen, S. H. Southworth, C. Bostedt, O. Travnikova, T. Marchenko, S.-K. Son, R. Santra, M. Simon, L. Young, and S. L. Sorensen: *A chemical understanding of the limited site-specificity in molecular inner-shell photofragmentation*. *Journal of Physical Chemistry Letters* **9**, 1156 (2018).
178. S. Bazzi, R. Welsch, O. Vendrell, R. Santra: *Challenges in XUV photochemistry simulations: A case study on ultrafast fragmentation dynamics of the benzene radical cation*. *Journal of Physical Chemistry A* **122**, 1004 (2018).
177. L. Young, K. Ueda, M. Gühr, P.H. Bucksbaum, M. Simon, S. Mukamel, N. Rohringer, K. C. Prince, C. Masciovecchio, M. Meyer, A. Rudenko, D. Rolles, C. Bostedt, M. Fuchs, D. A. Reis, R. Santra, H. Kapteyn, M. Murnane, H. Ibrahim, F. Légaré, M. Vrakking, M. Isinger, D. Kroon, M. Gisselbrecht, A. L'Huillier, H. J. Wörner, S. R Leone: *Roadmap of ultrafast x-ray atomic and molecular physics*. *Journal of Physics B: Atomic, Molecular and Optical Physics* **51**, 032003 (2018).
176. F. Theel, A. Karamatskou, R. Santra: *The fractal geometry of Hartree-Fock*. *Chaos* **27**, 123103 (2017).
175. G. Dixit, R. Santra: *Time-resolved ultrafast x-ray scattering from an incoherent electronic mixture*. *Physical Review A* **96**, 053413 (2017).
174. A. Karamatskou, R. Santra, O. Vendrell: *Ab initio investigation of nonlinear mode coupling in C₆₀*. *Journal of Physical Chemistry Letters* **8**, 5543 (2017).
173. C. Fortmann-Grote, A. A. Andreev, K. Appel, J. Branco, R. Briggs, M. Bussmann, A. Buzmakov, M. Garten, A. Grund, A. Hübl, Z. Jurek, N. D. Loh, M. Nakatsutsumi, L. Samoylova, R. Santra, E. A. Schneidmiller, A. Sharma, K. Steiniger: *Simulations of ultrafast x-ray laser experiments*. *Proceedings of SPIE* **10237**, 10237OS (2017).
172. C. Fortmann-Grote, A. Buzmakov, Z. Jurek, N.-T. Duane Loh, L. Samoylova, R. Santra, E. Schneidmiller, T. Tschentscher, S. Yakubov, C. H. Yoon, M. V. Yurkov, B. Ziaja-Motyka, A. P. Mancuso: *Start-to-end simulation of single-particle imaging using ultra-short pulses at the European X-ray Free-Electron Laser*. *IUCrJ* **4**, 560 (2017).
171. C. Fortmann-Grote, J. Bielecki, Z. Jurek, R. Santra, B. Ziaja-Motyka, A. P. Mancuso: *Simulations of single-particle imaging of hydrated proteins with x-ray free-electron lasers*. *Proceedings of SPIE* **10388**, 10388OM (2017).
170. M. M. Abdullah, Anurag, Z. Jurek, S.-K. Son, R. Santra: *Molecular-dynamics approach for studying the nonequilibrium behavior of X-ray-heated solid-density matter*. *Physical Review E* **96**, 023205 (2017). Erratum: *Physical Review E* **103**, 029901 (2021).
169. A. Baumann, S. Bazzi, D. Rompotis, O. Schepp, A. Azima, M. Wieland, D. Popova-Gorelova, O. Vendrell, R. Santra, M. Drescher: *Weak-field few-femtosecond VUV photodissociation dynamics of water isotopologues*. *Physical Review A* **96**, 013428 (2017).
168. M. Grosser, J. M. Slowik, R. Santra: *Attosecond x-ray scattering from a particle-hole wave packet*. *Physical Review A* **95**, 062107 (2017).
167. A. Rudenko, L. Inhester, K. Hanasaki, X. Li, S. J. Robotjazi, B. Erk, R. Boll, K. Toyota, Y. Hao, O. Vendrell, C. Bomme, E. Savelyev, B. Rudek, L. Foucar, S. H. Southworth, C. S. Lehmann, B. Kraessig, T. Marchenko, M. Simon, K. Ueda, K. R. Ferguson, M. Bucher, T. Gorkhover, S. Carron, R. Alonso-Mori, J. E. Koglin, J. Correa, G. J. Williams, S. Boutet, L. Young, C. Bostedt, S.-K. Son, R. Santra, D. Rolles: *Femtosecond response of polyatomic molecules to ultra-intense hard x-rays*. *Nature* **546**, 129 (2017).
166. M. Hollstein, R. Santra, D. Pfannkuche: *Correlation-driven charge migration following double ionization and attosecond transient absorption spectroscopy*. *Physical Review A* **95**, 053411 (2017).

165. S. Pabst, R. Santra: *Time-dependent configuration-interaction singles*. In "Computational Strong-Field Quantum Dynamics", edited by D. Bauer (De Gruyter, Berlin, 2017).
164. M. Sabbar, H. Timmers, Y.-J. Chen, A. K. Pymer, Z.-H. Loh, S. G. Sayres, S. Pabst, R. Santra, S. R. Leone: *State-resolved attosecond reversible and irreversible dynamics in strong optical fields*. *Nature Physics* **13**, 472 (2017).
163. A. M. Hanna, O. Vendrell, A. Ourmazd, R. Santra: *Laser control over the ultrafast Coulomb explosion of N_2^{2+} after Auger decay: A quantum-dynamics investigation*. *Physical Review A* **95**, 043419 (2017).
162. K. Toyota, S.-K. Son, R. Santra: *Interplay between relativistic energy corrections and resonant excitations in x-ray multiphoton ionization dynamics of Xe atoms*. *Physical Review A* **95**, 043412 (2017).
161. C. Arnold, O. Vendrell, R. Santra: *Electronic decoherence following photoionization: Full quantum-dynamical treatment of the influence of nuclear motion*. *Physical Review A* **95**, 033425 (2017).
160. S.-K. Son, O. Geffert, R. Santra: *Compton spectra of atoms at high x-ray intensity*. *Journal of Physics B: Atomic, Molecular and Optical Physics* **50**, 064003 (2017).
159. R. Santra, J. Schirmer: *Finite-temperature second-order many-body perturbation theory revisited*. *Chemical Physics* **482**, 355 (2017).
158. A. Karamatskou, R. Santra: *Time-dependent configuration-interaction-singles calculation of the 5p-subshell two-photon ionization cross section in xenon*. *Physical Review A* **95**, 013415 (2017).
157. S. Pabst, A. Sytcheva, O. Geffert, R. Santra: *Stability of the time-dependent configuration-interaction-singles method in the attosecond and strong-field regimes: A study of basis sets and absorption methods*. *Physical Review A* **94**, 033421 (2016).
156. L. Inhester, K. Hanasaki, Y. Hao, S.-K. Son, R. Santra: *X-ray multiphoton ionization dynamics of a water molecule irradiated by an x-ray free-electron laser pulse*. *Physical Review A* **94**, 023422 (2016).
155. R. E. Goetz, M. Merkel, A. Karamatskou, R. Santra, C. P. Koch: *Maximizing hole coherence in ultrafast photoionization of argon with an optimization by sequential parametrization update*. *Physical Review A* **94**, 023420 (2016).
154. D. Popova-Gorelova, J. Küpper, R. Santra: *Imaging electron dynamics with time- and angle-resolved photoelectron spectroscopy*. *Physical Review A* **94**, 013412 (2016).
153. M. M. Abdullah, Z. Jurek, S.-K. Son, R. Santra: *Calculation of x-ray scattering patterns from nanocrystals at high x-ray intensity*. *Structural Dynamics* **3**, 054101 (2016).
152. R. Santra, L. Young: *Interaction of intense x-ray beams with atoms*. In "Handbook of Synchrotron Light Sources and Free-Electron Lasers", edited by E. J. Jaeschke, S. Khan, J. R. Schneider, J. B. Hastings (Springer International Publishing, Switzerland, 2016).
151. Z. Jurek, S.-K. Son, B. Ziaja, R. Santra: *XMDYN and XATOM: versatile simulation tools for quantitative modeling of x-ray free-electron laser induced dynamics of matter*. *Journal of Applied Crystallography* **49**, 1048-1056 (2016).
150. R. Fung, A. M. Hanna, O. Vendrell, S. Ramakrishna, T. Seideman, R. Santra, A. Ourmazd: *Dynamics from noisy data with extreme timing uncertainty*. *Nature* **532**, 471 (2016).
149. C. H. Yoon, M. V. Yurkov, E. A. Schneidmiller, L. Samoylova, A. Buzmakov, Z. Jurek, B. Ziaja, R. Santra, N. D. Loh, T. Tschentscher, A. P. Mancuso: *A comprehensive simulation framework*

- for imaging single particles and biomolecules at the European X-ray Free-Electron Laser.* Scientific Reports **6**, 24791 (2016).
148. P. K. Mishra, O. Vendrell, R. Santra: *Subpicosecond energy transfer from a highly intense THz pulse to water: A computational study based on the TIP4P/2005 rigid-water-molecule model.* Physical Review E **93**, 032124 (2016).
147. E. Goetz, A. Karamatskou, R. Santra, C. P. Koch: *Quantum optimal control of photoelectron spectra and angular distributions.* Physical Review A **93**, 013413 (2016).
146. S. Pabst, D. Wang, R. Santra: *Driving Rabi oscillations at the giant dipole resonance in xenon.* Physical Review A **92**, 053424 (2015).
145. D. Popova-Gorelova, R. Santra: *Imaging interatomic electron current in crystals with ultrafast resonant x-ray scattering.* Physical Review B **92**, 184304 (2015).
144. L. Galli, S.-K. Son, T. R. M. Barends, T. A. White, A. Barty, S. Botha, S. Boutet, C. Caleman, R. B. Doak, M. H. Nanao, K. Nass, R. L. Shoeman, N. Timneanu, R. Santra, I. Schlichting, H. N. Chapman: *Towards phasing using high x-ray intensity.* IUCrJ **2**, 167 (2015).
143. Z. Li, O. Vendrell, R. Santra: *Ultrafast charge transfer of a valence double hole in glycine driven exclusively by nuclear motion.* Physical Review Letters **115**, 143002 (2015).
142. P. K. Mishra, O. Vendrell, R. Santra: *Ultrafast energy transfer from solvent to solute induced by subpicosecond highly intense THz pulses.* Journal of Physical Chemistry B **119**, 8080 (2015).
141. T. Tachibana, Z. Jurek, H. Fukuzawa, K. Motomura, K. Nagaya, S. Wada, P. Johnsson, M. Siano, S. Mondal, Y. Ito, M. Kimura, T. Sakai, K. Matsunami, H. Hayashita, J. Kajikawa, X.-J. Liu, E. Robert, C. Miron, R. Feifel, J. P. Marangos, K. Tono, Y. Inubushi, M. Yabashi, S.-K. Son, B. Ziaja, M. Yao, R. Santra, K. Ueda: *Nanoplasma formation by high intensity hard x-rays.* Scientific Reports **5**, 10977 (2015).
140. D. Popova-Gorelova, R. Santra: *Imaging instantaneous electron flow with ultrafast resonant x-ray scattering.* Physical Review B **91**, 184303 (2015).
139. V. Saxena, Z. Jurek, B. Ziaja, R. Santra: *Hydrodynamic model for picosecond propagation of laser-created nanoplasmas.* High Energy Density Physics **15**, 93 (2015).
138. M. Tilley, A. Karamatskou, R. Santra: *Wave-packet propagation based calculation of above-threshold ionization in the x-ray regime.* Journal of Physics B: Atomic, Molecular and Optical Physics **48**, 124001 (2015).
137. Y. Hao, L. Inhester, K. Hanasaki, S.-K. Son, R. Santra: *Efficient electronic structure calculation for molecular ionization dynamics at high x-ray intensity.* Structural Dynamics **2**, 041707 (2015).
136. L. Fang, Z. Jurek, T. Osipov, B. F. Murphy, R. Santra, N. Berrah: *Investigating dynamics of complex system irradiated by intense x-ray free electron laser pulses.* Journal of Physics: Conference Series **601**, 012006 (2015).
135. A. Aquila, A. Barty, C. Bostedt, S. Boutet, G. Carini, D. dePonte, P. Drell, S. Doniach, K. H. Downing, T. Earnest, H. Elmlund, V. Elser, M. Gühr, J. Hajdu, J. Hastings, S. P. Hau-Riege, Z. Huang, E. E. Lattman, F. R. N. C. Maia, S. Marchesini, A. Ourmazd, C. Pellegrini, R. Santra, I. Schlichting, C. Schroer, J. C. H. Spence, I. A. Vartanyants, S. Wakatsuki, W. I. Weis, G. J. Williams: *The linac coherent light source single particle imaging road map.* Structural Dynamics **2**, 041701 (2015).
134. T. Mazza, A. Karamatskou, M. Ilchen, S. Bakhtiarzadeh, A. J. Rafipoor, P. O’Keeffe, T. J. Kelly, N. Walsh, J. T. Costello, M. Meyer, R. Santra: *Sensitivity of nonlinear photoionization to resonance substructure in collective excitation.* Nature Communications **6**, 6799 (2015).

133. Y.-J. Chen, S. Pabst, A. Karamatskou, R. Santra: *Theoretical characterization of the collective resonance states underlying the xenon giant dipole resonance*. *Physical Review A* **91**, 032503 (2015).
132. B. Ziaja, Z. Jurek, N. Medvedev, V. Saxena, S.-K. Son, R. Santra: *Towards realistic simulations of macromolecules irradiated under the conditions of coherent diffraction imaging with an x-ray free-electron laser*. *Photonics* **2**, 256 (2015).
131. L. Galli, S.-K. Son, T. A. White, R. Santra, H. N. Chapman, M. H. Nanao: *Towards RIP using free-electron laser SFX data*. *Journal of Synchrotron Radiation* **22**, 249 (2015).
130. B. Ziaja, Z. Jurek, V. Saxena, R. Santra: *Modeling of nanoplasmas created from finite systems by ultrafast intense x-ray pulses*. *Contributions to Plasma Physics* **55**, 58 (2015).
129. N. Berrah, L. Fang, T. Osipov, Z. Jurek, B. F. Murphy, R. Santra: *Emerging photon technologies for probing ultrafast molecular dynamics*. *Faraday Discussions* **171**, 471 (2014).
128. Z. Li, M. E.-A. Madjet, O. Vendrell, R. Santra: *Core-level transient absorption spectroscopy as a probe of electron hole relaxation in photoionized $H^+(H_2O)_n$* . *Faraday Discussions* **171**, 457 (2014).
127. R. Santra, G. Dixit, J. M. Slowik: *Comment on "How to observe coherent electron dynamics directly"*. *Physical Review Letters* **113**, 189301 (2014).
126. H. Timmers, Z. Li, N. Shivaram, R. Santra, O. Vendrell, A. Sandhu: *Coherent electron hole dynamics near a conical intersection*. *Physical Review Letters* **113**, 113003 (2014).
125. J. M. Slowik, S.-K. Son, G. Dixit, Z. Jurek, R. Santra: *Incoherent x-ray scattering in single molecule imaging*. *New Journal of Physics* **16**, 073042 (2014).
124. S.-K. Son, R. Thiele, Z. Jurek, B. Ziaja, R. Santra: *Quantum-mechanical calculation of ionization-potential lowering in dense plasmas*. *Physical Review X* **4**, 031004 (2014).
123. B. F. Murphy, T. Osipov, Z. Jurek, L. Fang, S.-K. Son, M. Mucke, J. H. D. Eland, V. Zhaunerchyk, R. Feifel, L. Avaldi, P. Bolognesi, C. Bostedt, J. D. Bozek, J. Grilj, M. Gühr, L. J. Frasinski, J. Glowina, D. T. Ha, K. Hoffmann, E. Kukk, B. K. McFarland, C. Miron, E. Sistrunk, R. J. Squibb, K. Ueda, R. Santra, N. Berrah: *Femtosecond x-ray-induced explosion of C_{60} at extreme intensity*. *Nature Communications* **5**, 4281 (2014).
122. Z. Jurek, B. Ziaja, R. Santra: *Applicability of the classical molecular dynamics method to study x-ray irradiated molecular systems*. *Journal of Physics B: Atomic, Molecular and Optical Physics* **47**, 124036 (2014).
121. S. Pabst, R. Santra: *Spin-orbit effects in atomic high-harmonic generation*. *Journal of Physics B: Atomic, Molecular and Optical Physics* **47**, 124026 (2014).
120. Y.-J. Chen, S. Pabst, Z. Li, O. Vendrell, R. Santra: *Dynamics of fluctuations in a quantum system*. *Physical Review A* **89**, 052113 (2014).
119. E. Heinrich-Josties, S. Pabst, R. Santra: *Controlling the 2p hole alignment in neon via the 2s-3p Fano resonance*. *Physical Review A* **89**, 043415 (2014).
118. G. Dixit, J. M. Slowik, R. Santra: *Theory of time-resolved nonresonant x-ray scattering for imaging ultrafast coherent electron motion*. *Physical Review A* **89**, 043409 (2014).
117. G. Dixit, R. Santra: *Imaging ultrafast electronic motion by x-ray scattering*. *Journal of Physics: Conference Series* **488**, 012009 (2014).
116. A. Karamatskou, S. Pabst, Y.-J. Chen, R. Santra: *Calculation of photoelectron spectra within the time-dependent configuration-interaction singles scheme*. *Physical Review A* **89**, 033415 (2014). Erratum: *Physical Review A* **91**, 069907 (2015).

115. S. R. Leone, C. W. McCurdy, J. Burgdörfer, L. S. Cederbaum, Z. Chang, N. Dudovich, J. Feist, C. H. Greene, M. Ivanov, R. Kienberger, U. Keller, M. F. Kling, Z.-H. Loh, T. Pfeifer, A. N. Pfeiffer, R. Santra, K. Schafer, A. Stolow, U. Thumm; M. J. J. Vrakking: *What will it take to observe processes in 'real time'?* Nature Photonics **8**, 162 (2014).
114. J. Küpper, S. Stern, L. Holmegaard, F. Filsinger, A. Rouzée, A. Rudenko, P. Johnsson, A. V. Martin, M. Adolph, A. Aquila, S. Bajt, A. Barty, C. Bostedt, J. Bozek, C. Caleman, R. Coffee, N. Coppola, T. Delmas, S. Epp, B. Erk, L. Foucar, T. Gorkhover, L. Gumprecht, A. Hartmann, R. Hartmann, G. Hauser, P. Holl, A. Hömke, N. Kimmel, F. Krasniqi, K.-U. Kühnel, J. Maurer, M. Messerschmidt, R. Mosshammer, C. Reich, B. Rudek, R. Santra, I. Schlichting, C. Schmidt, S. Schorb, J. Schulz, H. Soltau, J. C. H. Spence, D. Starodub, L. Strüder, J. Thøgersen, M. J. J. Vrakking, G. Weidenspointner, T. A. White, C. Wunderer, G. Meijer, J. Ullrich, H. Stapelfeldt, D. Rolles, H. N. Chapman: *X-ray diffraction from isolated and strongly aligned gas-phase molecules with a free-electron laser*. Physical Review Letters **112**, 083002 (2014)
113. D. Krebs, S. Pabst, R. Santra: *Introducing many-body physics using atomic spectroscopy*. American Journal of Physics **82**, 113 (2014).
112. P. K. Mishra, O. Vendrell, R. Santra: *Ultrafast energy transfer to liquid water by sub-picosecond high-intensity terahertz pulses: An ab initio molecular dynamics study*. Angewandte Chemie International Edition **52**, 13685 (2013).
111. S. Pabst, R. Santra: *Strong-field many-body physics and the giant enhancement in the high-harmonic spectrum of xenon*. Physical Review Letters **111**, 233005 (2013).
110. S. Bhardwaj, S.-K. Son, K.-H. Hong, C.-J. Lai, F. X. Kärtner, R. Santra: *Recombination-amplitude calculations of noble gases, in both length and acceleration forms, beyond the strong-field approximation*. Physical Review A **88**, 053405 (2013).
109. K. Motomura, H. Fukuzawa, S.-K. Son, S. Mondal, T. Tachibana, Y. Ito, M. Kimura, K. Nagaya, T. Sakai, K. Matsunami, S. Wada, H. Hayashita, J. Kajikawa, X.-J. Liu, R. Feifel, P. Johnsson, M. Siano, E. Kukk, B. Rudek, B. Erk, L. Foucar, E. Robert, C. Miron, K. Tono, Y. Inubushi, T. Hatsui, M. Yabashi, M. Yao, R. Santra, K. Ueda: *Sequential multiphoton multiple ionization of atomic argon and xenon irradiated by x-ray free-electron laser pulses from SACLA*. Journal of Physics B **46**, 164024 (2013).
108. S.-K. Son, H. N. Chapman, R. Santra: *Determination of multiwavelength anomalous diffraction coefficients at high x-ray intensity*. Journal of Physics B **46**, 164015 (2013).
107. J. M. Slowik, R. Santra: *X-ray phase-contrast imaging: the quantum perspective*. Journal of Physics B **46**, 164016 (2013).
106. L. Müller, C. Gutt, B. Pfau, S. Schaffert, J. Geilhufe, F. Büttner, J. Mohanty, S. Flewett, R. Treusch, S. Düsterer, H. Redlin, A. Al-Shemmary, M. Hille, A. Kobs, R. Frömter, H. P. Oepen, B. Ziaja, N. Medvedev, S.-K. Son, R. Thiele, R. Santra, B. Vodungbo, J. Lüning, S. Eisebitt, G. Grübel: *Breakdown of the x-ray resonant magnetic scattering signal during intense pulses of extreme ultraviolet free-electron-laser radiation*. Physical Review Letters **110**, 234801 (2013).
105. H. Fukuzawa, S.-K. Son, K. Motomura, S. Mondal, K. Nagaya, S. Wada, X.-J. Liu, R. Feifel, T. Tachibana, Y. Ito, M. Kimura, T. Sakai, K. Matsunami, H. Hayashita, J. Kajikawa, P. Johnsson, M. Siano, E. Kukk, B. Rudek, B. Erk, L. Foucar, E. Robert, C. Miron, K. Tono, Y. Inubushi, T. Hatsui, M. Yabashi, M. Yao, R. Santra, K. Ueda: *Deep inner-shell multiphoton ionization by intense x-ray free-electron laser pulse*. Physical Review Letters **110**, 173005 (2013).
104. A. Karamatskou, S. Pabst, R. Santra: *Adiabaticity and diabaticity in strong-field ionization*. Physical Review A **87**, 043422 (2013).
103. G. Dixit, R. Santra: *Role of electron-electron interference in ultrafast time-resolved imaging of electronic wavepackets*. Journal of Chemical Physics **138**, 134311 (2013).

102. G. Dixit, J. M. Slowik, R. Santra: *Proposed imaging of the ultrafast electronic motion in samples using x-ray phase contrast*. Physical Review Letters **110**, 137403 (2013).
101. A. Wirth, R. Santra, E. Goulielmakis: *Real time tracing of valence-shell electronic coherences with attosecond transient absorption spectroscopy*. Chemical Physics **414**, 149 (2013).
100. B. Rudek, D. Rolles, S.-K. Son, L. Foucar, B. Erk, S. Epp, R. Boll, D. Anielski, C. Bostedt, S. Schorb, R. Coffee, J. Bozek, S. Trippel, T. Marchenko, M. Simon, L. Christensen, S. De, S. Wada, K. Ueda, I. Schlichting, R. Santra, J. Ullrich, A. Rudenko: *Resonance-enhanced multiple ionization of krypton at an x-ray free-electron laser*. Physical Review A **87**, 023413 (2013).
99. Z. Li, M. El-A. Madjet, O. Vendrell, R. Santra: *Correlated dynamics of the motion of proton-hole wave packets in a photoionized water cluster*. Physical Review Letters **110**, 038302 (2013).
98. S. Pabst, A. Sytcheva, A. Moulet, A. Wirth, E. Goulielmakis, R. Santra: *Theory of attosecond transient-absorption spectroscopy of krypton for overlapping pump and probe pulses*. Physical Review A **86**, 063411 (2012).
97. B. Ziaja, H. N. Chapman, R. Fäustlin, S. Hau-Riege, Z. Jurek, A. V. Martin, S. Toleikis, F. Wang, E. Weckert, R. Santra: *Limitations of coherent diffractive imaging of single objects due to their damage by intense x-ray radiation*. New Journal of Physics **14**, 115015 (2012).
96. N. Rohringer and R. Santra: *Strongly driven resonant Auger effect treated by an open-quantum-system approach*. Physical Review A **86**, 043434 (2012).
95. B. Rudek, S.-K. Son, L. Foucar, S. W. Epp, B. Erk, R. Hartmann, M. Adolph, R. Andritschke, A. Aquila, N. Berrah, C. Bostedt, J. Bozek, N. Coppola, F. Filsinger, H. Gorke, T. Gorkhover, H. Graafsma, L. Gumprecht, A. Hartmann, G. Hauser, S. Herrmann, H. Hirsemann, P. Holl, A. Hömke, L. Journal, C. Kaiser, N. Kimmel, F. Krasniqi, K.-U. Kühnel, M. Matysek, M. Messerschmidt, D. Miesner, T. Möller, R. Moshhammer, K. Nagaya, B. Nilsson, G. Potdevin, D. Pietschner, C. Reich, D. Rupp, G. Schaller, I. Schlichting, C. Schmidt, F. Schopper, S. Schorb, C. -D. Schröter, J. Schulz, M. Simon, H. Soltau, L. Strüder, K. Ueda, G. Weidenspointner, R. Santra, J. Ullrich, A. Rudenko, D. Rolles: *Ultra-efficient ionization of heavy atoms by intense x-ray free-electron laser pulses*. Nature Photonics **6**, 858 (2012).
94. Z. Jurek, R. Thiele, B. Ziaja, R. Santra: *Effect of two-particle correlations on x-ray coherent diffractive imaging studies performed with continuum models*. Physical Review E **86**, 036411 (2012).
93. R. Thiele, S.-K. Son, B. Ziaja, R. Santra: *Effect of screening by external charges on the atomic orbitals and photoinduced processes within the Hartree-Fock-Slater atom*. Physical Review A **86**, 033411 (2012).
92. R. W. Dunford, S. H. Southworth, D. Ray, E. P. Kanter, B. Krässig, L. Young, D. A. Arms, E. M. Dufresne, D. A. Walko, O. Vendrell, S.-K. Son, R. Santra: *Evidence for interatomic Coulombic decay in Xe K-shell-vacancy decay of XeF₂*. Physical Review A **86**, 033401 (2012).
91. G. Dixit, O. Vendrell, R. Santra: *Imaging electronic quantum motion with light*. Proceedings of the National Academy of Sciences of the United States of America **109**, 11636 (2012).
90. S.-K. Son, R. Santra: *Monte Carlo calculation of ion, electron, and photon spectra of xenon atoms in x-ray free-electron laser pulses*. Physical Review A **85**, 063415 (2012). Erratum: Physical Review A **92**, 03906 (2015).
89. A. Sytcheva, S. Pabst, S.-K. Son, R. Santra: *Enhanced nonlinear response of Ne⁹⁺ to intense ultrafast x-rays*. Physical Review A **85**, 023414 (2012).
88. S. Pabst, L. Greenman, D. A. Mazziotti, R. Santra: *Impact of multichannel and multipole effects on the Cooper minimum in the high-order-harmonic spectrum of argon*. Physical Review A **85**, 023411 (2012).

87. M. Madjet, O. Vendrell, R. Santra: *Ultrafast dynamics of photoionized acetylene*. Physical Review Letters **107**, 263002 (2011).
86. E. P. Kanter, B. Krässig, Y. Li, A. M. March, P. Ho, N. Rohringer, R. Santra, S. H. Southworth, L. F. DiMauro, G. Doumy, C. A. Roedig, N. Berrah, L. Fang, M. Hoener, P. H. Bucksbaum, S. Ghimire, D. A. Reis, J. D. Bozek, C. Bostedt, M. Messerschmidt, L. Young: *Unveiling and driving hidden resonances with high-fluence, high-intensity x-ray pulses*. Physical Review Letters **107**, 233001 (2011).
85. S.-K. Son, H. N. Chapman, R. Santra: *Multi-wavelength anomalous diffraction at high x-ray intensity*. Physical Review Letters **107**, 218102 (2011).
84. A. Wirth, M. Th. Hassan, I. Grguras, J. Gagnon, A. Moulet, T. T. Luu, S. Pabst, R. Santra, Z. A. Alahmed, A. M. Azzeer, V. S. Yakovlev, V. Pervak, F. Krausz, E. Goulielmakis: *Synthesized light transients*. Science **334**, 195 (2011).
83. B. Ziaja, H. N. Chapman, R. Santra, T. Laarmann, E. Weckert, C. Bostedt, T. Möller: *Heterogeneous clusters as a model system for the study of ionization dynamics within tampered samples*. Physical Review A **84**, 033201 (2011).
82. N. V. Kryzhevoi, R. Santra, L. S. Cederbaum: *Inner-shell single and double ionization potentials of aminophenol isomers*. Journal of Chemical Physics **135**, 084302 (2011).
81. R. Santra, V. S. Yakovlev, T. Pfeifer, Z.-H. Loh: *Theory of attosecond transient absorption spectroscopy of strong-field-generated ions*. Physical Review A **83**, 033405 (2011).
80. S.-K. Son, L. Young, R. Santra: *Impact of hollow-atom formation on coherent x-ray scattering at high intensity*. Physical Review A **83**, 033402 (2011). Erratum: Physical Review A **83**, 069906 (2011).
79. G. Doumy, C. Roedig, S.-K. Son, C. I. Blaga, A. D. DiChiara, R. Santra, N. Berrah, C. Bostedt, J. D. Bozek, P. H. Bucksbaum, J. P. Cryan, L. Fang, S. Ghimire, J. M. Glowia, M. Hoener, E. P. Kanter, B. Krässig, M. Kuebel, M. Messerschmidt, G. G. Paulus, D. A. Reis, N. Rohringer, L. Young, P. Agostini, L. F. DiMauro: *Nonlinear atomic response to intense ultrashort x-rays*. Physical Review Letters **106**, 083002 (2011).
78. S. Pabst, L. Greenman, P. J. Ho, D. A. Mazziotti, R. Santra: *Decoherence in attosecond photoionization*. Physical Review Letters **106**, 053003 (2011).
77. E. Goulielmakis, Z.-H. Loh, A. Wirth, R. Santra, N. Rohringer, V. S. Yakovlev, S. Zherebtsov, T. Pfeifer, A. M. Azzeer, M. F. Kling, S. R. Leone, F. Krausz: *Real-time observation of valence electron motion*. Nature **466**, 739 (2010).
76. L. Greenman, P. J. Ho, S. Pabst, E. Kamarchik, D. A. Mazziotti, R. Santra: *Implementation of the time-dependent configuration interaction singles method for atomic strong-field processes*. Physical Review A **82**, 023406 (2010).
75. L. Young, E. P. Kanter, B. Krässig, Y. Li, A. M. March, S. T. Pratt, R. Santra, S. H. Southworth, N. Rohringer, L. F. DiMauro, G. Doumy, C. A. Roedig, N. Berrah, L. Fang, M. Hoener, P. H. Bucksbaum, J. P. Cryan, S. Ghimire, J. M. Glowia, D. A. Reis, J. D. Bozek, C. Bostedt, M. Messerschmidt: *Femtosecond electronic response of atoms to ultraintense x-rays*. Nature **466**, 56 (2010).
74. S. Pabst, R. Santra: *Alignment of asymmetric-top molecules using multiple-pulse trains*. Physical Review A **81**, 065401 (2010). Erratum: Physical Review A **82**, 049901 (2010).
73. S. Pabst, P. J. Ho, R. Santra: *Computational studies of x-ray scattering from three-dimensionally-aligned asymmetric-top molecules*. Physical Review A **81**, 043425 (2010).
72. R. Santra: *Zerfall im Verbund*. Physik Journal **9** (4), 19 (2010).

71. T. E. Glover, M. P. Hertlein, S. H. Southworth, T. K. Allison, J. van Tilborg, E. P. Kanter, B. Krässig, H. R. Varma, B. Rude, R. Santra, A. Belkacem, L. Young: *Controlling x-rays with light*. Nature Physics **6**, 69 (2009).
70. H. R. Varma, M. F. Ciappina, N. Rohringer, R. Santra: *Above-threshold ionization in the x-ray regime*. Physical Review A **80**, 053424 (2009).
69. P. J. Ho, D. Starodub, D. K. Saldin, V. L. Shneerson, A. Ourmazd, R. Santra: *Molecular structure determination from x-ray scattering patterns of laser-aligned symmetric-top molecules*. Journal of Chemical Physics **131**, 131101 (2009).
68. R. Santra, N. V. Kryzhevoi, L. S. Cederbaum: *X-ray two-photon photoelectron spectroscopy: A theoretical study of inner-shell spectra of the organic para-aminophenol molecule*. Physical Review Letters **103**, 013002 (2009).
67. N. Rohringer, R. Santra: *Multichannel coherence in strong-field ionization*. Physical Review A **79**, 053402 (2009).
66. P. J. Ho, M. R. Miller, R. Santra: *Field-free molecular alignment for studies using x-ray pulses from a synchrotron radiation source*. Journal of Chemical Physics **130**, 154310 (2009).
65. R. Santra: *Concepts in x-ray physics*. Journal of Physics B **42**, 023001 (2009). Corrigendum: Journal of Physics B **42**, 169801 (2009).
64. H. R. Varma, L. Pan, D. Beck, R. Santra: *X-ray absorption near-edge structure of laser-dressed neon*. Physical Review A **78**, 065401 (2008).
63. P. J. Ho, R. Santra: *Theory of x-ray diffraction from laser-aligned symmetric-top molecules*. Physical Review A **78**, 053409 (2008).
62. A. S. Sandhu, E. Gagnon, R. Santra, V. Sharma, W. Li, P. Ho, P. Ranitovic, C. L. Cocke, M. M. Murnane, H. C. Kapteyn: *Observing the creation of electronic Feshbach resonances in soft x-ray-induced O₂ dissociation*. Science **322**, 1081 (2008).
61. I. A. Sulai, Q. Wu, M. Bishof, G. W. F. Drake, Z.-T. Lu, P. Mueller, R. Santra: *Hyperfine suppression of $2^3S_1 - 3^3P_J$ transitions in ^3He* . Physical Review Letters **101**, 173001 (2008).
60. C. Buth, R. Santra: *X-ray refractive index of laser-dressed atoms*. Physical Review A **78**, 043409 (2008).
59. E. P. Kanter, R. Santra, C. Höhr, E. R. Peterson, J. Rudati, D. A. Arms, E. M. Dufresne, R. W. Dunford, D. L. Ederer, B. Krässig, E. C. Landahl, S. H. Southworth, L. Young: *Characterization of the spatiotemporal evolution of laser-generated plasmas*. Journal of Applied Physics **104**, 073307 (2008).
58. C. Buth, R. Santra: *Rotational molecular dynamics of laser-manipulated bromotrifluoromethane studied by x-ray absorption*. Journal of Chemical Physics **129**, 134312 (2008).
57. N. Rohringer, R. Santra: *Resonant Auger effect at high x-ray intensity*. Physical Review A **77**, 053404 (2008).
56. R. Santra, R. W. Dunford, E. P. Kanter, B. Krässig, S. H. Southworth, L. Young: *Strong-field control of x-ray processes*. Advances in Atomic, Molecular, and Optical Physics **56**, 219 (2008).
55. E. R. Peterson, C. Buth, D. A. Arms, R. W. Dunford, E. P. Kanter, B. Krässig, E. C. Landahl, S. T. Pratt, R. Santra, S. H. Southworth, L. Young: *An x-ray probe of laser-aligned molecules*. Applied Physics Letters **92**, 094106 (2008).
54. C. Buth, R. Santra: *Theory of x-ray absorption by laser-aligned symmetric-top molecules*. Physical Review A **77**, 013413 (2008).

53. R. Santra, C. Buth, E. R. Peterson, R. W. Dunford, E. P. Kanter, B. Krässig, S. H. Southworth, L. Young: *Strong-field control of x-ray absorption*. Journal of Physics: Conference Series **88**, 012052 (2007).
52. S. H. Southworth, D. A. Arms, E. M. Dufresne, R. W. Dunford, D. L. Ederer, C. Höhr, E. P. Kanter, B. Krässig, E. C. Landahl, E. R. Peterson, J. Rudati, R. Santra, D. A. Walko, L. Young: *K-edge x-ray absorption spectroscopy of laser-generated Kr⁺ and Kr²⁺*. Physical Review A **76**, 043421 (2007).
51. N. Rohringer, R. Santra: *X-ray nonlinear optical processes using a self-amplified spontaneous emission free-electron laser*. Physical Review A **76**, 033416 (2007).
50. C. Buth, R. Santra, L. Young: *Electromagnetically induced transparency for x-rays*. Physical Review Letters **98**, 253001 (2007).
49. Z.-H. Loh, M. Khalil, R. E. Correa, R. Santra, C. Buth, S. R. Leone: *Quantum state-resolved probing of strong-field-ionized xenon atoms using femtosecond high-order harmonic transient absorption spectroscopy*. Physical Review Letters **98**, 143601 (2007).
48. C. Buth, R. Santra: *Theory of x-ray absorption by laser-dressed atoms*. Physical Review A **75**, 033412 (2007).
47. C. Höhr, E. R. Peterson, N. Rohringer, J. Rudati, D. A. Arms, E. M. Dufresne, R. W. Dunford, D. L. Ederer, E. P. Kanter, B. Krässig, E. C. Landahl, R. Santra, S. H. Southworth, L. Young: *Alignment dynamics in a laser-produced plasma*. Physical Review A **75**, 011403 (R) (2007).
46. N. Rohringer, A. Gordon, R. Santra: *Configuration-interaction-based time-dependent orbital approach for ab initio treatment of electronic dynamics in a strong optical laser field*. Physical Review A **74**, 043420 (2006).
45. Z. B. Walters, R. Santra, C. H. Greene: *Interaction of intense VUV radiation with large xenon clusters*. Physical Review A **74**, 043204 (2006).
44. R. Santra: *Imaging molecular orbitals using photoionization*. Chemical Physics **329**, 357 (2006).
43. R. Santra, R. W. Dunford, L. Young: *Spin-orbit effect on strong-field ionization of krypton*. Physical Review A **74**, 043403 (2006).
42. R. Santra: *Why complex absorbing potentials work: A discrete-variable-representation perspective*. Physical Review A **74**, 034701 (2006).
41. L. Young, D. A. Arms, E. M. Dufresne, R. W. Dunford, D. L. Ederer, C. Höhr, E. P. Kanter, B. Krässig, E. C. Landahl, E. R. Peterson, J. Rudati, R. Santra, S. H. Southworth: *X-ray microprobe of orbital alignment in strong-field ionized atoms*. Physical Review Letters **97**, 083601 (2006).
40. R. C. Bilodeau, C. W. Walter, I. Dumitriu, N. D. Gibson, G. D. Ackerman, J. D. Bozek, B. S. Rude, R. Santra, L. S. Cederbaum, N. Berrah: *Photo double detachment of CN⁻: Electronic decay from an inner-valence hole in molecular anions*. Chemical Physics Letters **426**, 237 (2006).
39. A. Gordon, F. X. Kärtner, N. Rohringer, R. Santra: *Role of many-electron dynamics in high harmonic generation*. Physical Review Letters **96**, 223902 (2006).
38. R. Santra, A. Gordon: *Three-step model for high-harmonic generation in many-electron systems*. Physical Review Letters **96**, 073906 (2006).
37. A. Gordon, R. Santra, F. X. Kärtner: *Role of the Coulomb singularity in high-order harmonic generation*. Physical Review A **72**, 063411 (2005).
36. R. Santra, K. Kirby: *Ab initio configuration-interaction investigation of optical transitions in K + He and K + H₂*. Journal of Chemical Physics **123**, 214309 (2005).

35. Y. Sajeev, R. Santra, S. Pal: *Correlated complex independent particle potential for calculating electronic resonances*. Journal of Chemical Physics **123**, 204110 (2005).
34. S. Feuerbacher, R. Santra: *Calculating molecular Rydberg states using the one-particle Green's function: Application to HCO and C(NH₂)₃*. Journal of Chemical Physics **123**, 194310 (2005).
33. R. Santra, E. Arimondo, T. Ido, C. H. Greene, J. Ye: *High-accuracy optical clock via three-level coherence in neutral bosonic ⁸⁸Sr*. Physical Review Letters **94**, 173002 (2005).
32. Y. Sajeev, R. Santra, S. Pal: *Analytically continued Fock space multireference coupled-cluster theory: Application to the ²Π_g shape resonance in e-N₂ scattering*. Journal of Chemical Physics **122**, 234320 (2005).
31. A. Larson, S. Tonzani, R. Santra, C. H. Greene: *Dissociative recombination of HCO⁺*. Journal of Physics: Conference Series **4**, 148 (2005).
30. R. Santra, J. M. Shainline, C. H. Greene: *Siegert pseudostates: completeness and time evolution*. Physical Review A **71**, 032703 (2005).
29. R. Santra, C. H. Greene: *Multiphoton ionization of xenon in the VUV regime*. Physical Review A **70**, 053401 (2004).
28. S. Scheit, V. Averbukh, H.-D. Meyer, N. Moiseyev, R. Santra, T. Sommerfeld, J. Zobeley, L. S. Cederbaum: *On the Interatomic Coulombic Decay in the Ne dimer*. Journal of Chemical Physics **121**, 8393 (2004).
27. R. Santra, K. V. Christ, C. H. Greene: *Properties of metastable alkaline-earth-metal atoms calculated using an accurate effective core potential*. Physical Review A **69**, 042510 (2004).
26. C. Buth, R. Santra, L. S. Cederbaum: *Non-Hermitian Rayleigh-Schrödinger perturbation theory*. Physical Review A **69**, 032505 (2004).
25. R. Santra, C. H. Greene: *Xenon clusters in intense VUV laser fields*. Physical Review Letters **91**, 233401 (2003).
24. C. Buth, R. Santra, L. S. Cederbaum: *Impact of interatomic electronic decay processes on Xe 4d hole decay in the xenon fluorides*. Journal of Chemical Physics **119**, 10575 (2003).
23. C. Buth, R. Santra, L. S. Cederbaum: *Ionization of the xenon fluorides*. Journal of Chemical Physics **119**, 7763 (2003).
22. V. Kokoouline, R. Santra, C. H. Greene: *Multichannel cold collisions between metastable Sr atoms*. Physical Review Letters **90**, 253201 (2003).
21. R. Santra, C. H. Greene: *Tensorial analysis of the long-range interaction between metastable alkaline-earth-metal atoms*. Physical Review A **67**, 062713 (2003).
20. I. B. Müller, R. Santra, L. S. Cederbaum: *Resonances and pseudoresonances in a potential with attractive Coulomb tail: A study using analytic-continuation techniques*. International Journal of Quantum Chemistry **94**, 75 (2003).
19. R. Santra, L. S. Cederbaum: *Coulombic energy transfer and triple ionization in clusters*. Physical Review Letters **90**, 153401 (2003). Erratum: Physical Review Letters **94**, 199901 (2005).
18. S. Feuerbacher, T. Sommerfeld, R. Santra, L. S. Cederbaum: *Complex absorbing potentials in the framework of electron propagator theory. II. Application to temporary anions*. Journal of Chemical Physics **118**, 6188 (2003).
17. R. Santra, L. S. Cederbaum: *Complex absorbing potentials in the framework of electron propagator theory. I. General formalism*. Journal of Chemical Physics **117**, 5511 (2002).

16. R. Santra, L. S. Cederbaum: *Non-Hermitian electronic theory and applications to clusters*. Physics Reports **368**, 1 (2002).
15. R. Santra, J. Zobeley, L.S. Cederbaum: *Electronic decay of valence holes in clusters and condensed matter*. Physical Review B **64**, 245104 (2001).
14. R. Santra, L. S. Cederbaum: *An efficient combination of computational techniques for investigating electronic resonance states in molecules*. Journal of Chemical Physics **115**, 6853 (2001).
13. J. Zobeley, R. Santra, L. S. Cederbaum: *Electronic decay in weakly bound hetero-clusters: Energy transfer versus electron transfer*. Journal of Chemical Physics **115**, 5076 (2001).
12. N. Moiseyev, R. Santra, J. Zobeley, L. S. Cederbaum: *Fingerprints of the nodal structure of autoionizing vibrational wave functions in clusters: interatomic Coulombic decay in Ne dimer*. Journal of Chemical Physics **114**, 7351 (2001).
11. T. Sommerfeld, R. Santra: *An efficient method to perform CAP/CI calculations for temporary anions*. International Journal of Quantum Chemistry **82**, 218 (2001).
10. R. Santra, J. Zobeley, L. S. Cederbaum, F. Tarantelli: *Intermolecular Coulombic decay of clusters*. Journal of Electron Spectroscopy and Related Phenomena **114-116**, 41 (2001).
9. T. Shiroka, C. Bucci, R. De Renzi, F. Galli, G. Guidi, G. H. Eaton, P. J. C. King, C. A. Scott, K. Träger, A. Breitrück, M. Diaz Trigo, A. Grossmann, K. Jungmann, J. Merkel, P. Neumayer, I. Reinhard, R. Santra, L. Willmann, V. Meyer, E. Roduner, R. Scheuermann, M. C. Charlton, P. Donnelly: *Production of pulsed ultraslow muons and first μ SR experiments on thin metallic and magnetic films*. Applied Magnetic Resonance **19**, 471 (2000).
8. R. Santra, J. Zobeley, L. S. Cederbaum, N. Moiseyev: *Interatomic Coulombic decay in van der Waals clusters and impact of nuclear motion*. Physical Review Letters **85**, 4490 (2000).
7. K. Träger, A. Breitrück, M. Diaz Trigo, A. Grossmann, K. Jungmann, J. Merkel, V. Meyer, P. Neumayer, B. Pacht, G. zu Putlitz, R. Santra, L. Willmann, G. Allodi, C. Bucci, R. De Renzi, F. Galli, G. Guidi, T. Shiroka, G. H. Eaton, P. J. C. King, C. A. Scott, G. W. Williams, E. Roduner, R. Scheuermann, M. C. Charlton, P. Donnelly, L. Pareti, G. Turilli: *Production of pulsed ultraslow muons and first μ SR experiments on thin metallic and magnetic films*. Physica B **289-290**, 662 (2000).
6. V. Meyer, S. N. Bagayev, P. E. G. Baird, P. Bakule, M. G. Boshier, A. Breitrück, S. L. Cornish, S. Dychkov, G. H. Eaton, A. Grossmann, D. Hübl, V. W. Hughes, K. Jungmann, I. C. Lane, Yi-Wei Liu, D. Lucas, Y. Matyugin, J. Merkel, G. zu Putlitz, I. Reinhard, P. G. H. Sandars, R. Santra, P. V. Schmidt, C. A. Scott, W. T. Toner, M. Towrie, K. Träger, L. Willmann, V. Yakhontov: *Pulsed laser spectroscopy in muonium and deuterium*. Hyperfine Interactions **127**, 197 (2000).
5. R. Santra, J. Zobeley, L. S. Cederbaum: *Inner-valence ionization of molecular anions and ultrafast relaxation by electron emission*. Chemical Physics Letters **324**, 416 (2000).
4. R. Santra, J. Breidbach, J. Zobeley, L. S. Cederbaum: *Parallel filter diagonalization: A novel method to resolve quantum states in dense spectral regions*. Journal of Chemical Physics **112**, 9243 (2000).
3. V. Meyer, S. N. Bagayev, P. E. G. Baird, P. Bakule, M. G. Boshier, A. Breitrück, S. L. Cornish, S. Dychkov, G. H. Eaton, A. Grossmann, D. Hübl, V. W. Hughes, K. Jungmann, I. C. Lane, Yi-Wei Liu, D. Lucas, Y. Matyugin, J. Merkel, G. zu Putlitz, I. Reinhard, P. G. H. Sandars, R. Santra, P. V. Schmidt, C. A. Scott, W. T. Toner, M. Towrie, K. Träger, L. Willmann, V. Yakhontov: *Measurement of the 1s-2s energy interval in muonium*. Physical Review Letters **84**, 1136 (2000).

2. R. Santra, L. S. Cederbaum, H. - D. Meyer: *Electronic decay of molecular clusters: non-stationary states computed by standard quantum chemistry methods*. Chemical Physics Letters **303**, 413 (1999).
1. V. Yakhontov, R. Santra, K. Jungmann: *Resonant three-photon ionization of hydrogenic atoms by a non-monochromatic laser field*. Journal of Physics B **32**, 1615 (1999).

Presentations for Scientific Audiences:

157. Invited speaker, 2024 MULTIPHOTON PROCESSES GORDON RESEARCH CONFERENCE (Bryant University, Rhode Island, USA, 2024): *Femtosecond and attosecond dynamics in liquid water*.
156. Invited speaker, INTERNATIONAL SCHOOL ON ULTRAFAST X-RAY & ATTOSECOND SCIENCE (Paris-Saclay University, France, 2024): *Femtosecond and attosecond dynamics in liquid water*.
155. Invited speaker, CAMOST-G20-S20 CONSORTIUM ON DISRUPTIVE SCIENCE FOR SUSTAINABLE DEVELOPMENT (joint initiative of IIT Tirupati and IISER Tirupati, Tirupati, India, 2023): *Science using x-ray free-electron lasers*.
154. Invited speaker, 7TH INTERNATIONAL SYMPOSIUM ON INTENSE FIELD, SHORT WAVELENGTH ATOMIC AND MOLECULAR PROCESSES (St. Saveur, Quebec, Canada, 2023): *Machine-learning approaches in ultrafast science*.
153. Invited speaker, INTERNATIONAL WORKSHOP ON PHOTOIONIZATION (IWP) & RESONANT INELASTIC X-RAY SCATTERING (RIXS) (Zao-cho, Japan, 2022): *Water, holes, and radicals*.
152. Invited speaker, PHYSICS COLLOQUIUM AT THE INDIAN INSTITUTE OF TECHNOLOGY (IIT) DELHI (Delhi, India, 2022): *Science using x-ray free-electron lasers*.
151. Invited speaker, CONFERENCE ON LASERS AND ELECTRO-OPTICS (San Jose, USA, 2020): *High-intensity x-ray science*.
150. Invited speaker, ELEVENTH INTERNATIONAL WORKSHOP ON RADIATION DAMAGE TO BIOLOGICAL SAMPLES, RD11 (Villigen, Switzerland 2020): *Quantitative simulation tools for predicting radiation damage driven by high-intensity x-ray pulses*.
149. Invited speaker, CMWS, DESY WATER WEEK (Hamburg, Germany, 2020): *Water, holes, and radicals*.
148. Invited speaker, 5TH INTERNATIONAL CONFERENCE ON ULTRAFAST STRUCTURAL DYNAMICS (Daejeon, South Korea, 2019): *Molecules at high x-ray intensity: Challenges for theory*.
147. Invited speaker, QUTIF ANNUAL MEETING (Oldenburg, Germany, 2019): *Molecules at high x-ray intensity: Challenges for theory*.
146. Invited speaker, XFEL SYMPOSIUM (Tohoku U., Japan, 2019): *Molecules at high x-ray intensity: Challenges for theory*.
145. Invited speaker, INTERNATIONAL WORKSHOP ON RADIATIVE PROPERTIES OF HOT DENSE MATTER (Hamburg, Germany, 2018): *Molecular imaging and plasma formation*.
144. Invited speaker, SYMPOSIUM "PHYSIK & ART(EFACT)" (Berlin, Germany, 2018): *Photons and Images*.
143. Invited speaker, 256TH ACS NATIONAL MEETING (Boston, USA, 2018): *Molecules at high x-ray intensity: Challenges for theory*.
142. Invited speaker, SCIENCE@FELS 2018 (Stockholm, Sweden, 2018): *Molecules at high x-ray intensity: Challenges for theory*.

141. Invited speaker, CONFERENCE ATOMS, MOLECULES AND MATERIALS IN EXTREME ENVIRONMENTS (Oslo, Norway, 2018): *Molecules at high x-ray intensity: Challenges for theory.*
140. Invited speaker, LEBENSWISSENSCHAFTLICHES WOCHENENDSEMINAR (Hamburg, Germany, 2018): *Processes at high x-ray intensity.*
139. Invited speaker, COMPUTATIONAL PHYSICS WORKSHOP ITAMP (Cambridge, USA, 2018): *Atoms and molecules at high x-ray intensity: dedicated software development.*
138. Invited speaker, COLLOQUIUM AT ICTP (Trieste, Italy, 2018): *Atoms in intense light fields.*
137. Invited speaker, JOINT ICTP-IAEA SCHOOL AND WORKSHOP ON FUNDAMENTAL METHODS FOR ATOMIC, MOLECULAR AND MATERIALS PROPERTIES IN PLASMA ENVIRONMENTS (Trieste, Italy, 2018): *Molecular imaging and plasma formation.*
136. Invited speaker, PHYSICS SEMINAR (Umea, Sweden, 2018): *Atoms in intense light fields.*
135. Invited speaker, DESY RESEARCH COURSE AND WATER SYMPOSIUM (Hamburg, Germany, 2018): *Adiabatic and nonadiabatic dynamics in water.*
134. Invited speaker, FRIAS JUNIOR RESEARCHER CONFERENCE (Freiburg, Germany, 2017): *Probing electronic quantum motion with x-rays.*
133. Invited speaker, FEMTO13 (Cancun, Mexico, 2017): *Electronic structure at high x-ray intensity.*
132. Invited speaker, THE 6TH INTERNATIONAL CONFERENCE ON ATTOSECOND PHYSICS (XI'AN, China, 2017): *Electronic coherence and charge transfer.*
131. Invited speaker, PHYSICAL CHEMISTRY COLLOQUIUM AT THE UNIVERSITY OF HAMBURG (Hamburg, Germany, 2016): *Extreme states of matter: From terahertz- to x-ray-driven dynamics.*
130. Invited speaker, PULSE INSTITUTE 10TH ANNIVERSARY SYMPOSIUM (SLAC Menlo Park, California, USA, 2016): *X-ray multiphoton physics: Challenges for theory.*
129. Invited speaker, CONFERENCE DYNAMIC PATHWAYS IN MULTIDIMENSIONAL LANDSCAPES (Berlin, Germany, 2016): *X-ray-driven dynamics and extreme states of matter.*
128. Invited speaker, XFEL WORKSHOP, (SLAC Menlo Park, California, USA, 2016): *Momentum density-density correlations.*
127. Invited speaker, ETTORE MAJORANA SCHOOL (Erice, Sicily 2016): *(i) X-ray multiphoton physics and radiation damage; (ii) X-ray multiphoton physics and imaging.*
126. Invited speaker, THEORETICAL CHEMISTRY COLLOQUIUM AT THE UNIVERSITY OF BOCHUM, (Bochum, Germany, 2016): *Extreme states of matter: From terahertz- to x-ray-driven dynamics.*
125. Invited speaker, IPTC-COLLOQUIUM AT THE UNIVERSITY OF TÜBINGEN (Tübingen, Germany, 2016): *Extreme states of matter: From terahertz- to x-ray-driven dynamics.*
124. Invited speaker, CECAM WORKSHOP (Lausanne, Switzerland 2016): *Electronic structure in high-intensity x-ray fields.*
123. Invited speaker, RESONANCE WORKSHOP (Trieste, Italy, 2015): *From Rabi oscillations to collective excitations.*
122. Invited speaker, COAXSA WORKSHOP (Hamburg, Germany, 2015): *Probing electronic quantum motion with x-rays.*
121. Invited speaker, NOBEL SYMPOSIUM ON FREE ELECTRON LASER RESEARCH (Sigtuna, Sweden, 2015): *Electronic structure in high-intensity x-ray fields.*
120. Invited speaker, WORKSHOP ON METHODS AND ALGORITHMS IN ELECTRONIC-STRUCTURE THEORY (Ringberg Castle, Germany, 2015): *Electronic structure in strong x-ray fields.*

119. Invited speaker, NORDITA, CONTROL OF ULTRAFAST QUANTUM PHENOMENA (Stockholm, Sweden, 2015): *Time-dependent configuration interaction singles on a grid: Applications.*
118. Invited speaker, COLLOQUIUM AT MAX-PLANCK-INSTITUTE FOR NUCLEAR PHYSICS (Heidelberg, Germany, 2015): *Matter excited by high-intensity x-ray pulses.*
117. Invited speaker, DPG SPRING MEETING (Heidelberg, Germany, 2015): *Electronic structure in high-intensity x-ray fields.*
116. Invited speaker, WORKSHOP "THE FUTURE OF AMO SCIENCE AT FLASH", (Hamburg, Germany, 2014): *Correlation effects in AMO physics.*
115. Invited speaker, INTERNATIONAL WORKSHOP ON "ATOMIC PHYSICS", MAX PLANCK INSTITUTE FOR THE PHYSICS OF COMPLEX SYSTEMS (Dresden, Germany, 2014): *The xenon 4d giant dipole resonance revisited.*
114. Invited speaker, FEL-ATTO CONFERENCE, UNIVERSITY COLLEGE LONDON (London, United Kingdom, 2014): *Theory of x-ray-induced electronic and molecular structure and dynamics.*
113. Invited speaker, GORDON RESEARCH CONFERENCE ON MULTIPHOTON PROCESSES (Waltham, Massachusetts, USA, 2014): *Theory of x-ray-induced electronic and molecular structure and dynamics.*
112. Invited speaker, DESY SCIENCE DAYS (Jesteburg, Germany, 2014): *Theory of x-ray-induced electronic and molecular structure and dynamics.*
111. Invited speaker, RÖNTGEN-WORKSHOP, UNIVERSITY OF JENA (Jena, Germany, 2014): *Electronic structure in high-intensity x-ray fields.*
110. Invited speaker, 5TH RINGBERG WORKSHOP ON SCIENCE WITH FELs (Ringberg Castle, Germany, 2014): *Electronic structure in high-intensity x-ray fields.*
109. Invited speaker, PHYSICS COLLOQUIUM AT THE UNIVERSITY OF BAYREUTH (Bayreuth, Germany, 2014): *Ultrafast x-ray atomic physics.*
108. Invited speaker, PHYSICAL CHEMISTRY COLLOQUIUM, ETH ZUERICH (Zuerich, Switzerland, 2013): *X-ray multiphoton ionization and the phase problem in coherent diffractive imaging.*
107. Invited speaker, DPG PHYSICS SCHOOL ON FREE-ELECTRON X-RAY LASER PHYSICS (Bad Honnef, Germany, 2013): *Electron dynamics and the phase problem.*
106. Invited speaker, ELECTRON DYNAMICS OF CHIRAL SYSTEMS ELCH SUMMER SCHOOL, UNIVERSITY OF KASSEL (Hofgeismar, Germany, 2013): *Hole dynamics and coherence.*
105. Invited speaker, GORDON RESEARCH CONFERENCE ON X-RAY SCIENCE (Stonehill College, Easton, MA, USA, 2013): *X-rays in the quantum world.*
104. Invited speaker, THE 38TH INTERNATIONAL CONFERENCE ON VACUUM ULTRAVIOLET AND X-RAY PHYSICS (VUVX-2013) (Hefei, China, 2013): *X-ray multiphoton ionization and the phase problem in coherent diffractive imaging.*
103. Invited speaker, SEMINAR AT ARGONNE NATIONAL LABORATORY (Argonne, Illinois, USA, 2013): *Nuclear and electronic dynamics triggered by photoionization.*
102. Invited speaker, SEMINAR AT ARGONNE NATIONAL LABORATORY (Argonne, Illinois, USA, 2013): *Imaging electronic quantum motion with light.*
101. Invited speaker, UK FEL FORUM MEETING (London, UK, 2013): *High-intensity x-ray interactions with heavy atomic species.*
100. Invited speaker, 2013 DAMOP MEETING OF THE AMERICAN PHYSICAL SOCIETY (Quebec, Canada, 2013): *Multiwavelength anomalous diffraction at high x-ray intensity.*

99. Invited speaker, CONFERENCE ON LASERS AND ELECTRO-OPTICS EUROPE (CLEO/EUROPE) AND THE INTERNATIONAL QUANTUM ELECTRONICS CONFERENCE (IQEC) 2013 (Munich, Germany, 2013): *Non-linear FEL science*.
98. Invited Speaker, THEORETICAL CHEMISTRY SEMINAR, UNIVERSITY OF HEIDELBERG (Heidelberg, Germany 2013): *Ultrafast x-ray atomic physics*.
97. Invited speaker, INSTITUTE SEMINAR, INSTITUT FÜR OPTIK UND QUANTENELEKTRONIK, UNIVERSITY OF JENA (Jena, Germany, 2013): *Ultrafast x-ray atomic physics*.
96. Invited breakout session leader, WORKSHOP ON "UNRAVELING THE INTERPRETATIONS OF ATTOSECOND MEASUREMENTS" (Washington, District of Columbia, USA, 2013)
95. Invited speaker, INTERNATIONAL WORKSHOP ON "ATOMIC PHYSICS", MAX PLANCK INSTITUTE FOR THE PHYSICS OF COMPLEX SYSTEMS (Dresden, Germany, 2012): *Ultrafast x-ray atomic physics*.
94. Invited speaker, INTERNATIONAL SYMPOSIUM ON FRONTIERS IN QUANTUM PHOTON SCIENCE (Hamburg, Germany, 2012): *Ultrafast x-ray atomic physics*.
93. Invited speaker, "FRONTIERS IN OPTICS 2012 / LASER SCIENCE XXVIII" (Rochester, New York, USA, 2012): *Imaging electronic quantum motion with light*.
92. Invited speaker, WORKSHOP ON "VISIONS FOR SWEDISH X-RAY LASER FACILITIES" (Lund, Sweden, 2012): *Probing electronic quantum motion with x-rays*.
91. Invited speaker, WORKSHOP ON "FRONTIERS IN INTENSE LASER-MATTER INTERACTION THEORY (FILMITH)" MAX PLANCK INSTITUTE OF QUANTUM OPTICS (Garching, Germany, 2012): *Ultrafast processes in Xenon*.
90. Invited speaker, WORKSHOP ON "SCIENCE WITH SEEDED FEL BEAMS", EUROPEAN XFEL (Hamburg, Germany, 2012): *Nonlinear processes in atoms*.
89. Invited speaker, 2012 CONFERENCE ON ULTRAFAST DYNAMIC IMAGING OF MATTER (Banff, Alberta, Canada, 2012): *Imaging electronic quantum motion with light*.
88. Invited speaker, WORKSHOP ON "X-RAYS IN THE FOURTH DIMENSION" (Chicago, Illinois, USA, 2012): *Probing electronic quantum motion with x-rays*.
87. Invited speaker, GORDON RESEARCH CONFERENCE ON PHOTOIONS, PHOTOIONIZATION AND PHOTODETACHMENT (Galveston, Texas, USA, 2012): *Nonlinear x-ray atomic physics*.
86. Invited speaker, PHYSICS COLLOQUIUM AT THE UNIVERSITY OF CALIFORNIA, LOS ANGELES (Los Angeles, California, USA, 2012): *Ultrafast processes at high x-ray intensity*.
85. Invited speaker, WEDNESDAY MEETING OF THE DESY PHOTON SCIENCE DIVISION (Hamburg, Germany, 2011): *Coherent diffractive imaging and electron dynamics*.
84. Invited speaker, INTERNATIONAL CONFERENCE ON THEORETICAL AND APPLIED PHYSICS AT IIT KHARAGPUR (Kharagpur, West Bengal, India, 2011): *X-ray physics at high intensity*.
83. Invited speaker, 2011 SSRL / LCLS ANNUAL USERS' MEETING, SLAC (Menlo Park, California, USA, 2011): *X-ray scattering and electron dynamics*.
82. Invited speaker, KICK-OFF WORKSHOP OF THE NORDITA PROGRAM "STUDYING QUANTUM MECHANICS IN THE TIME DOMAIN" (Stockholm, Sweden, 2011): *Hole dynamics and coherence*.
81. Invited speaker, SEVENTEENTH INTERNATIONAL CONFERENCE ON ATOMIC PROCESSES IN PLASMAS (Belfast, United Kingdom, 2011): *Atomic response to ultraintense x-rays*.
80. Invited speaker, PHYSICS COLLOQUIUM AT THE UNIVERSITY OF ROSTOCK (Rostock, Germany, 2011): *Ultrafast processes at high x-ray intensity*.
79. Invited speaker, WORKSHOP ON METHODS AND CODES FOR ATOMS AND MOLECULES IN STRONG LASER FIELDS (Dublin, Ireland, 2011): *Hole dynamics and coherence*.

78. Invited speaker, JOINT ATOMIC PHYSICS COLLOQUIUM OF THE INSTITUTE FOR THEORETICAL ATOMIC, MOLECULAR AND OPTICAL PHYSICS AND THE HARVARD UNIVERSITY PHYSICS DEPARTMENT (Cambridge, Massachusetts, USA, 2011): *Ultrafast processes at high x-ray intensity*.
77. Invited speaker, PHYSICS COLLOQUIUM AT THE UNIVERSITY OF AARHUS (Aarhus, Denmark, 2011): *Ultrafast processes at high x-ray intensity*.
76. Invited speaker, WORKSHOP ON RECENT PROGRESS ON SOFT- AND HARD-X-RAY FEL APPLICATIONS (Ringberg Castle, Germany, 2011): *High-intensity x-ray ionization using XATOM*.
75. Invited speaker, 2011 XFEL/HASYLAB USERS' MEETING (Hamburg, Germany, 2011): *Nonlinear x-ray absorption*
74. Invited speaker, THEORETICAL PHYSICS SEMINAR AT THE UNIVERSITY OF KIEL (Kiel, Germany, 2011): *Hole dynamics and coherence*.
73. Invited speaker, PHYSICS COLLOQUIUM AT THE UNIVERSITY OF KIEL (Kiel, Germany, 2011): *Ultrafast processes at high x-ray intensity*.
72. Invited speaker, QUANTUM OPTICS AND LASER SCIENCE SEMINAR AT IMPERIAL COLLEGE (London, Great Britain, 2010): *Hole dynamics and coherence*.
71. Invited speaker, COLLOQUIUM AT THE MAX PLANCK INSTITUTE OF QUANTUM OPTICS (Garching, Germany, 2010): *Ultrafast processes at high x-ray intensity*.
70. Invited speaker, PHYSICS COLLOQUIUM AT THE UNIVERSITY OF GÖTTINGEN (Göttingen, Germany, 2010): *Ultrafast processes at high x-ray intensity*.
69. Invited speaker, WORKSHOP ON "SCIENCE WITH FLASH" (Hamburg, Germany, 2010): *Hole dynamics and coherence*.
68. Invited speaker, BLACKBOARD LUNCH SEMINAR AT THE KAVLI INSTITUTE FOR THEORETICAL PHYSICS (Santa Barbara, California, USA, 2010): *X-ray Frontiers*.
67. Invited speaker, JAMES FRANCK INSTITUTE SEMINAR AT THE UNIVERSITY OF CHICAGO (Chicago, Illinois, USA, 2010): *X-ray physics at high intensity*.
66. Invited breakout session leader, WORKSHOP ON "THE FUTURE OF ULTRAFAST SOFT X-RAY SCIENCE" (Berkeley, California, USA, 2009): *AMO session on quantum phenomena: executive summary*.
65. Invited speaker, PHYSICAL CHEMISTRY SEMINAR AT WAYNE STATE UNIVERSITY (Detroit, Michigan, USA, 2009): *X-ray physics at high intensity*.
64. Invited speaker, 441ST WILHELM AND ELSE HERAEUS SEMINAR ON "ULTRAFAST X-RAY METHODS FOR STUDYING TRANSIENT ELECTRONIC STRUCTURE AND NUCLEAR DYNAMICS" (Bad Honnef, Germany, 2009): *High-intensity laser control of x-ray processes*.
63. Invited speaker, SECOND INTERNATIONAL CONFERENCE ON ATTOWECOND PHYSICS (Kansas State University, Manhattan, Kansas, USA, 2009): *Multiphoton physics in the x-ray domain*.
62. Invited speaker, PHYSICS COLLOQUIUM AT ARGONNE NATIONAL LABORATORY (Argonne, Illinois, USA, 2009): *High-intensity laser control of x-ray processes*.
61. Invited speaker, 237TH NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY (Salt Lake City, Utah, USA, 2009): *Multichannel coherence in strong-field ionization*.
60. Invited speaker, PHYSICS COLLOQUIUM AT PURDUE UNIVERSITY (West Lafayette, Indiana, USA, 2009): *High-intensity laser control of x-ray processes*.
59. Invited speaker, PHYSICS COLLOQUIUM AT THE UNIVERSITY OF CHICAGO (Chicago, Illinois, USA, 2008): *High-intensity laser control of x-ray processes*.

58. Invited speaker, 2008 LCLS/SSRL ANNUAL USERS' MEETING & WORKSHOPS, SLAC (Menlo Park, California, USA, 2008): *Multiphoton physics in the x-ray domain.*
57. Invited speaker, WORKSHOP ON "INTERACTION OF FREE-ELECTRON-LASER RADIATION WITH MATTER: RECENT EXPERIMENTAL ACHIEVEMENTS, CHALLENGES FOR THEORY", DESY (Hamburg, Germany, 2008): *Multiphoton physics in the x-ray domain.*
56. Invited speaker, INTERNATIONAL WORKSHOP ON TIME-RESOLVED X-RAY DYNAMICS AT THE MAX PLANCK INSTITUTE FOR THE PHYSICS OF COMPLEX SYSTEMS (Dresden, Germany, 2008): *Strong-field control of x-ray processes.*
55. Invited speaker, PHYSICAL CHEMISTRY SEMINAR AT NORTHWESTERN UNIVERSITY (Evanston, Illinois, USA, 2008): *Calculating resonances using a complex absorbing potential.*
54. Invited speaker, PHYSICS SEMINAR AT THE UNIVERSITY OF CHICAGO (Chicago, Illinois, USA, 2008): *X-ray physics at high intensity.*
53. Invited speaker, PHYSICS COLLOQUIUM AT THE UNIVERSITY OF COLORADO (Boulder, Colorado, USA, 2008): *X-ray physics at high intensity.*
52. Invited speaker, 38TH WINTER COLLOQUIUM ON THE PHYSICS OF QUANTUM ELECTRONICS (Snowbird, Utah, USA, 2008): *Strong-field control of x-ray absorption.*
51. Invited speaker, SEMINAR AT THE MAX PLANCK INSTITUTE FOR NUCLEAR PHYSICS (Heidelberg, Germany, 2007): *X-ray processes at high intensity.*
50. Invited speaker, THEORETICAL CHEMISTRY SEMINAR AT THE UNIVERSITY OF HEIDELBERG (Heidelberg, Germany, 2007): *Strong-field control of x-ray absorption.*
49. Invited speaker, CM/AMO SEMINAR AT THE UNIVERSITY OF MICHIGAN (Ann Arbor, Michigan, USA, 2007): *Strong-field control of x-ray absorption.*
48. Invited speaker, ARGONNE NATIONAL LABORATORY PHYSICS DIVISION SEMINAR (Argonne, Illinois, USA, 2007): *Strong-field control of x-ray absorption.*
47. Invited speaker, PHYSICS COLLOQUIUM AT ILLINOIS STATE UNIVERSITY (Normal, Illinois, USA, 2007): *Insight into the structure of matter using (lots of) particles of light.*
46. Invited speaker, PHYSICS COLLOQUIUM AT THE UNIVERSITY OF WISCONSIN-MILWAUKEE (Milwaukee, Wisconsin, USA, 2007): *Strong-field control of x-ray absorption.*
45. Invited speaker, WORKSHOP ON "SCIENCE FOR A NEW CLASS OF SOFT X-RAY LIGHT SOURCES" (Berkeley, California, USA, 2007): *X-ray physics at high time-resolution and at high intensity.*
44. Invited speaker, 2007 RESEARCH MEETING OF THE ATOMIC, MOLECULAR AND OPTICAL SCIENCES (AMOS) PROGRAM SPONSORED BY THE U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE, OFFICE OF BASIC ENERGY SCIENCES (Warrenton, Virginia, USA, 2007): *Strong-field control of x-ray absorption.*
43. Invited speaker, XXV INTERNATIONAL CONFERENCE ON PHOTONIC, ELECTRONIC AND ATOMIC COLLISIONS (Freiburg, Germany, 2007): *Strong-field control of x-ray absorption.*
42. Invited speaker, ARGONNE NATIONAL LABORATORY CHEMISTRY DIVISION SEMINAR (Argonne, Illinois, USA, 2007): *X-ray absorption by laser-aligned atoms and molecules.*
41. Invited speaker, "FINDUNGSSYMPIOSIUM" CENTER FOR FREE ELECTRON LASER STUDIES (HASYLAB, Hamburg, Germany, 2006): *Short-wavelength free-electron lasers: Opportunities for atomic, molecular, and optical physics.*
40. Invited speaker, FEL MEETING 2006: NEW SCIENCE WITH VUV/SOFT X-RAY FREE ELECTRON LASERS (Madison, Wisconsin, USA, 2006): *Multiphoton physics at short wavelengths.*

39. Invited speaker, GORDON RESEARCH CONFERENCE ON MULTIPHOTON PROCESSES (Tilton, New Hampshire, USA, 2006): *Dynamics of a laser-produced hole in a noble gas atom.*
38. Invited speaker, MEDIUM ENERGY PHYSICS SEMINAR AT ARGONNE NATIONAL LABORATORY (Argonne, Illinois, USA, 2006): *Cold alkaline-earth atoms.*
37. Speaker, 2006 DAMOP MEETING OF THE AMERICAN PHYSICAL SOCIETY (Knoxville, Tennessee, USA, 2006): *Three-step model for high-harmonic generation in many-electron systems.*
36. Invited speaker, THEORETICAL PHYSICS SEMINAR AT ARGONNE NATIONAL LABORATORY (Argonne, Illinois, USA, 2006): *Calculating resonances using a complex absorbing potential.*
35. Invited speaker, PHYSICS COLLOQUIUM AT WESTERN MICHIGAN UNIVERSITY (Kalamazoo, Michigan, USA, 2006): *Clusters in XUV radiation fields.*
34. Invited speaker, AMO PHYSICS SEMINAR AT OHIO STATE UNIVERSITY (Columbus, Ohio, USA, 2006): *Electron-correlation and strong-field effects in atoms, molecules, and clusters probed using synchrotron radiation.*
33. Invited speaker, INTERNATIONAL SEMINAR ON PROGRESS AND EXCITEMENT IN AMO PHYSICS (Tokyo, Japan, 2006): *AMO physics using synchrotron radiation.*
32. Invited speaker, ARGONNE NATIONAL LABORATORY CHEMISTRY DIVISION SEMINAR (Argonne, Illinois, USA, 2006): *Electron-correlation and strong-field effects in atoms, molecules, and clusters probed using synchrotron radiation.*
31. Invited speaker, INTERNATIONAL WORKSHOP ON ATOMIC PHYSICS (Dresden, Germany, 2005): *High-harmonic generation and molecular orbital imaging; probing optical strong-field processes with x-rays.*
30. Invited speaker, 2005 DAMOP MEETING OF THE AMERICAN PHYSICAL SOCIETY (Lincoln, Nebraska, USA, 2005): *Clusters in XUV radiation fields.*
29. Speaker, 2005 DAMOP MEETING OF THE AMERICAN PHYSICAL SOCIETY (Lincoln, Nebraska, USA, 2005): *Multiphoton ionization of xenon in the VUV regime.*
28. Invited speaker, ITAMP WORKSHOP ON ATTOSECOND SCIENCE: FUTURE APPLICATIONS IN PHYSICS AND CHEMISTRY (Cambridge, Massachusetts, USA, 2005): *Electronic decay of valence holes in clusters.*
27. Invited speaker, SEMINAR AT ARGONNE NATIONAL LABORATORY (Argonne, Illinois, USA, 2005): *Clusters in XUV radiation fields.*
26. Invited speaker, PHYSICS COLLOQUIUM AT THE UNIVERSITY OF NEBRASKA (Lincoln, Nebraska, USA, 2005): *Clusters in XUV radiation fields.*
25. Invited speaker, PHYSICS COLLOQUIUM AT SAN DIEGO STATE UNIVERSITY (San Diego, California, USA, 2005): *Clusters in XUV radiation fields.*
24. Invited speaker, PHYSICS COLLOQUIUM AT THE GEORGIA INSTITUTE OF TECHNOLOGY (Atlanta, Georgia, USA, 2005): *Clusters in XUV radiation fields.*
23. Invited speaker, PHYSICS COLLOQUIUM AT WESLEYAN UNIVERSITY (Middletown, Connecticut, USA, 2005): *Clusters in XUV radiation fields.*
22. Invited speaker, UCONN/ITAMP OPEN HOUSE (Storrs, Connecticut, USA, 2005): *Electronic decay of valence holes in clusters.*
21. Invited speaker, JILA SEMINAR (Boulder, Colorado, USA, 2004): *Atoms and clusters in intense VUV laser fields.*
20. Invited speaker, BERKELEY ATTOSECOND MURI PROJECT KICK OFF WORKSHOP (Berkeley, California, USA, 2004): *Electronic decay of valence holes in clusters.*

19. Invited speaker, WORKSHOP ON ULTRAFAST SCIENCE AND LCLS EXPERIMENTS (SLAC, Menlo Park, California, USA, 2004): *Cluster physics at high photon energies.*
18. Invited speaker, WORKSHOP ON TIME DOMAIN SCIENCE USING X-RAY TECHNIQUES (Future Scientific Directions for the Advanced Photon Source) (Fontana, Lake Geneva Area, Wisconsin, USA, 2004): *Xenon clusters in intense VUV laser fields.*
17. Speaker, 2004 DAMOP MEETING OF THE AMERICAN PHYSICAL SOCIETY (Tucson, Arizona, USA, 2004): *Xenon clusters in intense VUV laser fields.*
16. Speaker, 2004 WORKSHOP ON ULTRAFAST X-RAY SCIENCE (San Diego, California, USA, 2004): *Xenon clusters in intense VUV laser fields.*
15. Invited speaker, THEORETICAL CHEMISTRY SEMINAR AT THE UNIVERSITY OF HEIDELBERG (Heidelberg, Germany, 2003): *Cold collisions between metastable alkaline-earth atoms.*
14. Invited speaker, CONDENSED MATTER PHYSICS SEMINAR AT THE UNIVERSITY OF COLORADO (Boulder, Colorado, USA, 2003): *Clusters in XUV radiation fields.*
13. Invited speaker, JOINT ATOMIC PHYSICS COLLOQUIUM OF THE INSTITUTE FOR THEORETICAL ATOMIC, MOLECULAR AND OPTICAL PHYSICS AND THE HARVARD UNIVERSITY PHYSICS DEPARTMENT (Cambridge, Massachusetts, USA, 2003): *Cold collisions between metastable alkaline-earth atoms.*
12. Invited speaker, SECOND WORKSHOP ON COLD ALKALINE-EARTH ATOMS (Copenhagen, Denmark, 2003): *Cold collisions between metastable alkaline-earth atoms.*
11. Invited speaker, SEMINAR OF THE LASER PLASMA BRANCH AT THE NAVAL RESEARCH LABORATORY (Washington, District of Columbia, USA, 2003): *Electronic decay of valence holes in clusters.*
10. Poster presenter, GORDON RESEARCH CONFERENCE ON ATOMIC PHYSICS (Tilton, New Hampshire, USA, 2003): *Cold collisions between metastable alkaline-earth atoms.*
9. Speaker, 2003 DAMOP MEETING OF THE AMERICAN PHYSICAL SOCIETY (Boulder, Colorado, USA, 2003): 1. *Electronic decay of valence holes in clusters.* 2. *Tensorial analysis of the long-range interaction between metastable alkaline-earth atoms.*
8. Invited speaker, SEMINAR AT HASYLAB/DESY (Hamburg, Germany, 2002): *Electronic decay of valence holes in clusters.*
7. Invited speaker, SPRING MEETING OF THE DEUTSCHE PHYSIKALISCHE GESELLSCHAFT (Osnabrück, Germany, 2002): *Electronic decay of valence holes in clusters.*
6. Invited speaker, GORDON RESEARCH CONFERENCE ON PHOTOIONS, PHOTOIONIZATION AND PHOTODETACHMENT (Williamstown, Massachusetts, USA, 2001): *Electronic decay of valence holes in clusters.*
5. Poster presenter, XTH INTERNATIONAL CONFERENCE ON QUANTUM CHEMISTRY (Menton, France, 2000): 1. *Parallel filter diagonalization: a novel method to resolve quantum states in dense spectral regions.* 2. *Electronic decay of molecular clusters: non-stationary states computed by standard quantum chemistry methods.*
4. Poster presenter, RESONANCE PHENOMENA IN CHEMICAL PHYSICS (Haifa, Israel, 1999): *Electronic decay of molecular clusters: a complex absorbing potential study.*
3. Speaker, SPRING MEETING OF THE DEUTSCHE PHYSIKALISCHE GESELLSCHAFT (Heidelberg, Germany, 1999): *Elektronischer Zerfall von Molekülclustern.*
2. Speaker, SPRING MEETING OF THE DEUTSCHE PHYSIKALISCHE GESELLSCHAFT (Konstanz, Germany, 1998): *The influence of time-dependent laser-light phase and amplitude on resonant three-photon ionization of hydrogenic atoms.*

1. Poster presenter, 29TH CONFERENCE OF THE EUROPEAN GROUP FOR ATOMIC SPECTROSCOPY (Berlin, Germany, 1997): *Three-photon ionization of hydrogenic atoms by a non-monochromatic laser field*.

Outreach:

38. Speaker ["Was hat Röntgen mit Einstein zu tun?"], PRESENTATION AT IRENA SENDLER STADTTEILSCHULE (contribution to an outreach event called "Wir wollen´s wissen") (Hamburg, Germany, 2024).
37. Speaker ["Was hat Röntgen mit Einstein zu tun?"], PRESENTATION AT STADTTEILSCHULE LURUP (contribution to an outreach event called "Wir wollen´s wissen") (Hamburg, Germany, 2024).
36. Speaker ["Was hat Röntgen mit Einstein zu tun?"], PRESENTATION AT GYMNASIUM BUCKHORN (contribution to an outreach event called "Wir wollen´s wissen") (Hamburg, Germany, 2024).
35. Speaker ["Was hat Röntgen mit Einstein zu tun?"], PRESENTATION AT STADTTEILSCHULE BLANKENESE (contribution to an outreach event called "Wir wollen´s wissen") (Hamburg, Germany, 2023).
34. Speaker ["Was hat Röntgen mit Einstein zu tun?"], PRESENTATION AT STADTTEILSCHULE POPPENBÜTTEL (contribution to an outreach event called "Wir wollen´s wissen") (Hamburg, Germany, 2023).
33. Speaker ["Was hat Röntgen mit Einstein zu tun?"], PRESENTATION AT GYMNASIUM BLANKENESE (contribution to an outreach event called "Wir wollen´s wissen") (Hamburg, Germany, 2022).
32. Speaker ["Was hat Röntgen mit Einstein zu tun?"], PRESENTATION AT MARION DÖNHOF GYMNASIUM (contribution to an outreach event called "Wir wollen´s wissen") (Hamburg, Germany, 2022).
31. Speaker ["Was hat Röntgen mit Einstein zu tun?"], PRESENTATION AT GYMNASIUM ALLEE (contribution to an outreach event called "Wir wollen´s wissen") (Hamburg, Germany, 2022).
30. Speaker ["Was hat Röntgen mit Einstein zu tun?"], PRESENTATION AT GYMNASIUM MARIENTHAL (contribution to an outreach event called "Wir wollen´s wissen") (Hamburg, Germany, 2021).
29. Speaker ["Bei Licht betrachtet"], PRESENTATION AT GYMNASIUM ALLEE (contribution to an outreach event called "Wir wollen´s wissen") (Hamburg, Germany, 2020).
28. Speaker ["Bei Licht betrachtet"], PRESENTATION AT GELEHRTENSCHULE DES JOHANNEUMS (contribution to an outreach event called "Wir wollen´s wissen") (Hamburg, Germany, 2020).
27. Speaker ["Single-shot imaging: theoretical developments"], SCIENCE PRESENTATION ON THE OCCASION OF A VISIT OF THE JDPG ("junge Deutsche Physikalische Gesellschaft") to CFEL (Hamburg, Germany, 2017).
26. Speaker ["Bei Licht betrachtet"], PUBLIC GENERAL-EDUCATION PRESENTATION AT CHRISTIANSENS (contribution to an outreach event called "Wissen vom Fass") (Hamburg, Germany, 2017).
25. Speaker ["Materie - intensiv beleuchtet"], INTERNATIONAL PHYSICS OLYMPIAD (lecture at the 48th "Physik Olympiade") (Hamburg, Germany, 2017).
24. Speaker ["Was ist Licht? Was ist ein Laser? Welche Prozesse ruft Licht in Materie hervor?"], PUBLIC GENERAL-EDUCATION PRESENTATION AT ELBWERK (contribution to an outreach event called "Wissen vom Fass") (Hamburg, Germany, 2016).
23. Speaker ["Der photoelektrische Effekt in neuem Licht"], PUBLIC GENERAL-EDUCATION PRESENTATION AT UNIVERSITÄT HAMBURG (contribution to a public lecture series called "Physik im Alltag") (Hamburg, Germany, 2015).

22. Speaker ["Der photoelektrische Effekt in neuem Licht"], PUBLIC GENERAL-EDUCATION PRESENTATION AT DESY (contribution to a public lecture series called "WISSENSWERTE") (Hamburg, Germany, 2015).
21. Coordinator ["Lehrerfortbildung@DESY"], CONTINUING EDUCATION PROGRAM FOR TEACHERS (Hamburg, Germany, 2014).
20. Speaker ["Forschung mit Photonen bei DESY"], PRESENTATION FOR SCHOOL TEACHERS AT THE NAT ANNUAL MEETING (Hamburg, Germany, 2014).
19. Speaker ["Futuristisch in jeder Hinsicht: Das Center for Free-Electron Laser Science und seine Forschung"], PUBLIC GENERAL-EDUCATION PRESENTATION AT DESY (contribution to a public lecture series called "WISSENSWERTE") (Hamburg, Germany, 2014).
18. Speaker ["Was macht ein theoretischer Physiker in der Praxis?"], DESY SCIENCE CAFE (Hamburg, Germany, 2013).
17. Speaker ["Center for Free-Electron Laser Science"], DESY PUBLIC OPEN HOUSE 2013 (Hamburg, Germany, 2013).
16. Speaker ["Forschung mit Photonen bei DESY"], GENERAL-EDUCATION PRESENTATION FOR THE PARTICIPANTS OF A SUMMER ACADEMY OF THE STUDIENSTIFTUNG DES DEUTSCHEN VOLKES AND OF THE MAX WEBER-PROGRAMM BAYERN (Überlingen, Germany, 2012).
15. Scientific expert in science show with Delf Deike ["DESY meets India"], 823RD BIRTHDAY OF THE PORT OF HAMBURG (Hamburg, Germany, 2012).
14. Speaker ["Alles nur Theorie! Ein interaktives Quiz am Beispiel der Forschung mit Photonen"], DESY PUBLIC OPEN HOUSE 2011 (Hamburg, Germany, 2011).
13. Speaker ["DESY und die Geheimnisse der Materie"], PRESENTATION FOR ELEMENTARY SCHOOL CHILDREN AT BÜCHER PARADIES ISERBROOK (Hamburg, Germany, 2011).
12. Member of selection committee, AUSWAHLSEMINAR DER STUDIENSTIFTUNG DES DEUTSCHEN VOLKES (Neumünster, Germany, 2011).
11. Judge, CHICAGO AREA UNDERGRADUATE RESEARCH SYMPOSIUM (Chicago, Illinois, USA, 2010).
10. Moderator, CHICAGO REGIONAL MIDDLE SCHOOL SCIENCE BOWL (Argonne, Illinois, USA, 2010).
9. Speaker ["X-ray imaging of laser-controlled molecular motion"], ARGONNE PUBLIC OPEN HOUSE 2009 (Argonne, Illinois, USA, 2009).
8. Speaker ["A career in science"], MORTON FRESHMAN CENTER CAREER DAY (Cicero, Illinois, USA, 2008).
7. Judge, CHICAGO REGIONAL MIDDLE SCHOOL SCIENCE BOWL (Argonne, Illinois, USA, 2008).
6. Speaker ["A career in science"], MORTON EAST HIGH SCHOOL STUDENT CAREER DAY (Cicero, Illinois, USA, 2007).
5. Speaker ["Insight into the structure of matter using (lots of) particles of light"], MORAIN VALLEY COMMUNITY COLLEGE (Palos Hills, Illinois, USA, 2007).
4. Co-instructor, BOY SCOUT SCIENCE BADGE DAY (Argonne, Illinois, USA, 2007).
3. Judge, CHICAGO REGIONAL MIDDLE SCHOOL SCIENCE BOWL (Argonne, Illinois, USA, 2007).
2. Judge, MAERCKER SCHOOL DISTRICT 60 SCIENCE FAIR, WESTVIEW MIDDLE SCHOOL (Westmont, Illinois, USA, 2007).
1. Speaker ["Insight into the structure of matter using (lots of) particles of light"], ARGONNE PUBLIC OPEN HOUSE 2006 (Argonne, Illinois, USA, 2006).