Christopher G. Elles

Department of Chemistry University of Kansas Lawrence, Kansas 66045 elles@ku.edu (785) 864-1922 ellesgroup.ku.edu

RESEARCH INTERESTS

Condensed-phase chemical reaction dynamics; Excited-state dynamics of photochromic molecular switches, photo-triggers, and photoactive materials; Ultrafast laser spectroscopy; Time-resolved x-ray absorption spectroscopy

PROFESSIONAL EXPERIENCE

University of Kansas

Professor, Department of Chemistry, 2022-present

Associate Professor, Department of Chemistry, 2016-2022

Assistant Professor, Department of Chemistry, 2009-2016

National Science Foundation

Program Director, Division of Chemistry, 2020-2022

University of Rome "La Sapienza"

Visiting Professor, Department of Physics, Summer 2012

EDUCATION

Postdoc, University of Southern California and Argonne National Laboratory (jointly), 2004-2009

Research Project: Reaction mechanisms in the ionization of liquid water

Advisors: Stephen E. Bradforth (USC) and Robert A. Crowell (ANL)

Ph.D., Chemistry, University of Wisconsin-Madison, July 2004

Dissertation: Vibrational relaxation and photodissociation dynamics in solution

Advisor: F. Fleming Crim

B.S., Chemistry, Colorado State University, May 1999

Research Project: Characterization of non-aqueous and mixed-solute reverse micelles

Advisor: Nancy E. Levinger

SELECTED AWARDS AND HONORS

Editorial Advisory Board, Journal of Physical Chemistry Letters, 2023-2025

Finalist, Honor for an Outstanding Progressive Educator (H.O.P.E.) Award, Univ. of Kansas, 2016

J. Michael Young Academic Advisor Award, University of Kansas, 2016

National Science Foundation CAREER Award, 2012-2017

University of Rome Visiting Professorship, 2012

Kansas NSF EPSCoR First Award, 2011

Arthur Adamson Postdoctoral Research Award, University of Southern California, 2009

Excellence in Physical Chemistry Research Award, University of Wisconsin, 2004

Chemistry Undergraduate Research Award, Colorado State University, 1999

Sigma Xi Grant-in-Aid of Research, 1998

AFFILIATIONS

American Association for the Advancement of Science, 2004-present

American Chemical Society, 1998-present

Inter-American Photochemical Society, 2017-present

Sigma Xi Scientific Research Society, 2020-present

PUBLICATIONS

- 42. K. H. Burns, T. J. Quincy, and C. G. Elles, *Excited-state resonance Raman spectroscopy probes* the sequential two-photon excitation mechanism of a photochromic molecular switch, Journal of Chemical Physics, **157**, 234302 (2022).
- 41. M. Singh, P. Dhote, D. R. Johnson, S. Figueroa-Lazu, C. G. Elles, and Z. Boskovic, *Photochemical decarbonylation of oxetanone and azetidinone: Spectroscopy, computational models, and synthetic applications*, Angewandte Chemie, Int. Ed., **62**, e202215856 (2022).
- 40. K. H. Burns and C. G. Elles, *Ultrafast dynamics of a molecular switch from resonance Raman spectroscopy: Visible and UV excitation*, Journal of Physical Chemistry A, **126**, 5932 (2022).
- 39. V. Ramamurthy, P. Sen, and, C. G. Elles, *Ultrafast excited state dynamics of spatially confined organic molecules*, Journal of Physical Chemistry A, **126**, 4681 (2022).
- 38. M. Singh, B. Gaskins, D. R. Johnson, C. G. Elles, and Z. Boskovic, *Synthesis of cycloheptatriene-containing azetidine lactones*, Journal of Organic Chemistry, **87**, 15001 (2022). 10.1021/acs.joc.2c00367
- 37. D. Bhattacharyya, Y. Zhang, C. G. Elles, and S. E. Bradforth, *Electronic structure of liquid alkanes: A representative case of liquid hexanes and cyclohexane studied using polarization-dependent two-photon absorption spectroscopy*, Journal of Physical Chemistry A, **125**, 7988 (2021).
- 36. C. J. Otolski, A. Mohan Raj, V. Ramamurthy, and C. G. Elles, *Spatial confinement alters the ultrafast photoisomerization dynamics of azobenzenes*, Chemical Science, **11**, 9513 (2020).
- 35. K. H. Burns, P. Srivastava, and C. G. Elles, *Absolute cross sections of liquids from broadband simulated Raman scattering with femtosecond and picosecond pulses*, Analytical Chemistry, **92**, 10686 (2020).
- 34. M. S. Barclay, C. G. Elles, and M. Caricato, *On the discrepancy between experimental and calculated Raman intensities for conjugated phenyl and thiophene derivatives*, Journal of Physical Chemistry A, **124**, 4678 (2020).
- 33. W. C. Henke, C. J. Otolski, W. N. G. Moore, C. G. Elles, and J. D. Blakemore, *Ultrafast* spectroscopy of [Mn(CO)₃] complexes: Tuning the kinetics of light-driven CO release and solvent binding, Inorganic Chemistry, **59**, 2178 (2020).
- 32. M. S. Barclay, C. G. Elles, and M. Caricato, *Benchmark study of ground-state Raman spectra in conjugated molecules*, Journal of Chemical Theory and Computation, **16**, 612 (2020).
- 31. S. Mahvidi, C. G. Elles, B. S. Hadavand, Y. Yokoyama, F. Nourmohammadian, *Influence of protonation on the photochromic behavior, phase transfer and thermal stability of phenyl-amine-substituted diarylethenes*, Progress in Color, Colorants and Coatings, **13**, 105 (2020).
- 30. M. S. Barclay, M. Caricato, and C. G. Elles, Femtosecond stimulated Raman scattering from triplet electronic states: Experimental and theoretical study of resonance enhancements, Journal of Physical Chemistry A, 123, 7720 (2019).
- 29. D. Bhattacharyya, Y. Zhang, C. G. Elles, and S. E. Bradforth, *Electronic structure of liquid methanol and ethanol from polarization-dependent two-photon absorption spectroscopy*, Journal of Physical Chemistry A, **123**, 5789 (2019).
- 28. C. J. Otolski, A. Mohan Raj, G. Sharma, R. Prabhakar, V. Ramamurthy, and C. G. Elles, *Ultrafast trans→ cis photoisomerization dynamics of alkyl-substituted stilbenes in a supramolecular capsule*, Journal of Physical Chemistry A, **123**, 5061 (2019).
- 27. C. J. Otolski, A. Mohan Raj, V. Ramamurthy, and C. G. Elles, *Ultrafast dynamics of encapsulated molecules reveals new insight on the photoisomerization mechanism for azobenzenes*, Journal of Physical Chemistry Letters, **10**, 121 (2019).
- 26. T. J. Quincy, M. S. Barclay, M. Caricato, and C. G. Elles, *Probing dynamics in higher-lying electronic states with resonance-enhanced femtosecond stimulated Raman spectroscopy*, Journal of Physical Chemistry A, **122**, 8308 (2018).

- 25. M. S. Barclay, T. J. Quincy, D. B. Williams-Young, M. Caricato, and C. G. Elles, *Accurate assignments of excited-state resonance Raman spectra: A benchmark study combining experiment and theory*, Journal of Physical Chemistry A, **121**, 7937 (2017).
- 24. M. de Wergifosse, C. G. Elles, and A. I. Krylov, *Two-photon absorption spectroscopy of stilbene and phenanthrene: Excited-state analysis and comparison with ethylene and toluene*, Journal of Chemical Physics, **146**, 174102 (2017).
- 23. M. de Wergifosse, A. L. Houk, A. I. Krylov, and C. G. Elles, *Two-photon absorption spectroscopy of trans-stilbene, cis-stilbene, and phenanthrene: Theory and experiment*, Journal of Chemical Physics, **146**, 144305 (2017).
- 22. G. Batignani, E. Pontecorvo, C. Ferrante, M. Aschi, C. G. Elles, and T. Scopigno, *Visualizing excited-state dynamics of a diaryl thiophene: Femtosecond stimulated Raman scattering as a probe of conjugated molecules*, Journal of Physical Chemistry Letters, 7, 2981 (2016).
- 21. A. L. Houk, R. S. Givens, and C. G. Elles, *Two-photon activation of p-hydroxyphenacyl phototriggers: Toward spatially controlled release of diethyl phosphate and ATP*, Journal of Physical Chemistry B, **120**, 3178 (2016).
- 20. A. L. Houk, I. L. Zheldakov, T. A. Tommey, and C. G. Elles, *Two-photon excitation of trans-stilbene: Spectroscopy and dynamics of electronically excited states above S*₁, Journal of Physical Chemistry B, **119**, 9335 (2015).
- 19. B. Langdon, J. Garlick, X. Ren, D. J. Wilson, A. M. Summers, S. Zigo, M. F. Kling, S. Lei, C. G. Elles, E. Wells, E. D. Poliakoff, K. D. Carnes, V. Kumarappan, I. Ben-Itzhak, and C. A. Trallero-Herrero, *A carrier-envelope-phase stabilized terawatt class laser at 1 kHz with a wavelength tunable option*, Optics Express, 23, 4563 (2015).
- 18. C. L. Ward and C. G. Elles, *Cycloreversion dynamics of a photochromic molecular switch via one-photon and sequential two-photon excitation*, Journal of Physical Chemistry A, **118**, 10011 (2014).
- 17. E. Pontecorvo, C. Ferrante, C. G. Elles, and T. Scopigno, *Structural rearrangement accompanying the ultrafast electrocyclization reaction of a photochromic molecular switch*, Journal of Physical Chemistry B, **118**, 6915 (2014).
- 16. I. L. Zheldakov, O. Grinevich, A. Mejiritski, C. G. Elles, and D. C. Neckers, *Transient spectroscopy of 5,7-diiodo-3-butoxy-6-fluorone (DIBF)*, Photochemistry and Photobiology, **90**, 335 (2014).
- 15. L. Sarkany, J. M. Wasylenko, S. Roy, D. A. Higgins, C. G. Elles, and V. Chikan, *Investigation of fluorescence emission from CdSe nanorods in PMMA and P3HT/PMMA films*, Journal of Physical Chemistry C, **117**, 18818 (2013).
- 14. E. Pontecorvo, C. Ferrante, C. G. Elles, and T. Scopigno, *Optimally shaped narrowband pulses for femtosecond stimulated Raman spectroscopy in the range 330-750 nm*, Optics Express, **21**, 6866 (2013).
- 13. C. L. Ward and C. G. Elles, Controlling the excited-state reaction dynamics of a photochromic molecular switch with sequential two-photon excitation, Journal of Physical Chemistry Letters, 3, 2995 (2012).
- 12. I. L. Zheldakov, J. M. Wasylenko, and C. G. Elles, *Excited-state dynamics and efficient triplet formation in phenylthiophene compounds*, Physical Chemistry Chemical Physics, **14**, 6211 (2012).

Prior to joining KU:

- 11. O. Marsálek, C. G. Elles, P. A. Pieniazek, Eva Pluhařová, J. Vande Vondele, S. E. Bradforth, and P. Jungwirth, *Chasing charge localization and chemical reactivity following photoionization in liquid water*, Journal of Chemical Physics, **135**, 224510 (2011).
- 10. C. G. Elles, C. A. Rivera, Y. Zhang, P. A. Pieniazek, and S. E. Bradforth, *Electronic structure of liquid water from polarization-dependent two-photon absorption spectroscopy*, Journal of Chemical Physics, **130**, 084501 (2009).

- 9. C. G. Elles, I. A. Shkrob, R. A. Crowell, D. A. Arms, and E. C. Landahl, *Transient x-ray absorption spectroscopy of hydrated halogen atom*, Journal of Chemical Physics, **128**, 061102 (2008).
- 8. C. G. Elles, I. A. Shkrob, R. A. Crowell, and S. E. Bradforth, *Excited state dynamics of liquid water: Insight from the dissociation reaction following two-photon excitation*, Journal of Chemical Physics, **126**, 164503 (2007).
- 7. C. G. Elles, A. E. Jailaubekov, R. A. Crowell, and S. E. Bradforth, *Excitation-energy dependence* of the mechanism for two-photon ionization of liquid H₂O and D₂O from 8.3 to 12.4 eV, Journal of Chemical Physics, **125**, 044515 (2006).
- 6. C. G. Elles and F. F. Crim, *Connecting chemical dynamics in gases and liquids*, Annual Review of Physical Chemistry, **57**, 273 (2006).
- 5. L. Sheps, A. C. Crowther, C. G. Elles, and F. F. Crim, *Recombination dynamics and hydrogen abstraction reactions of chlorine radicals in solution*, Journal of Physical Chemistry A, **109**, 4296 (2005).
- 4. C. G. Elles, M. J. Cox, G. L. Barnes, and F. F. Crim, *Recombination and reaction dynamics following photodissociation of CH*₃*OCl in solution*, Journal of Physical Chemistry A, **108**, 10973 (2004).
- 3. C. G. Elles, M. J. Cox, and F. F. Crim, *Vibrational relaxation of CH₃I in the gas phase and in solution*, Journal of Chemical Physics, **120**, 6973 (2004).
- 2. C. G. Elles, D. Bingemann, M. M. Heckscher, and F. F. Crim, *Vibrational relaxation of CH₂I₂ in solution: Excitation level dependence*, Journal of Chemical Physics, **118**, 5587 (2003).
- 1. C. G. Elles and N. E. Levinger, *Reverse micelles solubilizing DMSO and DMSO/water mixtures*, Chemical Physics Letters, **317**, 624 (2000).

RECENT AND FORTHCOMING PRESENTATIONS

Chemistry and Dynamics in Complex Environments, Telluride, CO (June 2023)

21st Intl. Conference on Time-Resolved Vibrational Spectroscopy (TRVS), Amsterdam, NE (June 2023)

Department of Chemistry, University of Michigan, Ann Arbor, MI (February 2023)

Inter-American Photochemical Society (I-APS) Winter Meeting, Miramar Beach, FL (January 2023)

International Conference on Raman Spectroscopy (ICORS), Long Beach, CA (August 2022)

Intl. Chemical Congress of Pacific Basin Societies (Pacifichem), Honolulu, HI (December 2021)

Chemistry and Dynamics in Complex Environments, Telluride, CO (June 2021)

20th Intl. Conference on Time-Resolved Vibrational Spectroscopy (TRVS), Online (June 2021)

International Conference on Raman Spectroscopy (ICORS), Rome, Italy (August 2020-cancelled)

Spectroscopy and Dynamics on Multiple Potential Energy Surfaces, Telluride, CO (July 2020-cancelled)

Department of Chemistry, University of Wisconsin-Oshkosh, Oshkosh, WI (March 2020)

Department of Chemistry, Ripon College, Ripon, WI (March 2020)

Advanced Photon Source, User Science Seminar, Argonne National Laboratory, Lemont, IL (Dec. 2019)

Department of Chemistry, Missouri University of Science and Technology, Rolla, MO (Nov. 2019)

19th Intl. Conference on Time-Resolved Vibrational Spectroscopy (TRVS), Auckland, NZ (Sept. 2019)

International Conference on Photochemistry, Boulder, CO (July 2019)

Chemistry and Dynamics in Complex Environments, Telluride, CO (June 2019)

Department of Physics and Astronomy Colloquium, University of Kansas, Lawrence, KS (Feb. 2019)

Pacific Conference on Spectroscopy and Dynamics, San Diego, CA (January 2019)

Department of Chemistry, University of Nebraska-Omaha, Omaha, NE (November 2018)

Department of Chemistry, University of Rochester, Rochester, NY (October 2018)

Gordon Research Conference on Molecular Interactions and Dynamics, Easton, MA (July 2018)

Department of Chemistry, University of Miami, Miami, FL (March 2018)

Center for Photochemical Sciences, Bowling Green State University, Bowling Green, OH (Feb. 2018)

27th Inter-American Photochemical Society (I-APS) Winter Meeting, Sarasota, FL (January 2018)

FUNDING

Ultrafast Dynamics of Highly Excited Molecules in the Condensed Phase. National Science Foundation, \$485,331 (PI), 2020-2023

Broadband two-photon absorption spectroscopy for high-repetition rate lasers. National Science Foundation, \$397,788 (PI), 2019-2023

Designer chromophores for therapeutic carbon monoxide release via two-photon photochemistry. Hall Research Fund (KU), \$38,000 (co-PI), 2018-2019

Fast processes in optogenetic systems: Experiments and modeling. National Institutes of Health Center of Biomedical Research Excellence in Protein Structure and Function (COBRE-PSF), Pilot Grant (coinvestigator), \$20,000, 2017-2018

Collaborative research: Imaging and controlling ultrafast dynamics of atoms, molecules, and nanostructures. National Science Foundation, RII Track 2, \$156,059 sub-award, 2014-2017

Ultrafast dynamics of organic and molecular electronics components. American Chemical Society Petroleum Research Fund, \$100,000 (PI), 2013-2016

Controlling non-adiabatic reaction dynamics in solution: A window on the fundamental details of chemical reactions. National Science Foundation CAREER Award, \$650,000 (PI), 2012-2017

Controlling non-adiabatic dynamics in solution: One- and two-photon excitation of photochromic molecular switches. Kansas NSF EPSCoR First Award, \$71,264 (PI), 2011-2012

RESEARCH SUPPORT

Visualizing the Optical Control of Chemical Dynamics. Linac Coherent Light Source (LCLS), (Roseanne Sension, PI) 5 shifts (60 hours) beamtime, August 2022

TR-XAS study of structural changes in the photodecomposition of Mn CO₂ reduction catalysts. Advanced Photon Source (APS), (PI), 15 shifts (120 hours) beamtime, Dec. 2019

Time-resolved XAS study of the photo-degradation mechanism for manganese CO₂ reduction catalysts. Advanced Photon Source (APS), (PI), 18 shifts (144 hours) beamtime, June 2018

RESEARCH MENTORING

Current Students:

Daniel R. Johnson 6th year Ph.D.
Prasenjit (PJ) Srivastava 6th year Ph.D.
KateLynn White 1st year Ph.D.
Chase Courbot undergraduate

Visiting Scholars and Students:

Jamie Somers, Undergraduate Student, Dublin City University (summer 2022)

Prof. Jordan Mantha, Associate Professor, Mid-America Nazarene University (2016-18)

Sadegh Mahvidi, Graduate Student, Institute for Color Science, Tehran, Iran (2016-17)

Former Graduate and Postdoctoral Students:

Kristen H. Burns (Ph.D., *August 2022*) Faculty Specialist (tenure track), Western Michigan Postdoc, Boise State University

David A. Stierwalt (M.S., August 2019) Indianapolis, IN

Christopher J. Otolski (Ph.D., May 2019) Postdoc, Argonne National Laboratory

Timothy J. Quincy (Ph.D., August 2018) Asst. Prof., Lincoln Univ. (MO)

Amanda L. (Staker) Houk (Ph.D., Oct. 2015) Senior Scientist, Savannah River National Lab.

Jenna M. (Wasylenko) Lindsey Teacher, Lee's Summit High School (MO) Cassandra L. Ward (Ph.D., May 2014) Senior Research Scientist, Wayne State Univ. Dr. Igor L. Zheldakov (postdoc, 2010-13) Chemist, Eastman Chemical Company Former KU Undergraduates: Anna Jasko (B.S., Chemical Engineering, May 2023) Jessica E. Bair (B.S., Chemistry, May 2022) Grad Student, Chalmers U. (Sweden) Robert A. Castaneda (B.A., Chemistry, May 2022) Grad Student, Univ. North Carolina Emmaline R. Lorenzo (B.S., Chemistry/Honors, May 2018) Grad Student, Northwestern Univ. Whitney M. Harmon (B.S., Chemistry, May 2018) Grad Student, Univ. of Iowa Brooks Hidaka (B.S., Chemistry, May 2018) Roseville Area HS (MN) Jung Moon Suh (B.S., Chemistry, May 2018) Regina Mundi College (Canada) Nicholas Jackson (B.S., Chemistry, May 2017) Teacher, Olathe South HS (KS) Jorge L. Perez (UKanTeach; McNair Scholar) Gardner, KS Thomas Hurley (B.S., Chemical Engineering, May 2016) Peace Corps (Cameroon) Victoria L. Gunderson (B.A., Chemistry, May 2016) Assistant Brewer, Lawrence, KS Johnathon R. Bliss (B.S., Chemistry, May 2015) DataMap, Kansas City, MO Graham Oltjen (B.S., Chemistry, May 2014) Agilent Technologies William L. Cleek (B.S., Chemistry, May 2013) Medical Resident, U. Washington Heidi J. LeSage (B.S., Chemistry, May 2011) Pearson Education, Portland, OR Alyssa Auld (B.S., Chemistry Education, May 2010) Teacher, Mill Valley HS (KS) Summer NSF-REU Students: Julia Goeks (2022) Graduate School, University of Illinois Ryan Hamelin (2015) Cavu Group (MA) Darien J. Morrow (2014) Ph.D., Univ. of Wisconsin (2020) Ph.D., Univ. of Colorado (2020) Samantha L. Allen (2013) Tyler A. Tommey (2011) Ph.D., Univ. of Akron (2020) Ph.D., IUPUI (2017) Joseph M. Varberg (2010) **COURSES TAUGHT** CHEM 110 Introductory Chemistry CHEM 180 Chemistry Seminar I CHEM 511 Biological Physical Chemistry Laboratory CHEM 525 Physical Chemistry for Engineers CHEM 530 Physical Chemistry I CHEM 531 Physical Chemistry I Laboratory CHEM 535 Physical Chemistry II CHEM 536 Physical Chemistry II Laboratory CHEM 537 Physical Chemistry Laboratory CHEM 695 Chemistry Seminar II CHEM 700 Responsible Scholarship in the Chemical Sciences CHEM 750 Introduction to Quantum Mechanics CHEM 854 Chemical Kinetics and Dynamics PROFESSIONAL SERVICE University of Kansas: Faculty Senate Research Committee, 2019-20 Ad Hoc Committee on Student Evaluation of Teaching, 2018-19

College of Liberal Arts & Sciences:

Physical Sciences General Research Fund Review Committee, 2023

Faculty Senate & University Senate (elected), 2015-18 Undergraduate STEM Education Committee, 2013 Joint Committee on STEM Teacher Preparation (with School of Ed.), 2020

Committee on Undergraduate Studies and Advising (CUSA; elected), 2017-20

College Faculty Mentor Advisory Committee, 2018-20

College Faculty Mentor Program (for at-risk undergraduates), 2016-20

Committee on Graduate Studies (CGS), 2012-13, 2015

Department of Chemistry:

Graduate Affairs Committee, 2022-present

Graduate Admissions Committee (chair 2012-14), 2010-15, 2018-19, 2022-present

Faculty Mentor, Chemistry Graduate Student Organization (ChemGSO), 2017-20

Graduate Recruiting Weekend Committee (chair), 2019-20

Faculty Performance Review Committee (elected), 2016-19

Ad Hoc Integrated Science Building Atrium Art Committee (chair), 2017-18

Graduate Recruiting Committee, 2009-10, 2016-18

Chemistry REU Program Committee, 2015-16

Chair Advisory Committee, 2010-11, 2015-16

Physical Chemistry Faculty Search Committee, 2013

Department Chair Search Committee, 2013

Search Committee for Graduate Programs Assistant, 2012, 2014

Search Committee for Director of Instrumentation Teaching Laboratories, 2011

Physics Machine Shop Committee, 2011

Meetings/Symposia/Workshops Organized:

Spectroscopy Applied to Structure, Dynamics, and Imaging, American Chemical Society Midwest Regional Meeting (MWRM), Lawrence, KS (October 18-20, 2017)

Spectroscopy and Dynamics on Multiple Potential Energy Surfaces, 72nd International Symposium on Molecular Spectroscopy, Urbana-Champaign, IL (June 19-23, 2017)

High School Teacher Development Workshops (co-organizer and presenter):

Seeing the Unseen in Physical Sciences, Manhattan, KS (June 15-16, 2017)

Seeing the Unseen in Physical Sciences, Manhattan, KS (June 9-10, 2016)

Connecting the Physics of Waves and Electromagnetic Radiation with the Next Generation Science Standards (NGSS), Manhattan, KS (June 8-10, 2015)

Editorial Advisory Board:

Journal of Physical Chemistry Letters (2023-2025)

Proposal Reviews:

Department of Energy, National Science Foundation, Petroleum Research Fund, Ohio University Research Council, Czech Science Foundation (GACR), French National Research Agency (ANR), German Research Foundation (DFG), CRDF Global

Journal Reviews:

Accounts of Chemical Research, ACS Applied Materials and Interfaces, Advanced Materials, Applied Physics Letters, Applied Sciences, Chemical Physics, Chemical Physics Letters, Chemical Science, Chemistry- A European Journal, ChemPhotoChem, ChemPhysChem, Colloids and Surfaces, Inorganic Chemistry, Journal of the American Chemical Society, Journal of Chemical Physics, Journal of Computational Chemistry, Journal of Physical Chemistry, Journal of Physical Chemistry Letters, Nature, Nature Chemistry, Nature Communications, Optical Materials, Optics Letters, Photochemical and Photobiological Sciences, Photochemistry and Photobiology, Physical Chemistry Chemical Physics (PCCP), Science, Science Advances