CURRICULUM VITAE

Emily Ann Carter

Professional Address

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Education

1987 California Institute of Technology Pasadena, CA
- Degree: Ph. D. in Physical Chemistry Advisor: William A. Goddard III

1982 University of California, Berkeley Berkeley, CA
- Degree: B.S. (high honors) in Chemistry

Professional Positions

2023-present Associate Laboratory Director for Applied Materials and Sustainability Sciences, Princeton Plasma Physics Laboratory (PPPL)

Leading diversification of PPPL's research portfolio into the fundamental science of electromanufacturing, solar geoengineering, microelectronics, and quantum information. Established the Princeton University Associated Faculty appointment program at PPPL.

2022-present Senior Strategic Advisor for Sustainability Science at Princeton Plasma Physics Laboratory; Gerhard R. Andlinger Professor in Energy and the Environment; Professor of Mechanical and Aerospace Engineering, the Andlinger Center for Energy and the Environment, and Applied and Computational Mathematics; Associated Faculty of the Princeton Institute for Computational Science & Engineering and the High Meadows Environmental Institute, Princeton University

2022-present Executive Vice Chancellor and Provost Emerita and Distinguished Professor of Chemical and Biomolecular Engineering Emerita, University of California, Los Angeles

2019-2021 Executive Vice Chancellor and Provost, University of California, Los Angeles

As chief academic and operating officer, had the responsibility for the campus' day-to-day operations as well oversight of UCLA's entire academic enterprise, and worked with the Chancellor and leadership team to guide strategic planning, policy, and process development, define budgetary and advancement priorities, oversee faculty and executive leadership recruitment and retention, and support strategic initiatives across campus and beyond. Direct reports: 6 EVCP staff, 5 vice provosts, 19 deans, and 10 vice chancellors. Designed and launched: a widened scope for the Sustainable LA Grand Challenge to help the multicultural communities of LA to become exemplars for sustainable, resilient, equitable future cities worldwide; summer doctoral research fellowship programs; Rising to the Challenge actions in support of Black life; professional development programs for administrative leaders; innovative diverse faculty hiring strategies; transparent, equitable processes for administrative leadership appointments and compensation; improved institutional effectiveness via a "busting bureaucracy" working group and hub-and-spoke models for improved services; a campus-wide "DataX" initiative; and charged a group of deans to develop a cross-campus "Advancing Faculty Diversity" initiative. Recruited 10 outstanding and diverse senior leaders (six female, seven first-generation, LGBTQ, Asian American, Latinx, Black, and/or Native American). Each school/division/unit completed strategic plans focused on world-class excellence in the 21st century, which now inform budgets and hiring plans. Charged committees to learn from more than a year of remote work and education, and to re-envision the future of education and work. Their reports underpin ongoing efforts to improve work flexibility post-CoVID, campus-wide support of education innovation, and access to a UCLA education via expanded summer sessions. Contributed to development of a UC systemwide "grow our own" diverse pipeline from undergraduate to the professoriate.

2019-2021 Distinguished Professor in Chemical and Biomolecular Engineering, University of California, Los Angeles

2019-2021 Gerhard R. Andlinger Professor in Energy and the Environment, Emeritus, Professor of Mechanical and Aerospace Engineering and Applied and Computational Mathematics, Emeritus, and Senior Scholar in Mechanical and Aerospace Engineering, Princeton University

2016-2019 Dean of the School of Engineering and Applied Science, Princeton University

Oversaw 10 academic units comprising six departments and four interdisciplinary centers/institutes, 12 undergraduate certificate programs, as well as school-wide administration of undergraduate and graduate student affairs; faculty recruitment, retention, and advancement; space, facilities, and building services; development and alumni affairs; diversity and inclusion; communications; information technology operations; and administration, finance and planning. Finalized strategic plan and identified priorities therein; held cross-campus faculty retreats to articulate detailed visions for prioritized research initiatives; reallocated resources to hire inaugural Associate Dean for Diversity and Inclusion; revamped communications strategy and execution, including branding and marketing; established School-wide committees to share best practices and streamline operations; carried out peer analysis to inform long-term growth plans; increased industrial outreach; launched new first-year undergraduate curriculum to boost retention of underprepared students; established networking for female/URM faculty, extra-departmental mentoring for junior faculty, and in-person, community-wide training on fostering inclusion, preventing sexual harassment, and unconscious bias; spearheaded creation of multi-PI robotics laboratory; secured commitment to grow the school by 50%; and helped secure gift commitments of >$175M for endowed professorships, focused research teams, data science, bioengineering, robotics, the Metropolis Project, and funding for capital projects.

2011-2019	Gerhard R. Andlinger Professor in Energy and the Environment, Professor of Mechanical and Aerospace Engineering and Applied and Computational Mathematics, Associated Faculty in Chemistry, Chemical and Biological Engineering, the Princeton Institute for Computational Science and Engineering (PICSciE), the Princeton Institute for the Science and Technology of Materials (PRISM), the Princeton Environmental Institute (PEI), and the Andlinger Center for Energy and the Environment (ACEE), Princeton University
2010-2016	Founding Director, Andlinger Center for Energy and the Environment, Princeton University *Led effort to build entire human and physical infrastructure of a $100M enterprise; hired all original faculty (joint with departments) and staff; acted as lead faculty liaison for design and construction of a large, complex laboratory building; undertook extensive alumni outreach and fundraising beyond the founding gift; built a cross-campus intellectual community via establishing a web presence, a highlight seminar series, and multidisciplinary seed grants for research; launched a corporate affiliates program, undergraduate certificate programs with new multidisciplinary courses, undergraduate internship and graduate fellowship programs, a visitors program, and a public education project (https://acee.princeton.edu/distillates).*
2009-2014	Co-Director, Combustion Energy Frontier Research Center
2006 – 2011	Arthur W. Marks '19 Professor of Mechanical and Aerospace Engineering and Applied and Computational Mathematics, Associated Faculty in PICSciE, Chemistry, Chemical Engineering, and PRISM, Princeton University
2004 –2006	Professor of Mechanical and Aerospace Engineering and Applied and Computational Mathematics, Associated Faculty in PICSciE, Chemistry, Chemical Engineering, and PRISM, Princeton University
2002-2004	Professor of Chemistry and Materials Science and Engineering, University of California, Los Angeles
Sept. – Dec. 2001	Visiting Associate in Aeronautics, Division of Engineering and Applied Science, California Institute of Technology
Dec. 2000—2004	UCLA Director of Modeling and Simulation, California NanoSystems Institute
Sept.—Dec. 1999	Visiting Scholar, Department of Physics, Harvard University
Jan.—June 1996	Dr. Lee Visiting Research Fellow in the Sciences, Christ Church, Oxford University
1994—2002	Professor of Physical Chemistry, University of California, Los Angeles
1992—1994	Associate Professor of Physical Chemistry, University of California, Los Angeles
1988—1992	Assistant Professor of Physical Chemistry, University of California, Los Angeles
1987—1988	Postdoctoral Research Associate in Chemistry, University of Colorado, Boulder, Colorado (Advisor: James T. Hynes)

Research Activities

Development of accurate and efficient quantum mechanics simulation techniques, including pioneering embedded correlated wavefunction and orbital-free density functional theories. Discovery and design of materials for producing chemicals, materials, and fuels from renewable energy, with a specific emphasis on carbon dioxide utilization. Delivered over 600 invited/plenary lectures at conferences, universities, companies, and government laboratories worldwide. Trained 56

postdoctoral fellows and graduated 39 Ph.D.s in chemistry, chemical engineering, physics, applied mathematics, electrical engineering, and mechanical and aerospace engineering over a 36-year period.

Web of Science Researcher ID	P-4075-2014
ORCID:	0000-0001-7330-7554
Google Scholar:	https://scholar.google.com/citations?user=vluc7z8AAAAJ&hl=en
Github:	Codes developed in the Carter group are available through GitHub repositories: https://github.com/EACcodes

Awards and Honors

2024	Annabelle Lee Lecturer, Virginia Tech, Virginia
2024	Marsha I. Lester Award for Exemplary Impact in Physical Chemistry, American Chemical Society, Physical Chemistry Division
2024	Foreign Member, The Royal Society, London, Great Britain
2024	Covestro Lecturer, University of Pittsburgh, Department of Chemical and Petroleum Engineering
2024	William H. Nichols Medal, New York Section of the American Chemical Society
2023	Gilbert Newton Lewis Memorial Lecturer, University of California, Berkeley, College of Chemistry
2023	Robert S. Mulliken Award, University of Chicago, Department of Chemistry
2023	27th John Stauffer Lecturer in Chemistry, Stanford University
2022	Fellow, Royal Society of Chemistry
2022	Paint Branch Distinguished Lecturer in Applied Physics, University of Maryland, Institute for Research in Electronics and Applied Physics
2022	Richard S. H. Mah Lecturer, Northwestern University, Department of Chemical and Biological Engineering
2022	Harrison Shull Distinguished Lecturer, Indiana University Bloomington, Department of Chemistry
2021	Materials Theory Award, Materials Research Society
2020	Brumley D. Pritchett Lecturer, Georgia Institute of Technology, School of Materials Science and Engineering
2020	Member, European Academy of Sciences
2020	Chemistry & Biochemistry Distinguished Lecturer, University of California, Los Angeles
2019	John Scott Award, Board of City Trusts, Philadelphia, PA
2019	Camille & Henry Dreyfus Lectureship, University of Basel, Switzerland
2019	Inaugural WiSE Presidential Distinguished Lecturer, University of Southern California

2019 18th NCCR MARVEL Distinguished Lecturer, L'École Polytechnique Fédérale de Lausanne (EPFL), Switzerland

2019 Graduate Mentoring Award, McGraw Center for Teaching and Learning, Princeton University

2019 Distinguished Alumni Award, California Institute of Technology

2019 Eyring Lecturer in Molecular Sciences, Arizona State University

2019 Mildred Dresselhaus Memorial Lecturer, Ras Al Khaimah Centre for Advanced Materials, United Arab Emirates

2019 Dow Foundation Distinguished Lecturer, University of California, Santa Barbara

2018 C. R. Mueller Distinguished Lecturer, Purdue University

2018 CME Leadership Award for Interdisciplinary Innovation, New York Section of the American Chemical Society

2018 Donald L. Katz Lectureship in Chemical Engineering, University of Michigan

2018 ACS Award in Theoretical Chemistry, American Chemical Society

2017 College of Engineering Fall Distinguished Lecturer, University of California, Davis

2017 Emerson Center Lectureship Award, Emory University

2017 Fritz London Memorial Lecturer, Duke University

2017 Julian C. Smith Lecturer in Chemical and Biomolecular Engineering, Cornell University

2017 Albert J. Moscowitz Memorial Lecturer in Chemistry, University of Minnesota

2017 Distinguished Lecturer in Theoretical and Computational Chemistry, University of California, San Diego

2017 Outstanding Referee of the Physical Review journals

2017 Irving Langmuir Prize in Chemical Physics, American Physical Society

2016 Schiesser Lecturer, Lehigh University

2016 Pitzer Lecturer on Theoretical Chemistry, Ohio State University

2016 Almlöf–Gropen Lecturer, Centre for Theoretical and Computational Chemistry at the University of Oslo and the University of Tromsø, Norway

2016 R. H. Betts Memorial Award Lecturer, University of Manitoba, Winnipeg, Canada

2016 Fred Kavli Innovations in Chemistry Lecturer, American Chemical Society

2016 Member, National Academy of Engineering

2015 Joseph O. Hirschfelder Prize in Theoretical Chemistry, Theoretical Chemistry Institute at the University of Wisconsin, Madison

2014 Fellow, National Academy of Inventors

2014 Malcolm Dole Distinguished Summer Lecturer in Physical Chemistry, Northwestern University

2014 Ira Remsen Award, Maryland Section of the American Chemical Society, Johns Hopkins University

2014 Women in STEM Award for Outstanding Research Scholarship, Princeton University

2014 Linnett Visiting Professor of Chemistry, University of Cambridge

2013 Hoyt C. Hottel Lecturer in Chemical Engineering, Massachusetts Institute of Technology

2013 Kenneth S. Pitzer Lecturer, Department of Chemistry, University of California, Berkeley

2013 Mathematics of Planet Earth Simons Public Lecturer, Institute for Pure and Applied Mathematics, University of California, Los Angeles

2013 Lord Lecturer, Department of Chemistry, Allegheny College

2013 Sigillo D'Oro (Golden Sigillum) Medal, Italian Chemical Society, Scuola Normale Superiore, Pisa, Italy

2013 Article selected for *The Journal of Chemical Physics* 80th Anniversary Collection (Chen Huang and Emily A. Carter, "Potential-functional embedding theory for molecules and materials," *J. Chem. Phys.*, **135**, 194104 (2011).)

2013 Francis Clifford Phillips Lectureship, Xi Chapter of the Phi Lambda Upsilon National Honorary Chemical Society and the Department of Chemistry, University of Pittsburgh

2013 Tedori-Callinan Lectureship, Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania

2013 Naval Research Laboratory Distinguished Lectureship, Naval Research Laboratory, Washington, DC

2013 W. Allan Powell Lectureship, Virginia Section of the American Chemical Society and the University of Richmond

2012 Docteur Honoris Causa from L'École Polytechnique Fédérale de Lausanne, Switzerland (EPFL)

2012 Fellow, American Chemical Society

2012 Honorary Mathematical and Physical Sciences Distinguished Lecturer, National Science Foundation

2012 Dean's Distinguished Lecturer, College of Science and Technology, Temple University

2011 MIT Distinguished Speaker in Computational Science and Engineering, Massachusetts Institute of Technology

2011 August Wilhelm von Hofmann Lecture Award, German Chemical Society

2011 Jerome B. Cohen Lecturer in Materials Science and Engineering, Northwestern University

2011 Ernest Davidson Lecturer in Theoretical Chemistry, University of North Texas

2011 Gerhard R. Andlinger Professor in Energy and the Environment, Princeton University

2010 Molecular Foundry Distinguished Lecturer, Lawrence Berkeley National Laboratory

2010 Coover Lecturer in Chemistry, Iowa State University

2010 Material Simulation Distinguished Lecturer, Pennsylvania State University

2010 Pelz Memorial Lecturer in Mechanical and Aerospace Engineering, Rutgers University

2010 Noyes Lecturer in Physical Chemistry, University of Texas, Austin

2009 Member, International Academy of Quantum Molecular Science

2008 EaSTChem Visiting Fellow, Universities of Edinburgh and St. Andrews, Scotland

2008 Member, National Academy of Sciences

2008 Fellow, American Academy of Arts & Sciences

2008 Welch Distinguished Lecturer in Chemistry

2008 Coulson Lecturer in Theoretical Chemistry, University of Georgia

2008 Kivelson Lecturer in Physical Chemistry, University of California, Los Angeles

2007-08 Old Dominion Faculty Fellow, Council of the Humanities, Princeton University

2007 American Chemical Society Award for Computers in Chemical and Pharmaceutical Research

2006 Arthur W. Marks '19 Professor, Princeton University

2005 Merck-Frosst Lecturer in Chemistry, Concordia University

2004 Fellow, Institute of Physics

2002 Dean's Recognition Award for Research, University of California, Los Angeles

2002 McDowell Lecturer in Physical Chemistry, University of British Columbia, Canada

2000 Fellow, American Association for the Advancement of Science

1998 Fellow, American Physical Society

1998 Hanson-Dow Award for Excellence in Teaching, University of California, Los Angeles

1996-97 Defense Science Study Group Member

1996 Dr. Lee Visiting Research Fellowship in the Sciences, Christ Church, Oxford University, England

1995 Peter Mark Memorial Award, American Vacuum Society

1995 Fellow, American Vacuum Society

1993 Herbert Newby McCoy Research Award, University of California, Los Angeles

1993 Medal of the International Academy of Quantum Molecular Science

1993 Exxon Faculty Fellowship in Solid State Chemistry, American Chemical Society Inorganic Division Award

1993 Glenn T. Seaborg Research Award, University of California, Los Angeles

1993-95 Alfred P. Sloan Research Fellow

1992-97 Camille and Henry Dreyfus Teacher-Scholar Award

1990-91 Union Carbide Innovation Recognition Award

1989-90 Faculty Member of Distinction (Undergraduate Teaching Award), University of California, Los Angeles

1989-90 Union Carbide Innovation Recognition Award

1988-93 Camille and Henry Dreyfus Foundation Distinguished New Faculty Award

1988-93 National Science Foundation Presidential Young Investigator Award

1986-87 SOHIO Fellowship in Catalysis, California Institute of Technology (Caltech)

1985-86	International Precious Metals Institute and Gemini Industries Research Grant Award
1984	Sigma Xi, California Institute of Technology (Caltech)
1982-85	National Science Foundation Predoctoral Fellowship
1982	Phi Beta Kappa, University of California, Berkeley
1982	Mabel Kittredge Wilson Prize in Chemistry, University of California, Berkeley
1981-82	Bruce Howard Memorial Scholar, University of California, Berkeley
1981	Coblentz Society Award for Molecular Spectroscopy, University of California, Berkeley
1981	Mildred Jordan Sharp Torch and Shield Award, University of California, Berkeley
1979-80	Theodore and Edith Braun Scholar, University of California, Berkeley
1978-82	Alumni Scholar, University of California, Berkeley
1978-82	Regents Scholar, University of California, Berkeley

News/Media Interviews

2024	August 19, 2024 – Featured in Politico's E&E news regarding US reusing captured CO_2 for concrete, aviation fuel
	August 7, 2024 – Featured in National Academies news regarding NASEM report about the role for carbon dioxide utilization in U.S. economy and identifying research gaps and opportunities
2023	November 25 – Interview on the "Girl Power Gurus" podcast as an international leader in sustainability science
	October 29 – Featured in Forbes regarding energy efficiency as a panacea for power
	June 28 – Interview with David Zierler at the Caltech Heritage Project regarding the paramount issue of climate change and sustainability
	May 5 – Featured in C-Change Conversation regarding the processes of transforming CO_2 emissions from burning coal, oil, and gas into useful products
	April 3 – Featured in Vogue Business regarding Why Gucci's latest fragrance is made from recycled carbon
	April 1 – Featured in PAW regarding Princeton Plasma Physics Lab Takes on Sustainability Science
2022	December 8 – Featured in OilPrice.com regarding scientists inventing a new way to convert ammonia into hydrogen
	December 3 – Featured in SciTechDaily regarding a new catalyst turning a smelly gas byproduct into a cash cow
	December 2 – Featured in E&E News regarding NASEM report of capturing carbon dioxide and conversion into useful products is possible but requires extensive new infrastructure and large clean energy inputs
	December 1 – Featured in Innovation Map regarding Houston startup founders reporting on clean energy tech efficacy

December 1 – Featured in National Academies news regarding NASEM report that industry and government should begin planning carbon dioxide utilization in circular economy

November 28 – Featured in SciTechDaily regarding development of light-powered nanomaterial catalyst that could be key for hydrogen economy

November 28 – Featured in Green Car Congress regarding development of earth-abundant photocatalyst for conversion of ammonia into hydrogen

November 27 – Featured in Earth.com regarding unlocking hydrogen's potential as a green fuel

November 25 – Featured in Tech Xplore regarding researchers creating green fuel with the flip of a light switch

November 25 – Featured in Science Daily regarding a new inexpensive catalyst that could be key for hydrogen economy

November 25 – Featured in Techfragments regarding a catalyst using light to turn ammonia into hydrogen fuel

November 24 – Featured in Phys.org regarding a light-powered catalyst that could be key for hydrogen economy

November 24 – Featured in Mirage News regarding Rice lab's key light-activated nanomaterial for hydrogen economy

February 9 – Interview with Times Radio UK (in association with The Times and Sunday Times) regarding JET fusion energy breakthrough

January 4 – Interview with Times Radio UK (in association with The Times and Sunday Times) regarding China's fusion research

2021 December 7 – Featured for the 2021 MRS Materials Theory Award regarding quantum-derived materials solutions for a sustainable future

2020 January 17 – Featured in ACS Chemical & Engineering News regarding the development of an improved process for synthesis gas ("syngas") production

January 16 – Quoted in *LA Times* on carbon conversion entitled "Turning carbon into concrete could win UCLA team a climate victory — and $7.5 million"

2019 November 15 – Featured in *The Philadelphia Inquirer* article entitled "Philadelphia science prize goes to climate change and electronics researchers from Penn, UCLA"

October 21 – Interview with *Physics* Magazine entitled "Waiting for the Quantum Simulation Revolution"

May 29 – Interview with 'She Roars' Podcast on universities in the service of humanity at Princeton and beyond

January 25 – Quoted in *China Daily* on China's Vice-President Wang Qishan call on innovation, multilateralism, and shaping a shared future entitled "Global vision presented in Davos speech"

January 24 – Interview with Yahoo! Finance entitled "The focus on the 4th Industrial Revolution at Davos"

January 21 – Interview with Bloomberg TV on Engineering's value to society

2018 September 19 – Interview with *ACS Energy Letters* Editor-in-Chief, Prashant V. Kamat, "A Conversation with Emily Carter," *ACS Energy Lett.*, **3**, 2470 (2018)

2017 January 18 – Interview with Reuters Money on climate change, innovation, and women in tech, aired via Facebook Live

January 16 – Featured in a World Economic Forum article entitled "Smashing the glass ceiling: 6 Davos leaders explain how they did it"

2016 May 5 – Quoted in the New York Times on ExxonMobil's pursuit of carbon capture technology entitled "Exxon Mobil Backs FuelCell Effort to Advance Carbon Capture Technology"

January 19 – Published an Op-Ed in the Houston Chronicle entitled "In era of cheap oil, our choices are clear: consume more or spark change"

2014 February – Co-wrote a Change.org petition to "stop gender discrimination in science"; this, as well as a follow-up interview with Nature entitled "Chemists call for boycott over all-male speaker line up"

2010 February 26 – Featured in Popular Science and Science Daily News regarding the discovery of an equation for materials innovation

2009 June 12 – Interview with NJNews television regarding EFRC on Combustion Science, aired on Channel 13

2006 June 5 – Featured in the Princeton Weekly Bulletin entitled "Carter shapes future breakthroughs, one atom at a time, one student at a time"

2005 January 31 – Published an invited Op-Ed piece in the Daily Princetonian entitled "Few Women in the Sciences? It's the Culture, Stupid;" this, as well as a response by Paul R. Ehrlich

1999 August – Interview with German TV (Bayrischer Rundfunk) about research

Memberships in Professional Societies

The Royal Society; elected Foreign Member in 2024

Royal Society of Chemistry; elected Fellow in 2022

European Academy of Sciences; elected Member in 2020

National Academy of Engineering; elected Member in 2016

National Academy of Inventors; elected Fellow in 2014

International Academy of Quantum Molecular Science; elected Member in 2009

National Academy of Sciences; elected Member in 2008

American Academy of Arts and Sciences; elected Fellow in 2008

Institute of Physics; elected Fellow in 2004

American Association for the Advancement of Science (1999 -); elected Fellow in 2000

Materials Research Society (1998 -)

American Vacuum Society (1989 -); elected Fellow in 1995

American Physical Society (1984 -); elected Fellow in 1998

American Chemical Society (1981 -); elected Fellow in 2012

Editorial Services to Scholarly Publications

Co-Guest Editor, *The Journal of Physical Chemistry* (Virtual Special Issue), "Honoring Michael R. Berman," 2022-23

Member, Editorial Advisory Board, *Energy & Environmental Science*, 2021-

Member, Editorial Advisory Board, *Advanced Theory and Simulations*, 2017-

Member, Editorial Advisory Board, *Journal of the American Chemical Society*, 2017-

Member, Inaugural Editorial Advisory Board, *ACS Central Science*, 2015-18

Member, Editorial Advisory Board of *Journal of Physical Chemistry Letters,* 2014-15

Member, Editor-in-Chief Search Committee, *Science*, 2012-13

Member, Editorial Advisory Board of *Journal of Chemical Theory and Computation*, 2010-19

Member, Editor-in-Chief Search Committee, *Journal of Chemical Physics*, 2007-08

Member, Editorial Board of *Annual Review of Physical Chemistry*, 2006-10

Member, Editorial Advisory Board of *Accounts of Chemical Research*, 2005-07

Guest Editor, *Accounts of Chemical Research special issue on Computational and Theoretical Chemistry*, 2004-05

Member, Editor-in-Chief Search Committee, *Journal of Physical Chemistry*, 2003-04

Member, Editorial Board of *SIAM Journal on Multiscale Modeling, and Simulation*, 2001-07

Member, Editorial Board of *Modelling and Simulation in Materials Science and Engineering,* 2001-12

Member, Editorial Advisory Board of *ChemPhysChem*, 2000-14

Member, Editorial Board of *Journal of Chemical Physics,* 2000-02

Guest Editor, *Journal of Physical Chemistry William A. Goddard issue,* 1999-2000

Member, Advisory Editorial Board of *Chemical Physics Letters,* 1998-2009

Member, Advisory Editorial Board of *PhysChemComm*, 1998-2002

Member, Editorial Board of the *Encyclopedia of Chemical Physics and Physical Chemistry,* 1999-2001

Member, Editorial Advisory Board of *Journal of Physical Chemistry,* 1995-2000

Member, Editorial Advisory Board of *Surface Science*, 1994-99

Specialist Editor of *Computer Physics Communications,* 1993-94

Member, Editorial Advisory Board of *Molecular Simulation,* 1991-96

Referee for: Accounts of Chemical Research, ACS Applied Materials & Interfaces, ACS Catalysis, ACS Sustainable Chemistry & Engineering, Advanced Energy Materials, Advanced Functional Materials, American Chemical Society Symposium Series, Angewandte Chemie, Applied Physics Letters, Canadian Journal of Chemistry, Catalysis Letters, Catalysis Today, ChemCatChem, Chemical Communications, Chemical Physics, Chemical Physics Letters, Chemical Reviews, Energy & Environmental Materials, Energy & Environmental Science, Energy & Fuels, IEEE

Transactions on Plasma Science, Inorganic Chemistry, International Journal for Multiscale Computational Engineering, John Wiley & Sons, Ltd., Journal of Applied Physics, Journal of Chemical Physics, Journal of Computational Chemistry, Journal of Computational Physics, Journal of Materials Chemistry A, Journal of Molecular Catalysis, Journal of Organic Chemistry, Journal of Physical Chemistry, Journal of the American Chemical Society, Journal of Vacuum Science and Technology, Langmuir, Molecular Physics, Nanoscale, Nature, Nature Catalysis, Nature Chemistry, Nature Nanotechnology, Physica A, Physical Chemistry Chemical Physics, Physical Review B, Physical Review Letters, RSC Advances, Small, Solar RRL, Spectrochimica Acta, Surface and Coatings Technology, Surface Science, The European Physical Journal B, THEOCHEM, World Scientific Publishers.

PROFESSIONAL/COMMUNITY SERVICE

Referee for proposals submitted to the National Science Foundation, the Department of Energy, the American Chemical Society Petroleum Research Fund, the Army Research Office, the Air Force Office of Scientific Research, the International Science Foundation, Research Corporation, the Hong Kong Research Grants Council, the International Union of Pure and Applied Chemistry, the German-Israeli Foundation for Scientific Research & Development, University of California Energy Institute, the United States-Israel Binational Science Foundation, the Austrian Science Fund, Israel Science Foundation, and CECAM (European Centre for Atomic and Molecular Computations).

2025 Member, Scientific Advisory Board, Materials for Energy Conversion and Storage (MECS), Vienna Institute of Technology, Austria, 2025-

Outreach activities February 5 – Invited Speaker, "A Conversation about Climate Intervention Strategies: The Work Ahead," The Old Guard of Princeton, Princeton, NJ

2024 Chair, Scientific Advisory Board, Equatic, Inc., 2024-

Member, Sectional Committee 3 (Chemistry), The Royal Society, 2024-

Member, Stanford University Chemical Engineering External Advisory Committee, 2024

Outreach activities: September 18 – Presenter, "Carbon Utilization, Infrastructure, Research and Development: A Final Report," National Academies of Sciences, Engineering, and Medicine (NASEM) Division Committee on Engineering and Physical Sciences Meeting (held virtually), Washington, DC

August 19 – Presenter, "Carbon Utilization Infrastructure, Markets, and Research and Development: A Final Report," National Academies of Sciences, Engineering, and Medicine (NASEM) Public Briefing (held virtually), Washington, DC

August 7 – Presenter, "Carbon Utilization Infrastructure, Markets, and Research and Development: A Final Report," National Academies of Sciences, Engineering, and Medicine (NASEM) Sponsor Briefing, Pittsburgh, PA

March 25 – Invited Speaker, Lab Showcase: Meet the Princeton Plasma Physics Laboratory: Powering Possibilities for a Clean Energy Future," Federal Laboratory Consortium for Technology Transfer, Washington DC

March 21 – Invited Distinguished Panelist, Trends in Translational Research and Innovations in Material Science and Engineering," NAI-NJIT Forum on Sustainable Societies: Advances in Material Science and Engineering, Newark, NJ

2023 Co-Lead, Simons Foundation International Collaboration on Solar Radiation Management Science, 2023-

Member, John Scott Award Advisory Committee, 2023-

Member, Planning Committee for the 2023 Annual NAE Meeting Forum

Outreach activities: October 27 – Panel Moderator, Andlinger Center for Energy and the Environment Annual Meeting: Next-Generation Technologies for Carbon Capture, Utilization, and Storage, Princeton, NJ

October 23-25 – Chair, NASEM Webinar Series: Carbon Dioxide Utilization Markets, Infrastructure, Research and Development

September 18 – Invited Speaker, "Weighing Technology Choices for Climate Mitigation: Now, Later, or Never, and Where?" Princeton Human Values Forum (HVF), Princeton University

August 30 – Invited Speaker, "Applied Materials and Sustainability Sciences: New Directions for PPPL," Princeton Collaborative Research Facility (PCRF), Princeton Plasma Physics Lab

May 26 – Invited Speaker, "Seizing the Climate Mitigation Window: New Initiatives at PPPL and Princeton," Andlinger Center for Energy and the Environment, Princeton Reunions 2023

April 5 – Invited Panelist, Princeton NuEnergy U.S. Dept. of Energy EERE Grant Launch, "Innovation in NJ – Growing NJ's Clean Energy Economy"

March 15 – Invited Speaker, PPPL Young Professionals Network Spotlight Event

2022 Chair, Committee on Carbon Utilization Infrastructure, Markets, Research and Development, National Academies of Science, Engineering, and Medicine (NASEM) (2022-2024)

Member, Kavli Foundation Board of Directors, 2022-2026

Member, Visiting Committee for the California Institute of Technology Division of Chemistry and Chemical Engineering

Outreach activities: March 1-3 – Chair & Moderator, NASEM Webinar Series: Technology, Infrastructure, and Policy for Carbon Utilization

March 29 – Invited Presenter, NASEM Division on Engineering and Physical Sciences (DEPS) Committee Meeting

April 4 – Invited Guest Speaker, Princeton NuEnergy (PNE) FY2022 Q1 Quarterly Conference

April 27 – Invited Speaker, Collaborative Opportunities in Hydrogen RDD&D Workshop, Andlinger Center for Energy and the Environment, Princeton University

May 20 – Invited Speaker, "Transforming Carbon Dioxide for a Sustainable Future," Andlinger Center for Energy and the Environment, Princeton Reunions 2022

June 30 – Contributed Presenter, "National Academies Congressionally Mandated Study on Carbon Utilization Infrastructure, Markets, and RD&D," 19th International Conference on Carbon Dioxide Utilization (ICCDU), Princeton, NJ

September 14 – Keynote Speaker, "Keys to Becoming a Successful Faculty Member," Princeton Rising Stars in Physics Conference 2022, Princeton, NJ

September 19-20 – Workshop Organizer, Simons Foundation Science of Solar Geoengineering Workshop, New York, NY

November 30 – Presenter, "Carbon Dioxide Utilization Markets and Infrastructure: Status and Opportunities: A First Report," National Academies of Sciences, Engineering, and Medicine (NASEM) Congressional Briefing (held virtually), Washington, DC

December 1 – Presenter, "Carbon Dioxide Utilization Markets and Infrastructure: Status and Opportunities: A First Report," National Academies of Sciences, Engineering, and Medicine (NASEM) Public Briefing (held virtually), Washington, DC

December 5 – Invited Panelist, "A zero-emissions world is not a carbon-free world?" Deloitte-Andlinger Center Leadership Roundtable, Princeton, NJ

2021 Facilitator for the Research Corporation for Science Advancement (RSCA) 2021 Scialog Negative Emissions Science (NES) Conference

Member, Decadal External Review Committee for the Kavli Foundation

Outreach activities: October 29 – Invited Speaker: Sustainability and Plasma Sciences, Virtual Visit by the Honorable Jennifer M. Granholm, U.S. Secretary of Energy, Princeton Plasma Physics Laboratory (PPPL), Princeton, NJ

February 11 – Interview, An Intergenerational Chat Between STEMinists, United Nations (UN) Women for YOUth Newsletter (International Day of Women and Girls in Science), University of California, Los Angeles, Los Angeles, CA

February 22 – Invited Speaker/Panelist: The Carbon Continuum – Transition to a Net-Zero World, Institute for Carbon Management (ICM), University of California, Los Angeles, Los Angeles, CA

April 1 – Interview, Carbon sequestration: a critical but less-understood piece of the climate puzzle, Institute of the Environment and Sustainability (IoES), University of California, Los Angeles, Los Angeles, CA

April 1 – Invited Speaker/Panelist: Overcoming leadership challenges in digital teaching, Times Higher Education (THE) Live USA 2021, London, United Kingdom

2020 Member, Search Committee for University of California, Riverside Provost and Executive Vice Chancellor

Outreach activities: October 1 – Invited Speaker, Los Angeles Cleantech Incubator (LACI) Power Day, Los Angeles, CA

July 10 – Panelist, Higher Education Leadership, Virtual California Higher Education Sustainability Conference (CHESC), University of California, Santa Barbara, Santa Barbara, CA

2019 Member, NAE Dean's Roundtable on Linking Academic Engineering Research and Defense Basic Science, 2019-20

Member, External Advisory Committee of the University of Chicago Institute for Molecular Engineering

Member, External Review Committee of the Columbia University Fu Foundation School of Engineering and Applied Science

Outreach activities:

December 12 – Panelist, Way Forward and Actions – How is California Leading the Charge?, Environmental and Climate Change Literacy Project and Summit (ECCLPS), University of California, Los Angeles, Los Angeles, CA

November 12 – Round Table Panelist, Female Perspective, Jung Female Investigators' Program, University of Basel, Basel, Switzerland

October 1 – Featured Speaker, What is a University?, 10 Questions: Centennial Edition, University of California, Los Angeles, Los Angeles, CA

May 9 – College of Science and Technology Spring Commencement Speaker, Temple University, Philadelphia, PA

May 6 – Invited Speaker, Welcome Address, Building the Future: New Technological Frontiers in Cities, Princeton University, Princeton, NJ

April 28 – Featured Speaker, Johns Hopkins University Presidential Brunch Gathering on Sustainability, Johns Hopkins University, Baltimore, MD

February 25 – Session Chair on Computer Simulation, 11th Annual International Workshop on Advanced Materials (IWAM 2019), Ras Al Khaimah, United Arab Emirates

January 24 – Panelist, CNBC presents: A Just Energy Transition for the World Panel Discussion, World Economic Forum Annual Meeting 2019, Davos, Switzerland

January 24 – Panelist, The Promise and Progress of Bioengineering, World Economic Forum Annual Meeting 2019, Davos, Switzerland

2018

Member, 2019 Irving Langmuir Prize Selection Committee, 2018-19

Member, National Academies of Sciences, Engineering, and Medicine (NASEM) External Review Committee of the Gulf Research Program, 2018-19

Outreach activities:

October 4 – Invited Speaker, An Introduction to Engineering and Applied Science at Princeton, China Executive Summit 2018, Princeton University, Princeton, NJ

May 15 – Invited Speaker, ACS Princeton Local Section May Sectional Meeting, Princeton University, Princeton, NJ

April 7 – Keynote Speaker, AIChE Regional Conference, Princeton University, Princeton, NJ

January 26 – Invited Speaker, Women in Leadership Breakfast, Garden Court Hotel, Palo Alto CA

2017

Outreach activities:

October 25 – Speaker, Welcome: Thoughts on the Intersection of Biomedical Research and Data Science, Ahead of the Curve: New Frontiers in Biomedical Data Science, Princeton University, Princeton, NJ

October 18 – Organizing Committee Member and Panel Chair, New Directions in Carbon Dioxide Utilization, The Royal Society of London 2017 Sackler Forum on Dealing with Carbon Dioxide at Scale, Buckinghamshire, UK

September 6 – Invited Speaker, Overcoming Grand Challenges of the Twenty-First Century: The View from Princeton Engineering, Canyon Partners Research Retreat, Beverly Hills, CA

May 11 – Invited Speaker, Princeton Alumni Breakfast and Conversation, Henrietta's Table at The Charles Hotel, Cambridge, MA

April 26 – Invited Speaker, Annual Dinner of the Princeton Club of Chicago on The Future of Engineering at Princeton, University Club of Chicago, Chicago, IL

April 4 – Panelist, Women in COMP Post-Doctoral Breakfast, 253rd ACS Spring National Meeting, San Francisco, CA

February 8 – Invited Speaker, 55th Reunion Reception and Dinner with Princeton Class of 1962, New York Yacht Club, New York, NY

January 19 – IdeasLab Panelist, Responding to Climate Change with Princeton University, World Economic Forum Annual Meeting 2017, Davos, Switzerland

January 18 – Panelist, Princeton's Breakfast Panel: Income Inequality and Opportunities to Improve the Human Condition, World Economic Forum Annual Meeting 2017, Davos, Switzerland

2016 Member, Molecular Sciences Software Institute (MolSSI) Advisory Board, 2016-17

Member, Lawrence Berkeley National Laboratory (LBNL) Advisory Board, 2016-25

Member, Secretary of Energy Advisory Board Task Force on CO_2 Utilization and Negative Emissions, 2016-17 (https://www.energy.gov/seab/downloads/final-report-task-force-co2-utilization)
Member, ExxonMobil Corporate Strategic Research (CSR) Capability Reassessment Committee, 2016

Member, International Advisory Committee, World Association of Theoretical and Computational Chemists (WATOC) 2017 Conference

Outreach activities: December 2 – Invited Speaker, An Overview of Engineering Landscape and Princeton's School of Engineering and Applied Science, President's Retreat on Engineering, Princeton, NJ

November 15 – Invited Speaker, Sustainable Engineering and Development Society Dinner, Princeton University, Princeton, NJ

November 10 – Keynote Speaker, Celebrate Princeton Invention 2016, Princeton University, Princeton, NJ

October 4 – Invited Speaker, Women in Science Colloquium Dinner, Princeton University, Princeton, NJ

May 28 – Panel Moderator, Princeton Alumni-Faculty Forum, Out of the Box: What's New in Alternative Energy?, Princeton University, Princeton, NJ

May 18-20 – Organizer and Session Chair, Andlinger Center Building Opening Celebration and Symposium, Princeton University, Princeton, NJ

April 20 – Invited Speaker, Princeton Preview Faculty Panel, Princeton University, Princeton, NJ

2015 October 9 – Invited Speaker, Lead New Jersey Seminar on The Research Frontier in
Outreach activities: Energy and the Environment, Stonybrook-Millstone Watershed Association, Pennington, NJ

June 23 – Invited Speaker, Science & Storytelling NYC: NAS Speed Dating, Google NY, New York, NY

June 16 – Nassau Hall Society Speaker, Water, Energy, and the Environment, National Maritime Museum, Amsterdam, The Netherlands

April 26 – Presenter, 2015 NAS Awards Ceremony, Washington, DC

January 31 – Invited Speaker, Science on Saturday Lecture Series on The Road to a Sustainable Energy Future, Princeton Plasma Physics Laboratory, Princeton, NJ

2014 Member, Board on Energy and Environmental Systems, National Research Council, National Academy of Sciences, 2014-17

Member, 2015 National Academy of Sciences Award in Chemical Sciences Selection Committee

Member, SLAC National Accelerator Laboratory Scientific Policy Committee, 2014-16

Member, International Organizing Committee for the International Congress of Quantum Chemistry, 2014-17

Outreach activities: September 10 – Invited Speaker, Butler/PEI Energy Table Discussion & Dinner on The Future of Energy Technologies and Andlinger Center Resources, Butler College, Princeton University, Princeton, NJ

March 29 – Keynote Speaker, A Tale of Two Evolving Trajectories: Perspectives on a Life in Science and the Future of Energy, Women in STEM Symposium, Princeton University, Princeton, NJ

March 4 – Princeton Graduate Alumni Dinner Speaker, The Future of Energy (with Dean Vince Poor), Crowne Plaza Hotel, Palo Alto, CA

January 4 – After-Dinner Speaker, Food, Water, Energy and the Environment, Princeton Food Salon, Princeton, NJ

2013 Member, National Academy of Sciences Class Membership Committee, 2013-14

Advisory Council Liaison, NSF Mathematical and Physical Sciences Subcommittee on Optics and Photonics, 2013-14

Outreach activities: November 15 – Invited Speaker, Class of 1951 Mini-Reunion, Princeton University, Princeton, NJ

November 13 – Invited Speaker, Old Guard of Princeton, "Achieving a Sustainable Energy Future via Quantum Mechanics and the Andlinger Center," Princeton University, Princeton, NJ

June 26 – 2013 Princeton-CEFRC Summer School Career Panel Discussion, Princeton University, Princeton, NJ

June 19 – Panelist, Senate/NAS Science and Technology Policy Forum on Energy, Capitol Hill, Washington, DC

June 1 – Moderator, Princeton Alumni-Faculty Forum Panel, Can We Turn Things Around? Sustainability and Climate Change, Princeton, NJ

May 9 – Last Lecture for the Class of 2013, "Energy Choices for the 21st Century & Beyond," Princeton University, Princeton, NJ

January 9 – Invited Speaker, The Role of Science in Moving the Planet to Green Energy and a Sustainable Future, Nassau Club, Princeton, NJ

2012 Member, NSF Mathematical and Physical Sciences Advisory Council, 2012-15

Member, National Academy of Sciences Class Membership and Chemistry in Service to Society Committees, 2012-13

Chair, DOE-BES Council on Chemical and Biochemical Sciences, 2012-13

Outreach activities: October 19 – Panelist, What's Next in Energy, Aspire Colloquium, Princeton University, Princeton, NJ

June 2 – Moderator, Princeton Alumni-Faculty Forum Panel, Managing Our Expectations: Long-Term Energy Solutions, Princeton, NJ

May 31 – Panelist, Opportunities and Obstacles in Large-Scale Biomass Utilization – The Role of Chemical Sciences, Chemical Sciences Roundtable, Washington, DC

April 14 – Moderator, Energy Policy Panel, Princeton Colloquium on Public and International Affairs "The State of the States," Princeton, NJ

2011 Member, International Advisory Board of the Winton Programme for the Physics of Sustainability, Cambridge University, 2011-17

Outreach activities: July 14 – Moderator, A Conversation on Global Sustainability, Leading Through Change: A Princeton University Conference, Half Moon Bay, CA

May 25 – Panelist, A View from Senior EFRC Representatives, Science for our Nation's Energy Future, Energy Frontier Research Centers Summit & Forum, Washington, DC

April 16 - Keynote Speaker, Our Future, Our Challenge: 2011 High School Student Eco-Conference, Princeton Day School, Princeton, NJ

March 1 - Discussant, The Sunlight Derby – How to Win the Never-ending Race to Optimize Energy Risk in the 21st Century, JP Morgan Chase Global Markets Symposium, Key Biscayne, FL

February 12 – Moderator, Clean Energy Panel, Global China Connection Princeton International Conference, Princeton, NJ

2010 Chair, Energy Subdivision of the PHYS Division of the ACS, 2010-11

Member, Board on Chemical Sciences and Technology, National Research Council, National Academy of Sciences, 2010-12

Vice-Chair, DOE-BES Council on Chemical and Biochemical Sciences, 2010-11

July 26-27 – Invited Panelist and Speaker, OSTP/DOE Workshop on Computational Materials Science and Chemistry for Innovation

Outreach activities: October 15 – After dinner speaker at Princeton University's Aspire Leadership Assembly Dinner

February 19 – After dinner speaker at Princeton University's Annual Giving Reception and Dinner

2009 Conference co-organizer, "Chemical Carbon Mitigation – A Physiochemical Approach, *American Chemical Society Symposium*, Spring 2011, Anaheim, California, 2009-11

Co-organizer, DOE-BES workshop on Theories of Excited States in Molecules and Nanostructures, 2009-10

Chair-Elect, Energy Subdivision of the PHYS Division of the ACS, 2009-10

Outreach activities:	November 17 – Spoke at a Capitol Hill press conference about the impact of American Recovery and Reinvestment Act of 2009 investments in basic scientific research
	November 16 – Spoke at Princeton University Graduate School High Table about new projects in energy research
	March 25 – Invited Speaker on "Women in Research Computing," Office of Information Technology, Princeton University
2008	Member, DOE-BES Council on Chemical and Biochemical Sciences, 2008-11
	Member, International Advisory Board, 4th Multiscale Materials Modeling Conference, October 2008, Florida State University
2007	Member, NSF Workshop on Predictive Modeling of Materials at the Nanoscale
	Member, International Scientific Advisory Board, Centre of Excellence in Theoretical and Computational Chemistry, Norway, 2007-10
	Conference co-organizer, "Bold Predictions in Theoretical Chemistry: A Symposium in Honor of One of the Boldest, Bill Goddard, on the Occasion of his 70th Birthday, *American Chemical Society National Meeting*, August 2007, Boston, Massachusetts
Outreach activities:	Dec 14 - "Pizza with Professors in PRISM", Princeton University, Princeton, NJ
	Dec 13 - Panelist for workshop "Keys to Becoming a Successful Faculty Member," PICASso Career Workshop, Princeton University, Princeton, NJ
	Dec. 13 – Speaker, "Keys to Becoming a Successful Faculty Member," PICASso Career Workshop, Princeton University, Princeton, NJ
	April 19 – Speaker, "Mentoring in the Workplace," Office of Information Technology, Princeton University
2006	Member, NSF Review Panel for Cyber-Enabled Chemistry
	Member, DOE-BES Council for Chemical Sciences
	Member, Steering Committee for the Thomas Young Centre for Theory and Simulation of Materials, London, 2006-12
2005	Chair, American Conference on Theoretical Chemistry
	Chair, Division of Chemical Physics, American Physical Society
	Member, National Science Foundation Mathematical and Physical Sciences Theory Steering Committee
Outreach activities:	Sept 24 – Spoke about the need for women in engineering careers to 63 high school girls at the Mother-Daughter Luncheon hosted by Today's World Learning Center Foundation, Ryland Inn, Whitehouse, NJ
	Sept. 22 – Calculus Cameo on Combustion Dynamics to Princeton Freshmen.
	Sept. 12 - Member, Freshman Orientation Panel for the Princeton University Science and Technology Council
	February 4 – Spoke about Materials and Combustion Research to 110 high school girls on a SEAS outreach trip to New York City, organized by the National Coalition of Girls Schools

January 26 – What's in a Flame? (Combustion Chemistry) presentation at Community Park Elementary School Career Day

2004 Chair, Division of Chemical Physics, American Physical Society

International Advisory Committee, "Conference on Computational Physics," Genoa, Italy, 1-4 September, 2004

International Advisory Committee, 3rd International Conference on "Computational Modeling and Simulation of Materials" Acireale, Sicily, Italy, May 29-June 5, 2004

Symposium co-organizer, "Multiscale and Stochastic Modeling Methods," *SIAM Conference on Mathematical Aspects of Materials Science*, Los Angeles, CA, May 23-26, 2004

Program Chair, Division of Chemical Physics, American Physical Society March Meeting, Montreal, Canada, 22-26 March, 2004

Member, National Science Foundation Mathematical and Physical Sciences Theory Steering Committee

2003 Chair-Elect, Division of Chemical Physics, American Physical Society

Co-organizer, American Chemical Society Symposium, "New electronic structure methods: from molecules to materials," April, 2003

Member, Executive Committee for "Materials and Nanotechnology" Strategic Planning Workshop (Princeton University)

2002 Vice-Chair, Division of Chemical Physics, American Physical Society

Organizing Committee Member, Institute for Pure and Applied Math Workshop on Modeling and Simulation for Materials, 18-22 November, 2002

Conference co-organizer, "Molecular Modeling and Computation: Perspectives and Challenges," Center for Integrative Multiscale Modeling and Simulation, Caltech, Pasadena, CA, 15-16 November, 2002

Chair, Institute for Pure and Applied Mathematics Workshop on Linear Scaling Electronic Structure Methods, UCLA, 1-4 April, 2002

Host, Career-Day visitors, Marlborough School (Los Angeles), 25 March 2002.

2001 Two lectures, demonstrations, and video presentations etching and corrosion of materials at the UCLA University Elementary School (March 15, 2001)

Interviewed by graduate student minoring in Women Studies (May 15, 2001)

Panelist, Women in Science Faculty Roundtable (May 15, 2001)

2000 International Advisory Committee Member, 10th International Conference on Solid Films and Surfaces (ICSFS-10)

Member, Los Alamos National Laboratory Theoretical Division Advisory and Review Committee, 2000-05

Member, Physics and Astronomy Classification Scheme (PACS) Working Group, April 2000

Lecture on phases, molecular motion, energy, atomic structure, and molecular dynamics to 4th grade science students at Willows Community School in Los Angeles, March 17, 2000

1999 Sole Faculty Representative of the University of California system at the Science Coalition Signature Event, the purpose of which was to explain to Congress, in one-on-one meetings with Congressional Representatives or their staff, the importance of funding basic scientific research at Universities (Sept. 22, 1999)

Proposal Coordinator and Proposed Director of a UCLA Materials Research Science and Engineering Center (pre-proposal submitted Sept. 10, 1999)

Member, NSF Division of Materials Research Committee of Visitors, February 24-26, 1999

1998 Member, NSF Materials Research Science and Engineering Center Reverse Site Visit Review Panel, May 4-7, 1998

Reviewer for the National Research Council's Committee on Review and Evaluation of the Army Chemical Stockpile Disposal Program's Report on "Using Supercritical Water Oxidation to Treat Hydrolysate from VX Neutralization," February 3, 1998

1996 January 1996-December 1997: Executive Committee Member, Electronic Materials and Processing Division of the American Vacuum Society

1995 Panelist, Diversity Forum at the National Organization for the Professional Advancement of Black Chemists and Chemical Engineers, 20 April 1995

Conference co-organizer, "Metal-Metal Bonding: From Clusters to Surfaces," American Chemical Society National Meeting, Anaheim, CA, 2-7 April, 1995

American Chemical Society Awards Committee for the ACS Award for Encouraging Women into Careers in the Chemical Sciences (1995-1997)

1994-1997 Executive Committee Member, Division of Computational Physics of the American Physical Society

1994 Discussion Leader, Career Paths and Strategies for Success as a Woman in Science, at Caltech, 10 November 1994

Participant, Sigma Xi Planning Conference for the Sigma Xi 1995 Forum on Science Policy, 8-11 September 1994

1994 ACS Division of Physical Chemistry Procter & Gamble Award Committee

Panelist, Women in Science Roundtable Discussion: Personal Experiences, Strategies for Success, and a Look to the Future, University of Toronto, Canada, 19 May 1994

Discussion Leader, "On Issues Concerning Women in the Workplace," UCLA Chemistry and Biochemistry Department, 29 April 1994

University of California Regents Scholarship Interviewer, 16 April 1994

Panelist, 1994 Workshop on "Women in the Sciences: Rising to the Challenge," at UCLA, 27 January 1994

1993 Conference Chair, "14th Annual West Coast Theoretical Chemistry Conference," UCLA, CA, 17-19 June 1993

1992 Panelist, 1992 National Science Foundation Postdoctoral Fellowships in Chemistry

1992-1994 Executive Committee Member, Surface Science Division of the American Vacuum Society

1992-1995 Executive Committee Member, Division of Physical Chemistry of the American Chemical Society

1991 Conference co-organizer, "Richard B. Bernstein Memorial Symposium," Los Angeles, CA, 19-20 April 1991

Participant, "1991 Workshop on Chemical Education," University of Utah, Salt Lake City, Utah, 22-24 March 1991

1990 Conference co-organizer, "Physics, Chemistry, and Materials Science of Clusters", ONR Contractors Conference, Lake Arrowhead, CA, 21 - 23 January 1990

1989 Caltech/MIT High School Visitation Program (1989-1992)

List of Publications

475. A. D. Lele, Z. Shi, S. Khetan, E. A. Carter, J. M. P. Martirez, and Y. Ju, "Machine-learned force field for molecular dynamics simulation of non-equilibrium ammonia synthesis on iron catalysts," *Journal of Physical Chemistry C*, in press (2025).

474. J.-N. Boyn and E. A. Carter, "Elucidating and contrasting the mechanisms for Mg and Ca sulfate ion-pair formation with multi-level embedded quantum mechanics/molecular dynamics simulations," *Journal of Chemical Physics*, **161**, 224501 (2024). doi.org/10.1063/5.0235460.

473. E. A. Carter, S. Atsumi, M. Byron, J. Chen, S. Comello, M. Fan, B, Freeman, M. Fry, S. Jordaan, H. Mahgerefteh, A.-H. Park, J. Powell, A. R. Ramirez, V. Sick, S. Stewart, J. Trembly, J. Yang, J. Yuan, C. Wise, and E. Zeitler, "*Carbon Utilization Infrastructure, Markets, and Research and Development: A Final Report*," National Academies of Sciences, Engineering, and Medicine (NASEM). Washington DC: The National Academies Press. ISBN: 978-0-309-71775-5 (2024). doi: 10.17226/27732

472. E. A. Carter, "Our Role in Solving Global Challenges: An Opinion," *J. Am. Chem. Soc.*, **146**, 21193-21195 (2024). doi: 10.1021/jacs.4c07374

471. X. Wen, J.-N. Boyn, J. M. P. Martirez, Q. Zhao, and E. A. Carter, "Strategies to obtain reliable energy landscapes from embedded multireference correlated wavefunction methods for surface reactions," *Journal of Chemical Theory and Computation*, **20**, 6037-6048 (2024). doi: 10.1021/acs.jctc.4c00558

470. B. Bobell, J.-N. Boyn, J. M. P. Martirez, and E. A. Carter, "Modeling Bicarbonate Formation in an Alkaline Solution with Multi-Level Quantum Mechanics/Molecular Dynamics Simulations," *Molecular Physics Special Issue in Honour of Giovanni Ciccotti*, e2375370 (2024). doi: 10.1080/00268976.2024.2375370

469. X. Wen, J. M. P. Martirez, and E. A. Carter, "Plasmon-driven ammonia decomposition on Pd(111): Hole transfers role in changing rate-limiting steps," *ACS Catalysis*, **14**, 9539 (2024). doi: 10.1021/acscatal.4c01869

468. Z. Wei, J. M. P. Martirez, and E. A. Carter, "First-Principles Insights into the Thermodynamics of Variable-Temperature Ammonia Synthesis on Transition-Metal-Doped Cu (100) and (111)," *ACS Energy Lett.*, **9**, 3012 (2024). doi: 10.1021/acsenergylett.4c01100

467. A. G. Rajan, J. M. P. Martirez, and E. A. Carter, "Strongly Facet-Dependent Activity of Iron-Doped β-Nickel Oxyhydroxide for the Oxygen Evolution Reaction," *Phys. Chem. Chem. Phys. 25th Anniversary Special Issue*, **26**, 14721 (2024). doi: 10.1039/D4CP00315B

466. J.-N. Boyn and E. A. Carter, "Characterizing the Mechanisms of Ca and Mg Carbonate Ion-Pair Formation with Multi-Level Molecular Dynamics/Quantum Mechanics Simulations," *J. Phys. Chem. B*, **127,** 10824 (2023). doi: 10.1021/acs.jpcb.3c05369

465. A. Acosta, J. M. P. Martirez, N. Lim, J. P. Chang, and E. A. Carter, "Effect of thickness and surface composition on the stability of polarization in ferroelectric $Hf_xZr_{1-x}O_2$ thin films," *Phys. Rev. Mater.*, **7,** 124401 (2023). doi: 10.1103/PhysRevMaterials.7.124401

464. Z. Wei, J. M. P. Martirez, and E. A. Carter, "Introducing the Embedded Random Phase Approximation: H_2 Dissociative Adsorption on Cu(111) as an Exemplar," *J. Chem. Phys.*, **159**, 194108 (2023). doi: 10.1063/5.0181229

463. M. B. Bertagni, R. H. Socolow, J. M. P. Martirez, E. A. Carter, C. Greig, Y. Ju, T. Lieuwen, M.E. Mueller, S. Sundaresan, R. Wang, M. A. Zondlo, and A. Porporato, "Minimizing the Impacts of the Ammonia Economy on the Nitrogen Cycle and Climate," *Proc. Natl. Acad. Sci. U.S.A.,* **120,** e2311728120 (2023). doi: 10.1073/pnas.2311728120

462. J.-N. Boyn and E. A. Carter, "Probing pH-Dependent Dehydration Dynamics of Mg and Ca Cations in Aqueous Solutions with Multi-Level Quantum Mechanics/Molecular Dynamics Simulations," *J. Am. Chem. Soc.*, **145,** 20462 (2023). doi: 10.1021/jacs.3c06182

461. J. M. P. Martirez and E. A. Carter, "Solvent dynamics are critical to understanding carbon dioxide dissolution and hydration in water," *J. Am. Chem. Soc.*, **145,** 1256 (2023). doi: 10.1021/jacs.3c01283

460. E. A. Carter, M. A. Johnson, and S. R. Leone, "A Tribute to Michael R. Berman," *J. Phys. Chem. C,* **127,** 11421 (2023). doi: 10.1021/acs.jpcc.3c03070

459. R. B. Wexler, G. S. Gautam, R. Bell, S. Shulda, N. A. Strange, J. A. Trindell, J. D. Sugar, E. Nygren, S. Sainio, A. H. McDaniel, D. Ginley, E. A. Carter, and E. B. Stechel, "Multiple and nonlocal cation redox in Ca–Ce–Ti–Mn oxide perovskites for solar thermochemical applications," *Energy Environ. Sci.*, **16,** 2550 (2023). doi: 10.1039/d3ee00234a

458. R. B. Wexler, E. B. Stechel, and E. A. Carter, "Materials Design Directions for Solar Thermochemical Water Splitting," in *Solar Fuels*, Vol. 3, Nurdan Demirci Sankir & Mehmet Sankir, Eds. (Wiley-Scrivener, USA), 3-64 (2023). doi: 10.1002/9781119752097.ch1

457. L. Li, M. F. Calegari Andrade, R. Car, A. Selloni, and E. A. Carter, "Characterizing Structure-Dependent TiS_2/Water Interfaces using Deep-Neural-Network-Assisted Molecular Dynamics," *J. Phys. Chem. C*, **127**, 9750 (2023). doi: 10.1021/acs.jpcc.2c08581

456. J. Cai, Q. Zhao, W.-Y. Hsu, C. Choi, J. M. P. Martirez, C. Chen, J. Huang, E. A. Carter, and Y. Huang, "Highly Selective Electrochemical Reduction of CO_2 into Methane on Nanotwinned Cu," *J. Am. Chem. Soc.*, **145,** 9136 (2023). doi: 10.1021/jacs.3c00847

455. P. Chen, D. Fan, Y. Zhang, A. Selloni, E. A. Carter, C. B. Arnold, Y. Zhang, A. S. Gross, J. R. Chelikowsky, and N. Yao, "Observation of Electron Orbital Signatures of Single Atoms within Metal-Phthalocyanines using Atomic Force Microscopy," *Nat. Commun.*, **14,** 1460 (2023). doi: 10.1038/s41467-023-37023-9

454. E. A. Carter, S. Atsumi, M. Byron, A. Chuney, S. Comello, M. Fan, M. Fry, H. Mahgerefteh, E. Massetti, A.-H. Park, J. Powell, A. R. Ramírez, V. Sick, C. Wise, and E. Zeitler, "*Carbon Dioxide Utilization Markets and Infrastructure: Status and Opportunities: A First Report*," National Academies of Sciences, Engineering, and Medicine (NASEM), Washington, DC: The National Academies Press, ISBN 978-0-309-69327-1 (2023). doi: 10.17226/26703

453. Y. Yuan, L. Zhou, J. L. Bao, J. Zhou, A. Bayles, L. Yuan, M. Lou, M. Lou, S. Khatiwada, H. Robatjazi, E. A. Carter, P. Nordlander, and N. J. Halas, "Earth-abundant photocatalyst for H_2 generation from NH_3 with light-emitting diode illumination," *Science*, **378**, 889 (2022). doi: 10.1126/science.abn5636

452. L. Yuan, J. Zhou, M. Zhang, X. Wen, J. M. P. Martirez, H. Robatjazi, L. Zhou, E. A. Carter, P. Nordlander, and N. J. Halas, "Plasmonic Photocatalysis with Chemically and Spatially Specific Antenna-Dual Reactor Complexes," *ACS Nano*, **16**, 17365 (2022). doi: 10.1021/acsnano.2c08191

451. R. B. Wexler and E. A. Carter, "Oxygen-Chlorine Chemisorption Scaling for Seawater Electrolysis on Transition Metals: The Role of Redox," *Adv. Theory Simul.*, 2200592 (2022). doi: 10.1002/adts.202200592

450. J. M. P. Martirez and E. A. Carter, "First-Principles Insights into the Thermocatalytic Cracking of Ammonia-Hydrogen Blends on Fe(110): 1. Thermodynamics," *J. Phys. Chem. C*, **126**, 19733 (2022). (Virtual Special Issue: Honoring Michael R. Berman) doi: 10.1021/acs.jpcc.2c06003

449. Q. Zhao, J. M. P. Martirez, and E. A. Carter, "Charting C-C coupling pathways in electrochemical CO_2 reduction on Cu(111) using embedded correlated wavefunction theory," *Proc. Natl. Acad. Sci. U.S.A.*, **119**, e2202931119 (2022). doi: 10.1073/pnas.2202931119

448. Q. Zhao, J. M. P. Martirez, and E. A. Carter, "Electrochemical Hydrogenation of CO on Cu(100): Insights from Accurate Multiconfigurational Wavefunction Methods," *J. Phys. Chem. Lett.*, **13**, 10282 (2022). doi: 10.1021/acs.jpclett.2c02444

447. A. M. Teale, T. Helgaker, A. Savin, C. Adamo, B. Aradi, A. V. Arbuznikov, P W. Ayers, E. J. Baerends, V. Barone, P. Calaminici, E. Cancès, E. A. Carter, P. K. Chattaraj, H. Chermette, I. Ciofini, T. D. Crawford, F. D. Proft, J. F. Dobson, C. Draxl, T. Frauenheim, E. Fromager, P. Fuentealba, L. Gagliardi, G. Galli, J. Gao, P. Geerlings, N. Gidopoulos, P. M. W. Gill, P. Gori-Giorgi, A. Görling, T. Gould, S. Grimme, O. Gritsenko, H. J. A. Jensen, E. R. Johnson, R. O. Jones, M. Kaupp, A. M. Köster, L. Kronik, A. I. Krylov, S. Kvall, A. Laestadius, M. Levy, M. Lewin, S. Liu, P. -F. Loos, N. T. Maitra, F. Neese, J. P. Perdew, K. Pernal, P. Pernot, P. Piecuch, E. Rebolini, L. Reining, P. Romaniello, A. Ruzsinszky, D. R. Salahub, M. Scheffler, P. Schwerdtfeger, V. N. Staroverov, J. Sun, E. Tellgren, D. J. Tozer, S. B. Trickey, C. A. Ullrich, A. Vela, G. Vignale, T. A. Wesolowski, X. Xu, and W. Yang, "DFT exchange: sharing perspectives on the workhorse of quantum chemistry and materials science," *Phys. Chem. Chem. Phys.*, **24**, 28700 (2022). (Hot Article) doi: 10.1039/d2cp02827a

446. M. Lou, J. L. Bao, L. Zhou, G. N. Naidu, H. Robatjazi, A. I. Bayles, H. O. Everitt, P. Nordlander, E. A. Carter, and N. J. Halas, "Direct H_2S Decomposition by Plasmonic Photocatalysis: Efficient Remediation plus Sustainable Hydrogen Production," *ACS Energy Lett.*, **7**, 3666 (2022). doi: 10.1021/acsenergylett.2c01755

445. H. Robatjazi, A. Schirato, A. Alabastri, P. Christopher, E. A. Carter, P. Nordlander, and N. J. Halas, "Reply to: Distinguishing thermal from non-thermal contributions to plasmonic hydrodefluorination," *Nat. Catal.*, **5**, 247 (2022). doi: 10.1038/s41929-022-00768-5

444. S. Zhai, J. Nam, G. S. Gautam, K. Lim, J. Rojas, M. F. Toney, E. A. Carter, I.-H. Jung, W. C. Chueh, and A. Majumdar, "Thermodynamic guiding principles of high-capacity phase transformation materials for splitting H_2O and CO_2 by thermochemical looping," *J. Mater. Chem. A*, **10**, 3552 (2022). doi: 10.1039/d1ta10391a

443. A. Acosta, J. M. P. Martirez, N. Lim, J. P. Chang, and E. A. Carter, "Relationship between ferroelectric polarization and stoichiometry of HfO_2 surfaces," *Phys. Rev. Mater.*, **5**, 124417 (2021). doi: 10.1103/PhysRevMaterials.5.124417

442. L. Li, J. M. P. Martirez, and E. A. Carter, "Identifying an Alternative Hydride Transfer Pathway for CO_2 Reduction on CdTe(111) and $CuInS_2$(112) Surfaces," *Adv. Theory Simul.*, **5**, 2100413 (2021). doi: 10.1002/adts.202100413

441. O. Y. Long, G. S. Gautam, and E. A. Carter, "Assessing cathode property prediction *via* exchange-correlation functionals with and without long-range dispersion corrections," *Phys. Chem. Chem. Phys.*, **23**, 24726 (2021). doi: 10.1039/d1cp03163e

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PATENTS

Emily A. Carter, Robert B. Wexler, Sai Gautam Gopalakrishnan, and Ellen B. Stechel, *Perovskites for Solar Thermochemical Water and Carbon Dioxide Splitting.* Provisional Patent No.: 63/338093. Filed May 4, 2022. *Perovskites For Reduction-Re-Oxidation Thermochemical Water And Carbon Dioxide Splitting*. U.S. Utility Patent filed May 4, 2023.

Emily A. Carter, Robert B. Wexler, and Sai Gautam Gopalakrishnan, *$Cu_2CdGe(S,Se)_4$ Solar Cell Absorbers*. Provisional Patent No.: 63/056,111. Filed July 24, 2020. International Patent Application No. PCT/US2021/42160. Filed July 19, 2021; refiled January 23, 2023.

Emily A. Carter, Ananth Govind Rajan, and John Mark P. Martirez, *A Method of Generating Oxygen by Electrochemical Water Splitting at Optimized Conditions of pH, Temperature, and Pressure*. International Patent Application No.: PCT/IB2022/057592. Filed August 13, 2022. *Operating Conditions for Optimal High-Temperature, High-Pressure Operation of Water Oxidation Electrolyzers Using Mixed Iron/Nickel Oxyhydroxide Catalysts*. U.S. Foreign Filing License No.: 620,196.

Filed July 28, 2021. Indian Provisional Patent No.: 202141034520. Filed July 30, 2021. Indian Patent Issued April 28, 2023.

Emily A. Carter, Nima Alidoust, and Martina Lessio, *Multiple Band Gap Co-Ni Oxide Compositions and Applications Thereof*. Patent No.: US 10,256,361 B2. Issued April 9, 2019.

Emily A. Carter and Nima Alidoust, *p-Type Transparent Conducting Nickel Oxide Alloys.* Patent No.: US 10,079,189. Issued September 18, 2018.

Emily A. Carter and Maytal C. Toroker, *Wustite-Based Photoelectrodes with Lithium, Hydrogen, Sodium, Magnesium, Manganese, Zinc, and Nickel Additives.* Patent No.: US 9,735,306. Issued August 15, 2017.

Emily A. Carter and Ivan Milas, *Barium-Doped Bond Coats for Thermal Barrier Coatings*. Patent No.: US 7,927,714. Issued April 19, 2011.

Emily A. Carter and Emily A. Jarvis, *Supported Metal Catalyst with Improved Thermal Stability*. Patent No.: US 7,504,355. Issued March 17, 2009.

SEMINARS AND PAPER PRESENTATIONS (LAST FIVE YEARS ONLY)

A. Invited Seminars

October 25, 2024	"Carbon Dioxide Conversion for a Sustainable Future: Research and Policy," 2024 Annabelle Lee Lecture, Virginia Tech, VA
May 3, 2024	"How Quantum Mechanics Can Help Identify Mechanisms and Design Materials to Combat Climate Change," 2024 Covestro Lecture, University of Pittsburgh, PA
May 2, 2024	"How a Scientist/Engineer Can Help the Transition to a Net-Negative Emissions Civilization," 2024 Covestro Lecture, University of Pittsburgh, PA
March 20, 2024	"How Quantum Mechanics Can Help Identify Mechanisms and Materials to Combat Climate Change," HML Colloquia Series XX, KTH Royal Institute of Technology, Sweden (given virtually)
September 26, 2023	"How Quantum Mechanics Can Help Identify Mechanisms and Materials to Combat Climate Change," 2023 G. N. Lewis Memorial Lecture, University of California, Berkeley, CA
July 6, 2023	"How Quantum Mechanics Can Help Identify Mechanisms and Materials to Combat Climate Change," Zernike Institute of Advanced Materials Colloquium, University of Groningen, Groningen, The Netherlands
May 15, 2023	"How Quantum Mechanics Can Help Identify Mechanisms and Materials to Combat Climate Change," 2023 Richard S. Mulliken Lecture, University of Chicago, Chicago, IL
May 2, 2023	"Carbon Utilization and Other Needed Technologies for the Transition to Net Zero," High Meadows Environmental Institute Spring 2023 Faculty Seminar, Princeton University, Princeton, NJ

April 25, 2023 "How Quantum Mechanics Can Help Identify Mechanisms and Design Materials to Combat Climate Change," 27th John Stauffer Lectures in Chemistry, Stanford University, Palo Alto, CA

April 24, 2023 "How a Scientist/Engineer Can Help the Transition to a Net-Negative Emissions Civilization," 27th John Stauffer Lectures in Chemistry, Stanford University, Palo Alto, CA

February 17, 2023 "How Low Temperature Plasma Science Can Contribute to Society," PPPL Spring Graduate Student Seminar (AST 558), Plasma Physics Graduate Program, Princeton Plasma Physics Laboratory, Princeton, NJ

January 11, 2023 "How Quantum Mechanics Helps Identify Mechanisms and Discover Materials to Combat Climate Change," Department of Chemistry & Chemical Biology Seminar Series, McMaster University, Ontario, Canada (given virtually)

October 25, 2022 "How Quantum Mechanics Helps Identify Mechanisms and Discover Materials to Combat Climate Change," 2022 Paint Branch Distinguished Lecture in Applied Physics, University of Maryland, Institute for Research in Electronics and Applied Physics, College Park, MD.

May 5, 2022 "How Quantum Mechanics Helps Identify Mechanisms and Discover Materials to Combat Climate Change," 2022 Richard S. H. Mah Lecture on Modeling and Computation in Chemical Engineering, Northwestern University, Department of Chemical and Biological Engineering, Evanston, IL

April 14, 2022 "From Physical Chemistry to Engineering and Beyond: How to Make a Difference," Careers in Chemistry Inaugural Seminar Series, University of Washington, Seattle, WA (given virtually)

February 18, 2022 "Quantum Design of Materials for a Sustainable Future," Mechanical & Aerospace Engineering Spring 2022 Seminar Series, Princeton University, Princeton, NJ

January 26, 2022 "How Quantum Mechanics Helps Identify Mechanisms and Discover Materials to Combat Climate Change," 2022 Harrison Shull Distinguished Lecturer, Indiana University Bloomington, Department of Chemistry, Bloomington, IN (given virtually)

November 9, 2020 "Designing Materials for Sustainable Energy from First Principles," 2020 Brumley D. Pritchett Lecturer, Georgia Institute of Technology, School of Materials Science and Engineering, Atlanta, GA (given virtually)

B. Invited Lectures

August 20, 2024 "Marsha I. Lester Award for exemplary impact in physical chemistry," Invited Speaker at the *ACS Fall 2024 Meeting in the PHYS Awards session*, Denver, CO

August 18, 2024 "First principles insights into catalysis driven by clean electricity," Invited Speaker at the *ACS Fall 2024 Meeting in the Surfaces & Interfaces in Chemical & Biological Systems: Symposium in honor of Hai-Lung Dai session*, Denver, CO

August 7, 2024 "Public Briefing: National Academies of Science Report, Carbon Utilization Infrastructure Markets Research and Development," Invited Speaker at the *2024 FECM/NETL Carbon Management Research Project Review Meeting*, Pittsburgh, PA

July 10, 2024 "Contributions to Climate Change Mitigation through Quantum Simulations," *New Fellows Seminar*, The Royal Society, London, UK

June 13, 2024 "Back to the Future with Blue Moon Dynamics for Climate Change Intervention," Invited Speaker at the *2024 CECAM Workshop* on "From methods to applications: challenges and opportunities in contemporary simulations," École Normale Supérieure, Paris, France

April 30, 2024 "Initial Insights into Greener Ammonia Production from Quantum Simulations," Invited Speaker at the *2024 Annual Carbon Mitigation Initiative* Deep Dive on "Hydrogen & Ammonia Economies: Novel Technical Solutions & Environmental Implications," Princeton University, NJ

April 12, 2024 "A Physical Chemist's Journey to Combat Climate Change," Nichols Medal Award Address, *William H. Nichols Distinguished Symposium* on "Physical Chemistry and Sustainability," American Chemical Society (New York Chapter), White Plains, NY

November 6, 2023 "Carbon Removal Strategies 2030," invited webinar panelist, California Institute of Technology (Caltech), Pasadena, CA

June 15, 2023 "Carbon Dioxide Utilization: Insights from Quantum Based Simulations," Invited Speaker at the *Liquids, Glasses, and Other Adventures in Thermodynamics and Statistical Mechanics Symposium* in Celebration of Pablo Debenedetti's 70th Birthday, Princeton University, Princeton, NJ

May 29, 2023 "Carbon Dioxide Utilization Markets and Infrastructure: Status and Opportunities - A First Report from the U.S. National Academies of Sciences, Engineering, and Medicine," Invited Speaker at the *2023 Carbon Capture, Utilization and Storage Gordon Research Conference*, Les Diablerets, Switzerland

May 24, 2023 "CO_2 Capture via Carbonate Mineralization from Seawater," Invited Speaker at the *Princeton Catalysis Initiative Symposium*, Princeton University, Princeton, NJ

May 4, 2023 "Exploring green strategies for ammonia/hydrogen production," Invited Speaker at the *22nd Annual Meeting of the Carbon Mitigation Initiative*, Princeton University, Princeton, NJ

November 2, 2022 "Photo- and Electro-Catalysis via Embedded Correlated Wavefunction Theory: Examples and Outlook," Invited Speaker at the *Simons Foundation Initiative on Catalysis and Related Topics Workshop*, New York, NY.

August 29, 2022 "Catalyst Design and Discovery for Carbon Dioxide Utilization from First Principles," Invited Plenary Speaker at the *19th International Conference on Density-Functional Theory and its Applications* (DFT2022), Brussels, Belgium (given virtually).

August 22, 2022 "Replacing Fossil-Fuel-Driven Chemical Production by Photo- and Electro-catalysis Derived from Quantum Simulations," Invited Lecture at the *ACS Fall 2022 National Meeting*, Chicago, IL (given virtually).

May 23, 2022 "Sustaining the Planet Via (Photo)(Electro)Catalysis, from First Principles," Invited Keynote at the *27th North American Catalysis Meeting* (NAM27), New York, NY.

March 20, 2022 "Modeling of interfaces involved in sustainable energy technologies," Invited Lecture at the *ACS Spring 2022 National Meeting*, San Diego, CA (given virtually).

December 7, 2021 "Quantum-Derived Materials Solutions for a Sustainable Future," Invited Lecture and Invited Panelist at the *2021 MRS Fall Meeting & Exhibit*, Boston, MA (given virtually).

August 24, 2021 "Quantum chemistry off the beaten path," at the *ACS Fall 2021 National Meeting*, Atlanta, GA (held virtually).

August 22, 2021 "Mechanisms of (photo)electrochemical conversion of CO_2 to fuels from first principles," Invited Keynote at the *ACS Fall 2021 National Meeting*, Atlanta, GA (given virtually).

June 15, 2021 "Excited-State and Electrochemical Reactions at Materials Interfaces: High Fidelity Modeling Now and in the Future," Invited Keynote Lecture and Invited Panelist at the *Materials Research Society (MRS)/Kavli Future of Materials Virtual Workshop: Computational Materials Science, Focus on Non-Equilibrium and Excited-State Dynamics in Materials* (held virtually).

November 16, 2020 "Insights into Sustainable Energy Materials Optimization from First Principles," Opening Keynote at the *International Mechanical Engineering Congress & Exposition (IMECE) 2020 Virtual Meeting*, Portland, OR.

August 17-20, 2020 "Materials discovery for sustainable fuels from first principles," at the *ACS Fall 2020 National Meeting & Exposition*, San Francisco, CA. (Canceled due to COVID-19).

August 18, 2020 "Plasmon-induced excited-state catalysis understood via embedded correlated wavefunction theory," at the *ACS Fall 2020 National Meeting & Exposition*, San Francisco, CA (held virtually).

March 22, 2020 "Modeling of interfaces involved in sustainable energy technologies," at the *2020 ACS Spring National Meeting & Expo*, Philadelphia, PA. (Canceled due to COVID-19).

March 2, 2020 "Plasmon-induced excited-state catalysis understood via embedded correlated wavefunction theory," at the *2020 APS March Meeting*, Denver, CO. (Canceled due to COVID-19).

C. Invited Talks Given by Research Group Members

January 30, 2025 "Embedded Correlated Wavefunction Theory for Plasmonic Photocatalysis: Past, Present, and Future," at the *AFOSR MURI Kickoff Meeting; Combining Nonequilibrium Chemistries with Atomic Precision*, Rice University, Houston, TX. (presented by Mark Martirez)

March 13, 2024 "Quantum mechanical insights into light-driven reactions on metallic nanoparticles," at the *2024 Catalysis Society of New York Spring Symposium*, Agile Strategy Lab, New Jersey Institute of Technology, Newark, NJ. (presented by Mark Martirez)

January 11, 2024 "Can embedded multiconfigurational wavefunction methods reveal fresh insights into the electrochemical CO_2 reduction pathways on copper?," at the Lorentz-CECAM Workshop on "*Atomistic modelling of solid-liquid interfaces in electrocatalysis*," Leiden University, Leiden , The Netherlands. (to be presented by Mark Martirez)

August 13, 2023 Quantum-mechanical view of light-driven NH_3 activation on Pd- and Fe-decorated Al nanoparticles," at the *ACS Fall 2023 National Meeting & Exposition in the Division of Catalysis Symposium on Molecular and Heterogeneous Photocatalysts: Advances in Experiments and Theory*, San Francisco, CA. (presented by Mark Martirez)

June 23, 2023 "Understanding carbonate formation in aqueous solutions at the atomic level via multi-level quantum mechanics/molecular dynamics simulations," invited talk (direct invitation to Jan-Niklas Boyn) at the *ACS Central Regional Meeting*, Dearborn, MI.

March 21, 2023 "Capped density functional embedding theory for excited-state simulations of covalent compounds," at the *Lorentz Center workshop on "Accelerating theoretical spectroscopy for complex multiscale materials,"* Leiden University, Leiden, The Netherlands. (presented by Mark Martirez)

July 20, 2022 "Plasmonic heterogeneous catalysis: Excited-state surface chemistry understood via embedded correlated wavefunction theory, " at the *Centre Européen de Calcul Atomique et Moléculaire (CECAM) workshop on "Light-matter interaction and ultrafast nonequilibrium dynamics in plasmonic materials,"* University of Warwick, Coventry, England, United Kingdom. (presented by Mark Martirez)

August 19, 2020 "Accurate simulation of photochemical processes: From plasmon-driven photocatalysis to dye-sensitized photovoltaics," ACS PHYS Postdoctoral Award invited talk at the *ACS Fall 2020 National Meeting & Exposition*, San Francisco, CA. (presented by Mark Martirez)

July 14, 2020 "Density-functional-theory-based embedding theories for embedded correlated wavefunction description of molecules and surfaces," at the *Molecular Simulation with Machine Learning Online Workshop*, Princeton, NJ. (presented by Mark Martirez)

D. Contributed Talks and Presentations

Sept. 24, 2024 "First-Principles Insights into the Thermodynamics of Variable-Temperature Ammonia Synthesis on Transition-Metal-Doped Cu(100) and (111)," at the *Andlinger Center for Energy and the Environment Peer-led Seminar Series*, Princeton, NJ. (presented by Ziyang Wei)

Sept. 3, 2024 "Quantum mechanical insights into light-driven reactions on metallic nanoparticles," at the *XIX International Conference on Theoretical Aspects of Catalysis (ICTAC 2024)*, Seville, Spain. (presented by Mark Martirez)

August 21, 2024 "Toward understanding carbonate mineralization at the atomic level with multi-level quantum mechanics/molecular dynamics simulations," talk at the *ACS Fall 2024 Meeting in the Advances in CO2 Capture & Conversion: Mineralization, Direct Ocean Capture & Modeling session*, Denver, CO. (presented by Jan-Niklas Boyn)

August 21, 2024 "Accelerated embedding potential optimization by reconstructing the pseudo-valence electron density," talk *at the ACS Fall 2024 Meeting in the Addressing the Complexity of Correlated Quantum Many-Body Problems by Embedding & Downfolding session*, Denver, CO. (presented by Ziyang Wei)

August 3, 2024 "Embedded random phase approximation," talk at the *Emerging Frontiers in Computational Chemistry and Materials: A Symposium in Celebration of Emily Carter's Achievements*, Asilomar, Pacific Grove, CA. (presented by Ziyang Wei)

August 3, 2024 "Non-equilibrium alkane dehydrogenation via pulsed heating and quenching: A computational exploration," talk at the *Emerging Frontiers in Computational Chemistry and Materials: A Symposium in Celebration of Emily Carter's Achievements*, Asilomar, Pacific Grove, CA. (presented by Mark Martirez)

August 3, 2024 "Understanding the dynamics of Mg and Ca carbonate formation in aqueous solution from multi-level electronic structure simulations" talk at the *Emerging Frontiers in Computational Chemistry and Materials: A Symposium in Celebration of Emily Carter's Achievements*, Asilomar, Pacific Grove, CA. (presented by Jan-Niklas Boyn)

August 2, 2024 "Quantum Mechanics Simulation of Ammonia Formation by Nitrate Reduction on Copper Surfaces," poster at the *Emerging Frontiers in Computational Chemistry and Materials: A Symposium in Celebration of Emily Carter's Achievements*, Asilomar, Pacific Grove, CA. (presented by Vyshnavi Vennelakanti)

June 27, 2024 "Quantum Mechanics Simulation of Ammonia Formation by Nitrate Reduction on Copper Surfaces," poster at the *2024 Deep Modeling for Molecular Simulation* workshop, Princeton, NJ. (presented by Vyshnavi Vennelakanti)

June 17, 2024 "Toward understanding carbonate mineralization at the atomic level with multi-level quantum mechanics/molecular dynamics simulations," poster at the *2024 American Conference on Theoretical Chemistry*, Chapel Hill, NC. (presented by Jan-Niklas Boyn)

June 17, 2024 "Introducing the Embedded Random Phase Approximation: H2 Dissociative Adsorption on Cu(111) as an Exemplar," poster at the *2024 American Conference on Theoretical Chemistry*, Chapel Hill, NC. (presented by Ziyang Wei)

March 20, 2024 "Introducing the embedded random phase approximation: H_2 dissociative adsorption on Cu(111) as an exemplar," talk at the *ACS Spring 2024 Meeting & Exposition* in the *Division of Computers in Chemistry*, New Orleans, LA. (presented by Ziyang Wei)

Sept. 15, 2023 "DFT-Based Machine Learning Reactive Force Fields for Water and Aqueous NaCl and CO_2 Solutions," at the *High Meadows Environmental Institute's Summer of Learning Symposium*, Princeton University, Princeton, NJ. (presented by Huseyin Yagiz Devre)

August 14, 2023 "Toward understanding carbonate mineralization at the atomic level with multi-level electronic structure simulations," talk at the *ACS Fall 2023 National Meeting & Exposition* in the *Division of Energy and Fuels Symposium on Advances in Carbon Capture, Utilization, and Storage for a Sustainable Energy Future,* San Francisco, CA. (presented by Jan-Niklas Boyn)

June 23, 2023 "Understanding carbonate formation in aqueous solutions at the atomic level via multi-level quantum mechanics/molecular dynamics simulations,"talk at the *2023 ACS Central Regional Meeting* in the *Computational Chemistry from Electrons to Macromolecules* session, Dearborn, MI. (presented by Jan-Niklas Boyn)

March 28, 2023 "Understanding the dynamics of Mg and Ca carbonate formation in aqueous solution from multi-level electronic structure simulations" talk at the *ACS Spring 2023 National Meeting & Exposition* in the *Division of Physical Chemistry Symposium on Carbon Separation and Capture at the Atomistic Level: Theory and Experiment,* Indianapolis, IN. (presented by Jan-Niklas Boyn)

Nov. 15, 2022 "Crystal Features Controlling Oxygen Vacancy Formation in ABO_3 Perovskites," talk at the *2022 AIChE Annual Meeting*, Phoenix, AZ. (presented by Robert Wexler)

Nov. 14, 2022 "Modeling the Combined Effects of Temperature, Pressure, and pH on Oxygen Evolution Thermodynamics and Kinetics," talk at the *2022 AIChE Annual Meeting*, Phoenix, AZ. (presented by Ananth Govind Rajan)

Oct. 14, 2022 "Explaining plasmon-activated ammonia and hydrogen decomposition on Pd and Fe-decorated Al nanoparticles via first-principles atomic-scale simulations," poster at the *Andlinger Center for Energy and the Environment 2022 Annual Meeting*, Princeton, NJ. (presented by Xuelan Wen)

Oct. 14, 2022 "Plasmonic heterogeneous catalysis: Excited-state surface chemistry understood via embedded correlated wavefunction theory," poster at the *Andlinger Center for Energy and the Environment 2022 Annual Meeting*, Princeton, NJ. (presented by Mark Martirez)

July 26, 2022 "Explaining plasmon-activated ammonia and hydrogen decomposition on Pd and Fe-decorated Al nanoparticles via first-principles atomic-scale simulations," poster at the *American Conference on Theoretical Chemistry (ACTC) 2022*, Palisades Tahoe, CA. (presented by Xuelan Wen)

July 20, 2022 "Plasmonic heterogeneous catalysis: Excited-state surface chemistry understood via embedded correlated wavefunction theory," poster at the *Centre Européen de Calcul Atomique et Moléculaire (CECAM) workshop on "Light-matter interaction and ultrafast nonequilibrium dynamics in plasmonic materials,"* University of Warwick, Coventry, England, United Kingdom. (presented by Mark Martirez)

June 30, 2022 "Intuitive materials design for solar thermochemical carbon dioxide splitting," talk at the *19th International Conference on Carbon Dioxide Utilization (ICCDU)*, Princeton, NJ. (presented by Robert Wexler)

May 25, 2022 "Explaining plasmon-activated ammonia and hydrogen decomposition on Pd and Fe-decorated Al nanoparticles via first-principles atomic-scale simulations," poster at the *2022 AFOSR Molecular Dynamics and Theoretical Chemistry Program Review*, Arlington, VA. (presented by Xuelan Wen)

May 10, 2022 "Influence of Thickness and Surface Composition on the Stability of Ferroelectric Polarization in Ultrathin HfO_2," talk at the *2022 MRS Spring Meeting & Exhibit*, Honolulu, HI. (presented by Adrian Acosta)

March 16, 2022 "Crystal Features Controlling Oxygen Vacancy Formation in ABO_3 Perovskites," talk at the *APS March Meeting 2022*, Chicago, IL. (presented by Robert Wexler)

Feb. 9, 2022 "Perpendicular magnetic anisotropy in FeGa(110)/Pt(111) thin film interfaces," talk at the *TANMS Annual Research Strategy Meeting (ARSM) 2022 Virtual Symposia*, held virtually. (presented by Adrian Acosta)

Nov. 8, 2021 "Revisiting Electrochemical CO_2 Reduction on Copper: Reaction Mechanisms Revealed By Embedded Correlated Wavefunction Theory," talk at the *2021 AIChE Annual Meeting*, Boston, MA. (presented by Qing Zhao)

Oct. 25-28, 2021 "Characterization of Plasma-Thermal Cu ALE Processes and Etch Products," talk at the *AVS 67th Virtual Symposium*, Charlotte, NC. (presented by Xia "Gary" Sang)

Oct. 11, 2021 "Gas-Phase Directional Etching of Copper Via Surface Oxidation and Chemical Complexation," invited talk at the *240th ECS Digital Meeting*, Orlando, FL, held virtually. (presented by Prof. Jane Chang)

June 2, 2021 "Precise Control of Nanoscale Cu Etching via Gas-Phase Oxidation and Chemical Complexation," invited talk at the *239th ECS Digital Meeting with the 18th International Meeting on Chemical Sensors (IMCS)*, Chicago, IL. (presented by Prof. Jane Chang)

April 20, 2021 "First-Principles Screening of Ca-Ce-M-O (M = 3*d* transition metal) Oxide Perovskites for Solar Thermochemical Applications," talk at the *2021 Virtual MRS Spring Meeting & Exhibit*, Seattle, WA. (presented by Sai Gautam Gopalakrishnan)

April 20, 2021 "Designer Perovskites with Dual Reduction on A and B Sites; Lowering the Peak Temperature of Thermochemical Hydrogen Production Cycles," talk at the *2021 Virtual MRS Spring Meeting & Exhibit*, Seattle, WA. (presented by Robert Bell)

April 14, 2021 "Atomic-level understanding of sodium ion and water intercalation into titanium disulfide interlayers for water desalination," talk at the *ACS Spring 2021 National Meeting & Exposition*, San Antonio, TX, held virtually. (presented by Lesheng Li)

April 14, 2021 "Oxygen evolution at low-lattice-coordinated NiOOH sites for water oxidation: Mechanism and doping strategies," talk at the *ACS Spring 2021 National Meeting & Exposition*, San Antonio, TX, held virtually. (presented by Mark Martirez)

April 14, 2021 "Facet-Independent Oxygen Evolution Activity of Pure β-NiOOH: Different Chemistries Leading to Similar Overpotentials," talk at the *ACS Spring 2021 National Meeting & Exposition*, San Antonio, TX, held virtually. (presented by Ananth Govind Rajan)

April 13, 2021 "Marcus-Theory Based Microkinetic Model for pH- and Potential-Dependent Water Splitting," talk at the *ACS Spring 2021 National Meeting & Exposition*, San Antonio, TX, held virtually. (presented by Ananth Govind Rajan)

April 12, 2021 "Identification of a single-atom catalyst for electrochemical ammonia synthesis based on transition metal doped graphene-like GaN," talk at the *ACS Spring 2021 National Meeting & Exposition*, San Antonio, TX, held virtually. (presented by Lesheng Li)

April 6, 2021 "Discovering Competing Electrocatalytic Mechanisms and their Overpotentials: Automated Enumeration of Oxygen Evolution Pathways," talk at the *ACS Spring 2021 National Meeting & Exposition*, San Antonio, TX, held virtually. (presented by Ananth Govind Rajan)

April 6, 2021 "Efficient Machine-Learned Model for Oxide Perovskite Performance in Solar Thermochemical Technologies," talk at the *ACS Spring 2021 National Meeting & Exposition*, San Antonio, TX, held virtually. (presented by Robert Wexler)

March 16, 2021 "First-principles evaluation of Ca-Ce-M-O (M = 3*d* transition metal) oxide perovskites for solar thermochemical applications," talk at the *APS March Meeting 2021*, held virtually. (presented by Sai Gautam Gopalakrishnan)

Nov. 19, 2020 "Codoping Cu_2ZnSnS_4 with Cd, Ge, and Se: a recipe for suppressing deep traps," talk at the *ACS 2020 Virtual Postdoc Symposium*, San Francisco, CA. (presented by Robert Wexler)

Nov. 19, 2020 "Accurate simulation of photochemical processes: From plasmon-driven photocatalysis to dye-sensitized photovoltaics," talk at the *ACS 2020 Virtual Postdoc Symposium*, San Francisco, CA. (presented by Mark Martirez)

Nov. 17, 2020 "Suppressing Deep-Trap Formation in Cu_2ZnSnS_4-Based Solar Cells," talk at the *2020 American Institute of Chemical Engineers (AIChE) Virtual Annual Meeting*, San Francisco, CA. (presented by Robert Wexler)

Nov. 16, 2020 "Entropic Driving Forces of Ferrites for Two-Step Thermochemical Water and Carbon Dioxide Splitting," talk at the *International Mechanical Engineering Congress & Exposition (IMECE) 2020 Virtual Meeting*, Portland, OR. (presented by Shang Zhai)

Nov. 16, 2020 "Entropy Source Analysis for Ferrites in Two-Step Thermochemical Splitting of Water and Carbon Dioxide," talk at the *2020 American Institute of Chemical Engineers (AIChE) Virtual Annual Meeting*, San Francisco, CA. (presented by Shang Zhai)

Nov. 16, 2020 "Scratching the Surface: Simulating and Engineering the Interfaces of Materials for Sustainable Energy and Environmental Remediation," poster at the *2020 American Institute of Chemical Engineers (AIChE) Virtual Annual Meeting*, San Francisco, CA. (presented by Robert Wexler)

Nov. 16, 2020 "Revisiting Electrochemical CO_2 Reduction on Copper Via Embedded Correlated Wavefunction Theory," talk at the *2020 American Institute of Chemical Engineers (AIChE) Virtual Annual Meeting*, San Francisco, CA. (presented by Qing Zhao)

Nov. 16, 2020 "First-Principles Approaches for Accurate Predictions of Nanostructured Materials," poster at the *2020 American Institute of Chemical Engineers (AIChE) Virtual Annual Meeting*, San Francisco, CA. (presented by Qing Zhao)

Nov. 16, 2020 "Identification of a Single-Atom Catalyst for Electrochemical Ammonia Synthesis Based on Transition Metal Doped Graphene-like GaN," talk at the *2020 American Institute of Chemical Engineers (AIChE) Virtual Annual Meeting*, San Francisco, CA. (presented by Lesheng Li)

Aug. 17, 2020 "Codoping Cu_2ZnSnS_4 with Cd, Ge, and Se: a recipe for suppressing deep traps," talk at the *ACS Fall 2020 National Meeting & Exposition*, San Francisco, CA. (presented by Robert Wexler)

Aug. 17-20, 2020 "Reaction mechanisms of electrochemical CO_2 reduction on copper predicted by embedded correlated wavefunction theory," talk at the *ACS Fall 2020 National Meeting & Exposition*, San Francisco, CA. (presented by Qing Zhao) (Canceled due to COVID-19)

July 29, 2020 "Exchange-correlation functional challenges in modeling chalcogenides," poster at the *Virtual Conference on Theoretical Chemistry (VCTC)*, Stanford, CA. (presented by Robert Wexler)

July 28, 2020 "Computational design of kesterite solar cells via ion substitution," talk at the *Virtual Conference on Theoretical Chemistry (VCTC)*, Stanford, CA. (presented by Robert Wexler)

July 28, 2020 "Computational design of kesterite solar cells via ion substitution," panel at the *Virtual Conference on Theoretical Chemistry (VCTC)*, Stanford, CA. (presented by Robert Wexler)

March 26, 2020 "Tuning the catalytic performance of a hydride donor via surface doping in heterogeneous catalysis," talk at the *2020 ACS Spring National Meeting & Expo*, Philadelphia, PA. (presented by Shenzhen Xu) (Canceled due to COVID-19)

March 25, 2020 "Codoping Cu_2ZnSnS_4 with Ge and Se: Recipe for suppressing deep traps," talk at the *2020 ACS Spring National Meeting & Expo*, Philadelphia, PA. (presented by Robert Wexler) (Canceled due to COVID-19)

March 24, 2020 "Oxygen evolution at low-lattice-coordinated NiOOH sites: Doping strategies from divide-and-conquer DFT/hybrid-DFT," talk at the *2020 ACS Spring National Meeting & Expo*, Philadelphia, PA. (presented by Mark Martirez) (Canceled due to COVID-19)

March 24, 2020 "Revealing the facet-independent oxygen evolution activity of pure β-NiOOH using hybrid density functional theory: Different chemistries leading to similar overpotentials," talk at the *2020 ACS Spring National Meeting & Expo*, Philadelphia, PA. (presented by Ananth Govind Rajan) (Canceled due to COVID-19)

March 23, 2020 "Defect-mediated charge-carrier trapping and nonradiative recombination in WSe_2 monolayers," talk at the *2020 ACS Spring National Meeting & Expo*, Philadelphia, PA. (presented by Lesheng Li) (Canceled due to COVID-19)

March 22, 2020 "Modeling 3*d* transition metal oxides with optimal *U* values within a SCAN+*U* framework," talk at the *2020 ACS Spring National Meeting & Expo*, Philadelphia, PA. (presented by Sai Gautam Gopalakrishnan) (Canceled due to COVID-19)

March 22, 2020 "Exploring Ca-Ce-M-O (M = 3*d* transition metal) oxide perovskites for solar thermochemical applications," talk at the *2020 ACS Spring National Meeting & Expo*, Philadelphia, PA. (presented by Sai Gautam Gopalakrishnan) (Canceled due to COVID-19)

March 4, 2020 "Using density functional theory to evaluate Ca-Ce-M-O (M = 3d transition metal) oxide perovskites for solar thermochemical applications," talk at the *2020 APS March Meeting*, Denver, CO. (presented by Sai Gautam Gopalakrishnan) (Canceled due to COVID-19)

March 3, 2020 "Optimal *U* values for 3*d* transition metal oxides within a SCAN+*U* framework," poster at the *2020 APS March Meeting*, Denver, CO. (presented by Sai Gautam Gopalakrishnan) (Canceled due to COVID-19)

March 3, 2020 "Suppressing deep-trap formation in Cu2ZnSnS4-based solar cells," talk at the *2020 APS March Meeting*, Denver, CO. (presented by Robert Wexler) (Canceled due to COVID-19)

E. Invited Seminars and Lectures Declined (2022 onward; earlier years not recorded)

2026 Invited Speaker at the "sMaR&T Seminar Series," Materials Research and Technology Department, Luxembourg Institute of Science and Technology (LIST), Luxembourg.

2025 Invited Colloquium Speaker at the Department of Physics & Astronomy, University of Delaware, DE.

2025 Invited Plenary Speaker at the SLAC National Accelerator Laboratory on "*Driving critical chemical transformations with photons, electrons, and catalysts*," Menlo Park, CA.

2025 Invited Speaker at the "DGIST (virtual) Lecture Series," Energy Science and Engineering Department, Daegu Gyeongbuk Institute of Science & Technology (DGIST), Daegu, Korea.

Dec. 15-20, 2025 Invited Speaker at the Pacifichem 2025 session on the "*Challenges for Artificial Photosynthesis: Regulating Organic-Inorganic Functional Interfaces for Disruptive Solar Fuels Research*," Honolulu, HI.

Oct. 12-16, 2025 Invited Keynote Speaker at the 248th Meeting of The Electrochemical Society on *"Computational Electrochemistry,"* Chicago, IL.

Aug. 25-28, 2025 Invited Speaker at the "First principles modelling of interfaces for energy storage and conversion" Symposium at the *Psi-k 2025 Conference*, Lausanne, Switzerland.

July 23, 2025 Invited Speaker at the *2025 Dynamics at Surfaces Gordon Research Conference,* Plymouth, NH.

July 22-25, 2025 Invited Speaker at the special session on "Advanced Theoretical Methods in Nanoplasmonics and Molecular Plasmonics," *at the 15th International Conference on Metamaterials, Photonic Crystals and Plasmonics (META 2025)*, Malaga, Spain.

June 30-July 4, 2025 Invited Plenary Speaker at the *12th International Conference on Materials for Advanced Technologies (ICMAT)*, Materials Research Society (MRS), Singapore.

June 24-25, 2025 Distinguished Invited Speaker at the *International Symposium on AI for Electrochemistry* (*i*SAIEC 2025), Xiamen University, China.

June 22-27, 2025 Invited Speaker at the *13th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2025)*, Oslo, Norway.

June 8-13, 2025 Invited Plenary Speaker at the *13th International Conference on Chemical Kinetics*, Tahoe City, CA.

March 29, 2025 Invited Keynote Speaker at the *Forum on Digitalization Promoting Innovation in Large Enterprises — AI Empowering Industrial Development*, Beijing, China.

Feb. 10-14, 2025 Invited Speaker at *Energy Week@Penn*, University of Pennsylvania, Philadelphia, PA.

Dec. 16-20, 2024 Invited Plenary Speaker at the *Conference on Advances in Chemistry for Energy and Environment (CACEE-2024)*, Tata Institute of Fundamental Research, Mumbai, India.

Dec. 1-6, 2024	Invited Speaker at the 2024 Materials Research Society Meeting on "*Plasmas for Materials Science—Opportunities at the Interface*," Boston, MA.
Nov. 12-15, 2024	Invited Speaker at the "Exploring Chiral Nanostructured Materials and Plasmonics for Energy Applications" Symposium at the *nanoGE Materials for Sustainable Development (MATSUS Fall 24) Conference*, Lausanne, Switzerland.
Nov. 7, 2024	Invited Panelist at "*The Impact of Environment on Human Health*" Symposium, Princeton, NJ.
Oct. 27-Nov. 1, 2024	Invited Speaker at the *Women in Catalysis* symposium at the 2024 AIChE Meeting, San Diego, CA.
Oct. 6-11, 2024	Invited Lecturer at the PRiME 2024 Symposium on "*Fundamentals of Carbon Dioxide Reduction*," Honolulu, HI.
Sep. 30, 2024	Invited Speaker at the 77th Gaseous Electronics Conference (2024) on "*The Road to a Sustainable Energy Future and the Role of Plasmas*," San Diego, CA.
Sep. 22-25, 2024	Invited Speaker at the *International Conference on Molecular Electronic Structure*, Pescara, Italy.
Sep. 8, 2024	Invited Plenary Speaker at the *Banff International Research Station (BIRS), of the Institute for Advanced Study in Mathematics (IASM), Symposium*, Hangzhou, China.
July 14-18, 2024	Invited Speaker at the *10th International Congresses on Ceramics (ICC10)* on "*Green Ceramics for Clean Energy and Sustainability*," Montreal, Quebec, Canada.
July 9-11, 2024	Keynote Speaker at the *GLObal Conference for Women Leaders and Emerging Researchers in Material Sciences (GLOW 2024)*, Nanyang Technological University, Singapore.
June 20-24, 2024	Invited Lecturer at the *CIMTEC 2024 - Global Conference on "Materials in an Explosively Growing Informatics World,"* Montecatini Terme, Italy.
June 17-19, 2024	Invited Speaker at the *3rd Edition of the NanoSeries Conference on Nanotechnology*, Centro De Congressos Do Instituto Superior Técnico, University of Lisbon, Portugal.
June 6-9, 2024	Invited Speaker at the *10th Irsee Symposium at Schwäbisches Bildungszentrum on "Complexity at catalytically relevant interfaces,"* Irsee, Germany.
March 17-21, 2024	Invited Speaker at the *American Chemical Society (ACS) Spring 2024 National Meeting* on "*The Role of Fundamental Interfacial Processes in Electrocatalysis under Division of Catalysis Science & Technology (CATL)*," New Orleans, LA.
March 4-8, 2024	Invited Lecturer at the 2024 APS March Meeting Focus Session on "*Density Functional Theory in Chemical Physics*," Minneapolis, MN.
Feb. 21, 2024	Invited Lecturer at the 2024 Presidential Lecture Series in Physics on "*Atmosphere: Earth to Exoplanets,"* New York, NY.
2023-2024	Invited Speaker at the *Catalysis Society of Metropolitan New York*, NY.
Dec. 11-12, 2023	Invited Lecturer at the *Royal Society Discussion on "Green carbon for the chemical industry of the future,"* at the Royal Society, London, England, UK.
Nov. 8, 2023	Keynote Speaker at *New Jersey Institute of Technology Research Day*, New Jersey Institute of Technology, Newark, NJ.
Oct. 25-27, 2023	Plenary Lecturer at the *Sustainable Energy Workshop* at Brown University, Providence, RI.

Oct. 23-26, 2023	Invited Lecturer at the *Exploration Conference "Interfaces and Mixing in Fluids, Plasmas, Materials,"* Kavli Institute for Theoretical Physics, University of California, Santa Barbara, Santa Barbara, CA.
Oct. 9-10, 2023	Invited Keynote Speaker at the "*4th International Conference on Condensed Matter & Applied Physics,*" Bikaner, Rajasthan, India.
Sep. 11-14, 2023	Invited Lecturer at the *59th Symposium on Theoretical Chemistry (STC 2023)*, Zürich, Switzerland.
Sep. 10-14, 2023	Invited Speaker at the *Climate Sustainability Workshop* at Spelman College, Atlanta, GA.
July 11-12, 2023	Invited Panelist & Speaker at the *Climate Crossroads Summit at the National Academies,* Washington, D.C.
June 14-16, 2023	Plenary Speaker at the *Australasian Leadership Computing Symposium,* Canberra, Australia.
June 8, 2023	Panelist and guest of honor at the *Fourth Research Frontiers Forum, Climate Change and National Security: Goals, Gaps, and Game Changer*, Applied Physics Laboratory, Johns Hopkins University, Laurel, MD.
June 4-8, 2023	Invited Speaker at the *Canadian Chemistry Conference and Exhibition (CSC 2023)*, Vancouver, British Columbia.
May 28-June 2, 2023	Invited Keynote Speaker at the *243rd Electrochemical Society (ECS) Meeting*, Boston, MA.
March 26-30, 2023	Invited Lecturer at the *ACS Spring 2023 National Meeting*, Indianapolis, IN.
Nov. 15, 2022	Invited Lecturer at the *2022 AIChE Annual Meeting in Honor of Professor Keith E. Gubbins' 85th Birthday*, Phoenix, AZ.
Nov. 9-12, 2022	Invited Facilitator at the *2022 Scialog NES Meeting*, Tucson, AZ.
Aug. 25-30, 2022	Invited Sectional Lecturer at the *26th International Congress of Theoretical and Applied Mechanics (ICTAM2024)*, Daegu, Korea.
July 21, 2022	Invited Distinguished Lecturer at the *U.S. Naval Research Laboratory (NRL) Chemistry Division 2022 Colloquium Series,* Washington, DC.
July 18, 2022	Invited Plenary Lecturer at the *DOE Closing the Carbon Cycle Workshop*, Richland, WA.
July 10-13, 2022	Invited Plenary Lecturer at the *NWChem-30 Conference*, Vancouver, BC.
July 10-13, 2022	Invited Keynote Speaker at the *ACS Colloid and Surface Science Symposium*, Golden, CO.
June 16-19, 2022	Invited Speaker at the *Schwäbisches Bildungszentrum 9th Irsee Symposium*, Irsee, Germany.

Current Extramural Funding Sources

Department of Energy, Basic Energy Sciences

Department of Energy, Fusion Energy Sciences

BP

Department of Defense, Multidisciplinary University Research Initiative