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

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

As chief academic and operating officer, works with the Chancellor and leadership team to guide strategic planning, policy, and process development, define budgetary and advancement priorities, and support strategic initiatives across campus and beyond.

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

2019-present 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 efficient and accurate quantum mechanics simulation techniques, including embedded correlated wavefunction and orbital-free density functional theories. Discovery and design of molecules and materials for sustainable energy, including converting sunlight to electricity and producing chemicals and fuels from renewable energy. Delivered over 560 invited/plenary lectures at conferences, universities, companies, and government laboratories worldwide. Trained 50 postdoctoral fellows and trained/graduated 39 Ph.D.s in chemistry, chemical engineering, physics, applied mathematics, electrical engineering, and mechanical and aerospace engineering over a 32-year period.

ResearcherID: 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

2020 Member, European Academy of Sciences

2020 UCLA Chemistry & Biochemistry Distinguished Lecturer, University of California, Los Angeles

2019 2019 John Scott Award, Board of City Trusts, Philadelphia, PA

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

2019 2019 Distinguished Alumni Award, California Institute of Technology
https://www.youtube.com/watch?v=5llW6KVZEmg

2019 Spring 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 2018 C. R. Mueller Distinguished Lecturer, Purdue University

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

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

2018 2018 ACS Award in Theoretical Chemistry, American Chemical Society

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

2017 2017 Emerson Center Lectureship Award, Emory University

2017 2017 Fritz London Memorial Lecturer, Duke University

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

2017 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 2017 Irving Langmuir Prize in Chemical Physics, American Physical Society

2016 2016 Schiesser Lecturer, Lehigh University

2016 2016 Pitzer Lecturer on Theoretical Chemistry, Ohio State University

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

2016 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 2015-16 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 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 2014 Linnett Visiting Professor of Chemistry, University of Cambridge

2013 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 2013 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, Penn 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

2007-2008 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, UCLA

2002 McDowell Lecturer in Physical Chemistry, University of British Columbia

2000 Fellow, American Association for the Advancement of Science

1998 Fellow, American Physical Society

1998 Hanson-Dow Award for Excellence in Teaching, UCLA

1996-1997 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, UCLA

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, UCLA

1993-1995 Alfred P. Sloan Research Fellow

1992-1997 Camille and Henry Dreyfus Teacher-Scholar Award

1990-1991	Union Carbide Innovation Recognition Award
1989-1990	Faculty Member of Distinction (Undergraduate Teaching Award), UCLA
1989-1990	Union Carbide Innovation Recognition Award
1988-1993	Camille and Henry Dreyfus Foundation Distinguished New Faculty Award
1988-1993	National Science Foundation Presidential Young Investigator Award
1986-1987	SOHIO Fellowship in Catalysis, Caltech
1985-1986	International Precious Metals Institute and Gemini Industries Research Grant Award
1984	Sigma Xi, Caltech
1982-1985	National Science Foundation Predoctoral Fellowship
1982	Phi Beta Kappa, UC Berkeley
1982	Mabel Kittredge Wilson Prize in Chemistry, UC Berkeley
1981-1982	Bruce Howard Memorial Scholar, UC Berkeley
1981	Coblentz Society Award for Molecular Spectroscopy, UC Berkeley
1981	Mildred Jordan Sharp Torch and Shield Award, UC Berkeley
1979-1980	Theodore and Edith Braun Scholar, UC Berkeley
1978-1982	Alumni Scholar, UC Berkeley
1978-1982	Regents Scholar, University of California, Berkeley

NEWS/MEDIA INTERVIEWS

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

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

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

Member, Editorial Advisory Board, *Journal of the American Chemical Society*, 2017-2023

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

Member, Editorial Advisory Board of *Journal of Physical Chemistry Letters,* 2014-2015

Member, Editor-in-Chief Search Committee, *Science*, 2012-2013

Member, Editorial Advisory Board of *Journal of Chemical Theory and Computation*, 2010-2019

Member, Editor-in-Chief Search Committee, *Journal of Chemical Physics*, 2007-2008

Member, Editorial Board of *Annual Review of Physical Chemistry*, 2006-2010

Member, Editorial Advisory Board of *Accounts of Chemical Research*, 2005-2007

Guest Editor, *Accounts of Chemical Research special issue on Computational and Theoretical Chemistry*, 2004-2005

Member, Editor-in-Chief Search Committee, *Journal of Physical Chemistry*, 2003-2004

Member, Editorial Board of *SIAM Journal on Multiscale Modeling, and Simulation*, 2001-2007

Member, Editorial Board of *Modelling and Simulation in Materials Science and Engineering,* 2001-2012

Member, Editorial Advisory Board of *ChemPhysChem*, 2000-2014

Member, Editorial Board of *Journal of Chemical Physics,* 2000-2002

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*, 1994-1999

Specialist Editor of *Computer Physics Communications,* 1993-1994

Member, Editorial Advisory Board of *Molecular Simulation,* 1991-1996

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 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).

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, 2019-2020

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 https://www.youtube.com/watch?v=rnXFXUVaBOo

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, 2018-2019

Member, National Academies of Sciences, Engineering, and Medicine (NASEM) External Review Committee of the Gulf Research Program, 2018-2019

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 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

Outreach activities:

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, 2016-2017

Member, Lawrence Berkeley National Laboratory (LBNL) Advisory Board, 2016-2022

Member, Secretary of Energy Advisory Board Task Force on CO_2 Utilization, 2016

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 Energy and the Environment, Stonybrook-Millstone Watershed Association, Pennington, NJ

Outreach activities:

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, 2014-2017

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

Member, SLAC National Accelerator Laboratory Scientific Policy Committee, 2014-2016

Member, International Organizing Committee for the International Congress of Quantum Chemistry, 2014-2017

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, 2013-2014

Advisory Council Liaison, NSF Mathematical and Physical Sciences Subcommittee on Optics and Photonics, 2013-2014

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, 2012-2015

Member, National Academy of Sciences Class Membership and Chemistry in Service to Society Committees, 2012-2013

Chair, DOE-BES Council on Chemical and Biochemical Sciences, 2012-2013

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, 2011-2017

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, 2010-2011

Member, Board on Chemical Sciences and Technology, National Research Council, National Academy of Sciences, 2010-2012

Vice-Chair, DOE-BES Council on Chemical and Biochemical Sciences, 2010-2011

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, 2009-2011

Co-organizer, DOE-BES workshop on Theories of Excited States in Molecules and Nanostructures, 2009-2010

Chair-Elect, Energy Subdivision of the PHYS Division of the ACS, 2009-2010

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 – Talk on "Women in Research Computing," Office of Information Technology, Princeton University

2008 Member, DOE-BES Council on Chemical and Biochemical Sciences, 2008-2011

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, 2007-2010

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 – Talk on "Keys to Becoming a Successful Faculty Member," PICASso Career Workshop, Princeton University, Princeton, NJ

April 19 - Talk on "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 - 2012

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, 2000-2005.

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 (preproposal 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 Panel Member, 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 Proctor & Gamble Award Committee

Panel Member, 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

Panel Member, 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 Panel Member, 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)

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426. A. G. Rajan and E. A. Carter, "Microkinetic Model for pH- and Potential-Dependent Oxygen Evolution During Water Splitting on Fe-Doped β-NiOOH," *Energy Environ. Sci.*, in press (2020).

425. A. G. Rajan and E. A. Carter, "Discovering Competing Electrocatalytic Mechanisms and their Overpotentials: Automated Enumeration of Oxygen Evolution Pathways," *J. Phys. Chem. C*, in press (2020).

424. A. Gupta, A. G. Rajan, E. A. Carter, and H. A. Stone, "Ionic Layering and Overcharging in Electrical Double Layers in a Poisson-Boltzmann Model," *Phys. Rev. Lett.*, in press (2020).

423. J. M. P. Martirez, J. L. Bao, and E. A. Carter, "First Principles Insights into Plasmon-Induced Catalysis," *Annu. Rev. Phys. Chem.*, in press (2020).

422. A. J. Tkalych, H. Zhuang, and E. A. Carter, "An Integrated Methodology for Screening Hydrogen Evolution Reaction Catalysts: Pt/Mo_2C as an Example," in *Computational Materials, Chemistry, and Biochemistry: From Bold Initiatives to the Last Mile (In Honor of William A. Goddard's Contributions to Science and Engineering)*, Vol. 284, pp. ##-##, Richard Muller & Sadasivan Shankar, Eds. (Springer Series in Materials Science), ISBN 978-3-030-18777-4, in press (2021).

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419. A. G. Rajan, J. M. P. Martirez, and E. A. Carter, "Why do we use the materials and operating conditions we use for heterogeneous (photo)electrochemical water splitting?," *ACS Catal.*, **10**, 11177 (2020). doi: 10.1021/acscatal.0c01862

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416. R. B. Wexler, G. S. Gautam, and E. A. Carter, "Exchange-Correlation Functional Challenges in Modeling Quaternary Chalcogenides," *Phys. Rev. B*, **102**, 054101 (2020). doi: 10.1103/PhysRevB.102.054101

415. H. Robatjazi, J. L. Bao, L. Zhou, M. Zhang, P. Christopher, E. A. Carter, P. Nordlander, and N. J. Halas, "Plasmon-driven carbon-fluorine (C(sp^3)-F) bond activation with mechanistic insights into hot-carrier-mediated pathways," *Nat. Catal.* **3**, 564 (2020). doi: 10.1038/s41929-020-0466-5

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NON-PEER REVIEWED ARTICLES (LAST FIVE YEARS ONLY)

1. E. A. Carter, "In era of cheap oil, our choices are clear: consume more or spark change,"*Houston Chronicle*, 19 Jan. 2016.

PATENTS

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.

Emily A. Carter, Sai Gautam Gopalakrishnan, and Ellen B. Stechel, *Ca-Ce-M-O (M = Mn, Fe, and V) Oxide Perovskites as Solar Thermochemical Water and Carbon Dioxide Splitters*. Provisional Patent No.: 63/039,207. Filed June 15, 2020.

Emily A. Carter, Lesheng Li, and John Mark P. Martirez, *Mo-doped graphene-like GaN monolayer as electrocatalyst for artificial ammonia synthesis via nitrogen reduction reaction*. Provisional Patent No.: 63/033,325. Filed June 2, 2020.

Emily A. Carter and John Mark P. Martirez, *Fe-Cu and Fe-Ag as Primary-Secondary Co-dopants into NiOOH for Enhanced Electrochemical Molecular Oxygen Evolution Catalysis*. Provisional Patent No.: 62/948,392. Filed December 16, 2019

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

January 22, 2020 "Artificial Photosynthesis Mechanisms and Materials Optimization from First Principles," UCLA Chemistry & Biochemistry Distinguished Lecture, University of California, Los Angeles, Los Angeles, CA.

November 13, 2019 "Unconventional Quantum Mechanics Methods for Design of Materials for Sustainable Energy Technologies," 2019 Camille & Henry Dreyfus Lectureship (technical), University of Basel, Basel, Switzerland.

November 11, 2019 "Artificial Photosynthesis Mechanisms and Materials Optimization from First Principles," 2019 Camille & Henry Dreyfus Lectureship (general), University of Basel, Basel, Switzerland.

October 7, 2019 "Unconventional Quantum Mechanics Methods for Design of Materials for Sustainable Energy Technologies," University of Southern California, Los Angeles, CA.

October 7, 2019 "Quantum Mechanics and the Future of the Planet," Inaugural WiSE Presidential Distinguished Lecture, University of Southern California, Los Angeles, CA.

June 17, 2019 "Quantum Simulations of Sustainable Energy Materials," 18th NCCR MARVEL Distinguished Lecturer, L'École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland.

March 21, 2019 "Sustainable Energy Materials from First Principles," Spring 2019 Eyring Lecture in Molecular Sciences, Arizona State University, Tempe, AZ.

Feb. 8, 2019 "Strategies to Build a Healthy Intellectual Ecosystem for All," Graduate Students for Diversity in Science (GSDS) Diversity Seminar, University of California, Santa Barbara, Santa Barbara, CA.

Feb. 8, 2019 "Sustainable Energy Materials from First Principles," 2019 Dow Foundation Distinguished Lecture, University of California, Santa Barbara, Santa Barbara, CA.

Nov. 29, 2018 "Theoretical Chemistry's Role in Providing Sustainable Energy," 2018 C. R. Mueller Distinguished Lecture, Purdue University, West Lafayette, IN.

May 2, 2018 "Mechanisms for Sustainable Fuel and Chemical Production from First Principles," 2018 Donald L. Katz Lectureship in Chemical Engineering, University of Michigan, Ann Arbor, MI.

April 20, 2018 "Mechanisms for Sustainable Fuel and Chemical Production from First Principles," Physical Chemistry/Chemical Physics Colloquium, University of Colorado-Boulder, Boulder, CO.

Dec. 5, 2017 "Quantum Solutions for Sustainable Energy," College of Engineering Fall Distinguished Lecture, University of California, Davis, Davis, CA.

Aug. 31, 2017 "Atomic-Scale Assessment of First-Wall Materials for Fusion Reactors: Insights and Challenges for Materials Simulations," High Energy Science Seminar, Lawrence Livermore National Laboratory, Livermore, CA.

April 25, 2017 "Quantum Mechanical Solutions for Our Energy Future," 2017 Fritz London Memorial Lecture, Departments of Chemistry and Physics, Duke University, Durham, NC.

April 14, 2017 "How Quantum Mechanics Helps Discover Materials for Sustainable Energy," 2017 Julian C. Smith Lectures in Chemical and Biomolecular Engineering (public), Cornell University, Ithaca, NY.

April 13, 2017 "Sustainable Production of Fuels and Chemicals from First Principles," 2017 Julian C. Smith Lectures in Chemical and Biomolecular Engineering (technical), Cornell University, Ithaca, NY.

March 23, 2017 "Sustainable Production of Fuels and Chemicals from First Principles," 2017 Albert J. Moscowitz Memorial Lecture, Department of Chemistry, University of Minnesota, Minneapolis, MN.

Jan. 31, 2017 "How a Theoretical Chemist Contributes to Producing Sustainable Fuels and Chemicals," Distinguished Lecture in Theoretical and Computational Chemistry, University of California, San Diego, San Diego, CA.

Oct. 17, 2016 "Sustainable Energy Phenomena from First Principles: From Fuel Cells to Fusion," 2016 Pitzer Lecture on Theoretical Chemistry, Ohio State University, Columbus, OH.

Sept. 28, 2016 "Artificial Photosynthesis: Revelations from Quantum Mechanics, " Molecular Biology Butler Seminar, Princeton University, Princeton, NJ

Sept. 22, 2016 "Understanding Photoelectrocatalysis from First Principles," 2016 Schiesser Lecture, Department of Chemical and Biomolecular Engineering, Lehigh University, Bethlehem, PA.

June 17, 2016 "Quantum Solutions for a Sustainable Energy Future," 2016 Almlöf–Gropen Lecture, Centre for Theoretical and Computational Chemistry at the University of Oslo, Oslo, Norway.

June 13, 2016 "Quantum Solutions for a Sustainable Energy Future," 2016 Almlöf–Gropen Lecture, Centre for Theoretical and Computational Chemistry at the University of Tromsø, Tromsø, Norway.

April 6, 2016 "The Future of Energy," 2016 R. H. Betts Memorial Lecture (public), University of Manitoba, Winnipeg, Manitoba, Canada.

April 6, 2016 "Understanding Photoelectrocatalysis from First Principles," 2016 R. H. Betts Memorial Lecture (technical), University of Manitoba, Winnipeg, Manitoba, Canada.

Feb. 10, 2016 "Assessing First Wall Materials at the Atomic Scale and Energy Writ Large at Princeton," 2015-2016 Colloquium, Princeton Plasma Physics Laboratory, Princeton, NJ.

Oct. 21, 2015 "Quantum Mechanics without Wavefunctions," Joseph O. Hirschfelder Lectures in Theoretical Chemistry, University of Wisconsin-Madison, Madison, WI.

Oct. 20, 2015 "Renewable Fuels and Chemicals from Photoelectrocatalysis," Joseph O. Hirschfelder Lectures in Theoretical Chemistry, University of Wisconsin-Madison, Madison, WI.

Oct. 19, 2015 "(Photo)electrocatalysis: Theory and Mechanisms of Charge Transfer at Metal Surfaces," Joseph O. Hirschfelder Lectures in Theoretical Chemistry, University of Wisconsin-Madison, Madison, WI.

Oct. 2, 2015 "Assessing First Wall Materials at the Atomic Scale and Energy Writ Large at Princeton," Culham Centre for Fusion Energy Seminar, Oxford, UK.

Sept. 30, 2015 "Overcoming Grand Challenges in Energy," Inaugural Grand Challenges in Molecular Science and Engineering Seminar, Imperial College, London, UK.

B. Invited Lectures

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

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

Aug. 26, 2019 "Optimization of carbon dioxide reduction at functionalized semiconductor electrodes," at the *257th ACS Fall National Meeting*, San Diego, CA.

Aug. 26, 2019 "Sustainable electrolysis of water from first principles," at the *257th ACS Fall National Meeting*, San Diego, CA.

May 27, 2019 "Photo/Electro-Catalytic Fuel Production from First Principles," at the *2019 Spring E-MRS Meeting*, Nice, France.

May 21, 2019 "Photo/Electro-Catalytic Fuel Production from First Principles," at the *2019 AFOSR Molecular Dynamics/Theoretical Chemistry Program Review*, Washington, DC.

March 30, 2019 "How Quantum Mechanics Can Help Solve the World's Energy Problems," at the *William A. Goddard III's 82nd Birthday Celebration Symposium*, California Institute of Technology, Pasadena, CA.

Feb. 24, 2019 "Sustainable Energy Materials from First Principles," Mildred Dresselhaus Memorial Lecture plenary talk at the *11th Annual International Workshop on Advanced Materials (IWAM 2019)*, Ras Al Khaimah, United Arab Emirates.

Oct. 5, 2018 "Fuels from Sunlight," at *She Roars: Celebrating Women in Princeton*, Princeton, NJ.

Oct. 2, 2018 "Advances in Quantum Embedding Theories," at the *2018 SciDAC Annual Meeting*, Berkeley, CA.

Aug. 21, 2018 "Sustainable production of fuels and chemicals," CME Leadership Award keynote talk at the *256th ACS Fall National Meeting*, Boston, MA.

Aug. 19, 2018 "*Ab initio* potential energy surfaces and dynamics for sustainable chemistry," at the *256th ACS Fall National Meeting*, Boston, MA.

Aug. 14, 2018 "Intricacies of Electrochemical Interfaces from First Principles," at the *2018 Gerischer Electrochemistry Today 2018 Meeting*, Boulder, CO.

June 24, 2018 "Mechanisms for Sustainable Fuel and Chemical Production from First Principles," at the *International Conference on Theoretical Aspects of Catalysis (ICTAC) 2018*, Los Angeles, CA.

June 11, 2018 "Mechanism for Solar Fuel Production from First Principles," at the *3rd International Conference on Proton Coupled Electron Transfer (PCET) 2018*, Blowing Rock, NC.

March 20, 2018 "Theoretical chemistry's role in providing sustainable energy," ACS Award in Theoretical Chemistry Lecture at the *255th ACS Spring National Meeting*, New Orleans, LA.

March 20, 2018 "Insights from Ab Initio Potential Energy Surfaces and Molecular Dynamics for Sustainable Energy Technologies," at the *Dreyfus Symposium at the 255th ACS Spring National Meeting*, New Orleans, LA.

March 19, 2018 "Advances in orbital-free density functional theory simulations of materials," at the *255th ACS Spring National Meeting*, New Orleans, LA.

Feb. 8, 2018 "Theory of Plasmon-Induced Excited State Catalysis," at the *AFOSR MURI Program Review Meeting*, Houston, TX.

Jan. 29, 2018 "Functionalized Semiconductor Surfaces for Carbon Dioxide Photoreduction: Insights from Theory," at the *Gordon Research Conference on Renewable Energy: Solar Fuels*, Ventura, CA.

Nov. 2, 2017 "Quantum Mechanics Derived Solutions for Sustainable Energy," keynote lecture at the *2017 Emerson Center Lectureship Award Symposium*, Emory University, Atlanta, GA.

Sept. 26, 2017 "Mechanisms for Sustainable Fuel and Chemical Production from First Principles," keynote lecture at the *ACS Innovation in Energy Conversion: A Physical Chemistry Perspective*, Dalian, China.

Sept. 25, 2017 "Mechanisms for Sustainable Fuel and Chemical Production from First Principles," keynote lecture at the *5th International Workshop on Nanotechnology, Renewable Energy & Sustainability*, Xi'an, China.

July 19, 2017 "Quantum Solutions for Sustainable Energy," at the *American Conference on Theoretical Chemistry (ACTC) 2017*, Boston, MA.

July 7, 2017 "At Last: Understanding Photoelectrocatalytic Reduction of CO2," plenary lecture at the *2nd International Solar Fuels (ISF2) Conference*, San Diego, CA.

May 16, 2017 "Sustainable energy solutions from first principles," plenary lecture at the *BES-CTC PI Meeting*, Gaithersburg, MD.

May 9, 2017 "Artificial Photosynthesis from First Principles," at the *2017 Connaught Global Challenge Symposium: CO_2 Chemistry Solutions to Climate Change*, Toronto, Ontario, Canada.

April 3, 2017 "Understanding photoelectrocatalysis from first principles," keynote lecture at the *251st ACS Spring National Meeting*, San Francisco, CA.

April 2, 2017 "First principles optimization of novel solar cell materials," at the *251st ACS Spring National Meeting*, San Francisco, CA.

March 15, 2017 "In the Footsteps of Irving Langmuir: Physical Chemistry in Service of Society," The Irving Langmuir Prize in Chemical Physics Lecture at the *2017 APS March Meeting*, New Orleans, LA.

March 13, 2017 "Pushing the Envelope Beyond Standard Density Functional Theory for Simulations of Zero Emission Energy Materials," at the *2017 APS March Meeting*, New Orleans, LA.

March 2, 2017 "Mechanisms of Photoelectrochemical Production of Fuel Precursors from First Principles," at the *Gordon Research Conference on Nanomaterials for Applications in Energy Technology*, Ventura, CA.

Jan. 18, 2017 "Ask About: Artificial Photosynthesis," at the *World Economic Forum Annual Meeting 2017*, Davos, Switzerland.

Dec. 7, 2016 "Quantum Mechanical Modeling of Plasmon-Induced Chemistry," at the *AFOSR MURI Program Review Meeting*, Houston, TX.

Aug. 28, 2016 "Modelling Photoelectrochemistry from First Principles," plenary lecture at the *Theory and Applications of Computational Chemistry (TACC) 2016 Conference*, University of Washington, Seattle, WA.

Aug. 19, 2016 "Optimization of Novel Photovoltaic Materials from First Principles," at the *Penn Conference in Theoretical Chemistry 2016*, Philadelphia, PA.

May 25, 2016 "Mechanistic Insights into CO_2 Reduction on Semiconductor Photoelectrodes," at the *2016 Molecular Dynamics Annual Program Review Meeting*, Arlington, VA.

May 19, 2016 "Introducing Princeton's Andlinger Center for Energy and the Environment," at the *Andlinger Center Building Opening Celebration and Symposium*, Princeton, NJ.

March 14, 2016 "Quantum Solutions for a Sustainable Energy Future," The Fred Kavli Innovations in Chemistry Lecture at the *251st ACS Spring National Meeting*, San Diego, CA.

Jan. 25, 2016 "Photoelectrochemical and electrochemical CO_2 reduction: Theoretical investigations," at the *AFOSR MURI Annual Review Meeting*, San Diego, CA.

Jan. 21, 2016 "Materials for Sustainable Energy," keynote lecture at *The Academy of Medicine, Engineering & Science of Texas (TAMEST) 2016 Annual Conference*, Dallas, TX.

Dec. 19, 2015 "Modelling Heterogeneous Photoelectrocatalysis from First Principles," keynote lecture at the *Pacifichem 2015 Congress*, Honolulu, HI.

Dec. 15, 2015 "Excited States in Condensed Matter from Embedded Correlation Wavefunction Theory," at the *Pacifichem 2015 Congress*, Honolulu, HI.

Dec. 3, 2015 "Photochemistry via Plasmonic Metal Nanoparticles from First Principles," at the *2015 MRS Fall Meeting*, Boston, MA.

Dec. 1, 2015 "Theoretical Characterization of Photoelectrochemistry of GaP," at the *2015 MRS Fall Meeting*, Boston, MA.

Nov. 30, 2015 "Advances in Theory and Algorithms for Orbital-Free Density Functional Theory," at the *2015 MRS Fall Meeting*, Boston, MA.

Oct. 5, 2015 "Quantum Mechanical Evaluation of Photoelectrocatalysis," at the *Dorothy Crowfoot Hodgkin (DCH) Symposium*, Zurich, Switzerland.

Aug. 19, 2015 "From local correlated wavefunction theory to petascale orbital-free density functional theory," at the *250th ACS Fall National Meeting*, Boston, MA.

C. Invited Talks Given by Research Group Members

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)

Dec. 2, 2019 "Recent Work Involving Orbital-Free Density Functional Theory," at the *2019 MRS Fall Meeting,* Boston, MA. (presented by Chuck Witt)

Sept. 12, 2019 "Tutorial on Alternate Versions of Orbital-Free Density Functional Theory," at the Density Functionals for Many-Particle Systems: Mathematical Theory and Physical Applications of Effective Equations Workshop, Singapore. (presented by Chuck Witt)

Sept. 5, 2019 "Tutorial on Kinetic Energy Density Functionals for Orbital-Free Density Functional Theory," at the *Density Functionals for Many-Particle Systems: Mathematical Theory and Physical Applications of Effective Equations Workshop*, Singapore. (presented by Chuck Witt)

June 13, 2019 "Chemical blueprint of an efficient electrocatalytic oxygen evolution catalyst," at the *2019 CECAM Workshop: Electrochemical energy storage: Theory meets industry*, Paris, France. (presented by Mark Martirez)

Apr. 25, 2019 "Using SCAN+U Calculations and the Sub-Lattice Formalism to Estimate Off-Stoichiometry in Oxides," at the *2019 MRS Spring Meeting*, Phoenix, AZ. (presented by Sai Gautam Gopalakrishnan)

March 31, 2019 "Embedded correlated wavefunction methods based on DFT embedding with a unique embedding potential," at the *255th ACS Spring National Meeting*, Orlando, FL. (presented by Xing Zhang)

March 13, 2019 "Properties of Liquid Sn and Liquid LiSn Alloys from First Principles," at the *US-Japan and International Workshop on Power and Particle Control in DEMO Fusion Reactor by Liquid Metal Plasma-Facing Components*, Princeton Plasma Physics Laboratory, Princeton, NJ. (presented by Beatriz Gonzalez del Rio)

Nov. 27, 2018 "Describing Light-Driven Catalysis on Surface-Doped Plasmonic Metals via Embedded Correlated Wavefunction Theories," at the *2018 MRS Fall Meeting*, Boston, MA. (presented by Mark Martirez)

Nov. 26, 2018 "Role of functional defects in Cu_2ZnSnS_4 solar cells," at the *2018 MRS Fall Meeting*, Boston, MA. (presented by Sai Gautam Gopalakrishnan)

Oct. 24, 2018 "Ab initio modeling of light-driven catalysis on surface-doped plasmonic metals," at the *FACSS SciX 2018 Conference*, Atlanta, GA. (presented by Mark Martirez)

Aug. 20, 2018 "Advances in nontraditional density-based electronic structure theories," at the *256th ACS Fall National Meeting*, Boston, MA. (presented by Xing Zhang)

March 19, 2018 "Quantum mechanical description of excited-state catalysis on metals for nanoplasmonics," at the *255th ACS Spring National Meeting*, New Orleans, LA. (presented by Mark Martirez)

March 19, 2018 "First-principles investigation of adsorbed hydrogenated N-heterocycles as hydride shuttles for catalytic CO2 reduction on p-GaP photoelectrodes," at the *255th ACS Spring National Meeting*, New Orleans, LA. (presented by Martina Lessio)

Dec. 19, 2017 "Fast and Accurate Methods: From Local Configuration Interaction to Orbital-Free Density Functional Theory," at the *2017 CECAM Workshop: Expeditious Methods in Electronic Structure Theory and Many Body Techniques*, Tel Aviv, Israel. (presented by Johannes Dieterich)

Nov. 27, 2017 "Advances in Orbital-Free Density Functional Theory Simulations of Materials," at the *2017 MRS Fall Meeting*, Boston, MA. (presented by Chuck Witt)

Aug. 21, 2017 "Local correlation in molecules and condensed matter: Methods and applications," at the *254th ACS Fall National Meeting*, Washington, DC. (presented by Johannes Dieterich)

May 9, 2017 "TigerCI: local multi-reference configuration interaction," at the *MolSSI Workshop on Core Software Blocks in Quantum Chemistry*, Asilomar, CA. (presented by Johannes Dieterich)

April 5, 2017 "Plasmon-induced excited-state heterogeneous catalysis on surface-doped metallic nanoparticles," at the *251st ACS Spring National Meeting*, San Francisco, CA. (presented by Mark Martirez)

April 2, 2017 "The Holy Grail: Chemistry enabling an economically viable CO_2 capture, utilization, and storage strategy," invited poster at the *Accounts of Chemical Research* Distinguished Scientists Poster Session, *251st ACS Spring National Meeting*, San Francisco, CA. (presented by Thomas Senftle)

April 2, 2017 "Pyridine Co-catalysis impacting CO_2 reduction over semiconductor photoelectrodes," at the *251st ACS Spring National Meeting*, San Francisco, CA. (presented by Thomas Senftle)

Feb. 28, 2017 "Computational Materials Discovery: From Reduced Pt Catalysts to Lightweight Alloys," at the *2017 TMS Annual Meeting & Exhibition*, San Diego, CA. (presented by Houlong Zhuang)

Nov. 28, 2016 "Excited-State Heterogeneous Catalysis on Metallic Nanoparticles," at the *2016 MRS Fall Meeting & Exhibit*, Boston, MA. (presented by Mark Martirez)

July 19, 2016 "Embedded Correlated Wavefunction Methods and their Application to Plasmon-Enhanced HeterogeneousCatalysis," at the *Congress of the International Society of Theoretical Chemical Physics (ISTCP) 2016*, Grand Forks, ND. (presented by Caroline Krauter)

June 4, 2016 "New developments in reduced scaling wavefunction and linear scaling density functional theories," at the *LUEST 2016 Conference*, Telluride, CO. (presented by Johannes Dieterich)

May 16, 2016 "Plasmonic hydrogen activation on Al and Pd: theoretical study using embedded correlated wave function methods," at the *AFOSR MURI Meeting*, Rice University, Houston, TX. (presented by Caroline Krauter)

May 16, 2016 "Excited State Dissociation Pathway for N_2 on Fe-substituted Plasmon-Active Au," at the *AFOSR MURI Meeting*, Rice University, Houston, TX. (presented by Mark Martirez)

March 16, 2016 "How do surface reconstructions affect CO_2 reduction over GaP, CdTe, and $CuInS_2$ photoelectrodes?" at the *251st ACS Spring National Meeting*, San Diego, CA. (presented by Thomas Senftle)

March 15, 2016 "Density functional embedding theory within the projector-augmented-wave formalism," at the *251st ACS Spring National Meeting*, San Diego, CA. (presented by Kuang Yu)

March 14, 2016 "Role of charge-transfer excitations in Au-Fe alloys for heterogeneous N_2 dissociation catalysis," at the *251st ACS Spring National Meeting*, San Diego, CA. (presented by Mark Martirez)

March 14, 2016 "Embedded correlated wavefunction methods for plasmon-induced photocatalysis," at the *251st ACS Spring National Meeting*, San Diego, CA. (presented by Caroline Krauter)

March 13, 2016 "First-principles investigation of the role of pyridinium and adsorbed dihydropyridine in pyridine-catalyzed CO_2 reduction on p-GaP photoelectrodes," at the *251st ACS Spring National Meeting*, San Diego, CA. (presented by Martina Lessio)

D. Contributed Talks and Presentations

August 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)

August 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) (Cancelled 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) (Cancelled 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) (Cancelled 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) (Cancelled 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) (Cancelled 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) (Cancelled 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) (Cancelled 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) (Cancelled 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) (Cancelled 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) (Cancelled 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) (Cancelled due to COVID-19)

Nov. 13, 2019 "Probing the Oxygen Evolution Reaction Efficacy of NiOOH (0001) and (10-10) Using Hybrid Density Functional Theory," poster at the *American Institute of Chemical Engineers (AIChE) 2019 Meeting*, Orlando, FL. (presented by Ananth Govind Rajan)

Nov. 11, 2019 "Modeling Thermodynamics and Kinetics at 2D Material Interfaces: Applications in Synthesis, Nanopore Formation, Wetting, and Catalysis," talk at the *American Institute of Chemical Engineers (AIChE) 2019 Meeting*, Orlando, FL. (presented by Ananth Govind Rajan)

Sept. 24, 2019 "Orbital-Free Density Functional Theory: Foundations and Recent Work," invited seminar at the U.S. Navy Research Laboratory, Washington, DC. (presented by Chuck Witt)

April 3, 2019 "Estimating off-stoichiometry using density functional theory-based calculations and the sub-lattice formalism," talk at the *255th ACS Spring National Meeting*, Orlando, FL. (presented by Sai Gautam Gopalakrishnan)

March 7, 2019 "Response in the local, non-negative kinetic energy density of a perturbed free electron gas: Potential functionals and density functionals (with implications for orbital-free density functional theory)," talk at the *2019 APS March Meeting*, Boston, MA. (presented by Chuck Witt)

March 7, 2019 "First-Principles Molecular Dynamics Study of Liquid LiSn as a Plasma-Facing Component," talk at the *2019 APS March Meeting*, Boston, MA. (presented by Beatriz Gonzalez del Rio)

Nov. 27, 2018 "2-pyridinide as an active catalytic intermediate for CO_2 reduction on p-GaP photoelectrodes: lifetime and selectivity," talk at the *2018 MRS Fall Meeting*, Boston, MA. (presented by Shenzhen Xu)

Nov. 26, 2018 "Need for a SCAN+U framework to describe the oxidation energetics of transition metal oxides," poster at the *2018 MRS Fall Meeting*, Boston, MA. (presented by Sai Gautam Gopalakrishnan)

Nov. 9, 2018 "Quantum Mechanical Evaluation of Alternative Photovoltaic Materials," poster at the *7th Annual Meeting of the Princeton E-ffiliates Partnership*, Princeton, NJ. (presented by Sai Gautam Gopalakrishnan)

Oct. 29, 2018 "Liquid LiSn as a Plasma-Facing Component: A Molecular Dynamics Study 2018," poster at the *Annual AIChE Student Conference*, Pittsburgh, PA. (presented by Emily de Jong); First Place, Materials Division VII Section, *AIChE Undergraduate Poster Competition*

Aug. 21, 2018 "Effects of Cd and Ag doping in Cu_2ZnSnS_4 solar cells," talk at the *XXVII International Materials Research Congress (IMRC)*, Cancun Mexico. (presented by Sai Gautam Gopalakrishnan)

June 13, 2018 "Discovering and Understanding New Catalytic Materials for Sustainable Chemical Conversion via Quantum Mechanics," poster at the *Princeton E-ffiliates Partnership 2018 Retreat*, New York, NY. (presented by Mark Martirez)

June 12, 2018 "Density functional embedding theory with an accurate Kohn-Sham inversion scheme and space truncation," poster at the *Penn Conference in Theoretical Chemistry 2018*, Philadelphia, PA. (presented by Xing Zhang)

June 12, 2018 "Improved Optimized Effective Potential Procedure for Potential Functional Embedding Theory," poster at the *Penn Conference in Theoretical Chemistry 2018*, Philadelphia, PA. (presented by Qi Ou)

May 23, 2018 "Understanding Heterogeneous Photochemical Conversion Processes from First Principles," poster at the *AFOSR Molecular Dynamics and Theoretical Chemistry Program Review 2018,* Albuquerque, NM. (presented by Mark Martirez)

May 22, 2018 "Quantum Mechanical Evaluation of Alternative Photovoltaic Materials," poster at the *2018 BES-CTC PI Meeting*, Gaithersburg, MD. (presented by Sai Gautam Gopalakrishnan)

March 8, 2018 "Globally-Optimized Local Pseudopotentials for (Orbital-Free) Density Functional Theory Simulations of Liquids and Solids," talk at the *2018 APS March Meeting*, Boston, MA. (presented by Beatriz Gonzalez del Rio)

March 5, 2018 "Orbital-free density functional theory with atom-centered density matrices," talk at the *2018 APS March Meeting*, Boston, MA. (presented by Chuck Witt)

Nov. 7, 2017 "Structural, Electronic, and Chemical Properties of β-NiOOH from First Principles," poster at the *2017 Annual Research Computing Day*, Princeton, NJ. (presented by Alexander Tkalych)

Nov. 7, 2017 "Orbital-Free Density Functional Theory With Atom-Centered Density Matrices," poster at the *2017 Annual Research Computing Day*, Princeton, NJ. (presented by Chuck Witt)

Nov. 7, 2017 "Photocatalyzed Hydrogen Desorption from Palladium Surfaces Assisted by Localized Surface Plasmon Resonances," poster at the *2017 Annual Research Computing Day*, Princeton, NJ. (presented by Vincent Spata)

Oct. 31, 2017 "The Role of Surface-Bound Dihydropyridine Analogs in Pyridine-Catalyzed CO2 Reduction over Semiconductor Photoelectrodes," talk at the *2017 AIChE Annual Meeting*, Minneapolis, MN. (presented by Tom Senftle)

Oct. 31, 2017 "Quantum Mechanical Description of Excited-State Heterogeneous Catalysis Via Embedded Correlated Wavefunction Methods," talk at the *2017 AIChE Annual Meeting*, Minneapolis, MN. (presented by Mark Martirez)

Aug. 22, 2017 "Density-to-potential inversions in density functional theory with atom-centered bases and multiwavelet bases," talk at the *254th ACS Fall National Meeting*, Washington, DC. (presented by Xing Zhang)

Aug. 22, 2017 "Orbital-free density functional theory with atom-centered density matrices," talk at the *254th ACS Fall National Meeting*, Washington, DC. (presented by Chuck Witt)

Aug. 21, 2017 "Orbital-free density functional theory with atom-centered density matrices," poster at the *254th ACS Fall National Meeting (ACS Sci-Mix Poster Session)*, Washington, DC. (presented by Chuck Witt)

Aug. 2 & 3, 2017 "Photocatalyzed Hydrogen Desorption from Palladium Surfaces Assisted by Localized Surface Plasmon Resonances," poster at the *Gordon Research Seminar on Dynamics at Surfaces*, Newport, RI. (presented by Vincent Spata)

Aug. 2 & 3, 2017 "Excited-State Heterogeneous Catalysis on Surface-Doped Plasmonic Nanoparticles," poster at the *Gordon Research Seminar on Dynamics at Surfaces*, Newport, RI. (presented by Mark Martirez)

June 26 & 27, 2017 "Orbital free density functional theory with atom-centered density matrices," poster at the *ES 2017 Workshop: Recent Developments in Electronic Structure Methods*, Princeton, NJ. (presented by Chuck Witt)

May 24, 2017 "Structural, Electronic, and Chemical Properties of β-NiOOH from First Principles," poster at the *AFOSR Molecular Dynamics and Theoretical Chemistry Program Review 2017,* Albuquerque, NM. (presented by Alexander Tkalych)

Dec. 7, 2016 "Modeling Local Excited-States on Surface Reactive Sites: An Exploration of Plasmon-Catalyzed CH_4 Dehydrogenation on Ru-functionalized Cu and N_2 Dissociation on Fe-functionalized Au," poster at the *AFOSR MURI Program Review Meeting*, Houston, TX. (presented by Mark Martirez)

Dec. 7, 2016 "Photocatalytic Hydrogen Desorption from Pd Surfaces with Embedded Correlated Wavefunction Methods," poster at the *AFOSR MURI Program Review Meeting*, Houston, TX. (presented by Vincent Spata)

Nov. 15, 2016 "Implications of surface reconstructions impacting CO_2 reduction over semiconductor photoelectrodes," talk at the *2016 AIChE Annual Meeting*, San Francisco, CA. (presented by Tom Senftle)

Aug. 19, 2016 "Mechanisms of plasmon-induced photocatalytic reactions described by embedded correlated wave function methods," talk at the *Penn Conference in Theoretical Chemistry 2016*, Philadelphia, PA. (presented by Caroline Krauter)

May 19, 2016 "Using Quantum Mechanics and Monte Carlo Simulations to Optimize Copper-Zinc-Tin-Sulfide (CZTS) Solar Cells," poster at the *Andlinger Center Building Opening Celebration and Symposium*, Princeton, NJ. (presented by Kuang Yu)

May 19, 2016 "Surface Functionalization of Plasmon-Active Au for Sustainable Ammonia Synthesis," poster at the *Andlinger Center Building Opening Celebration and Symposium*, Princeton, NJ. (presented by Mark Martirez)

May 19, 2016 "How do surface reconstructions affect Py-catalyzed CO_2 reduction over semiconductor photoelectrodes?," poster at the *Andlinger Center Building Opening Celebration and Symposium*, Princeton, NJ. (presented by Tom Senftle)

May 19, 2016 "Understanding and Tuning the Hydrogen Evolution Reaction on Pt-Covered Tungsten Carbide Cathodes," poster at the *Andlinger Center Building Opening Celebration and Symposium*, Princeton, NJ. (presented by Houlong Zhuang)

May 19, 2016 "Structural and Electronic Features of β-$Ni(OH)_2$ and β-NiOOH from First Principles," poster at the *Andlinger Center Building Opening Celebration and Symposium*, Princeton, NJ. (presented by Alex Tkalych)

May 19, 2016 "Pyridine-catalyzed CO_2 reduction on p-GaP electrodes: new mechanistic insights from first-principles investigations," poster at the *Andlinger Center Building Opening Celebration and Symposium*, Princeton, NJ. (presented by Martina Lessio)

May 19, 2016 "Plasmon-induced hydrogen activation on aluminum nanoparticles." poster at the *Andlinger Center Building Opening Celebration and Symposium*, Princeton, NJ. (presented by Caroline Krauter)

May 16, 2016 "Using Quantum Mechanics and Monte Carlo Simulations to Optimize Copper-Zinc-Tin-Sulfide (CZTS)Solar Cells," poster at the *BES-CTC PI Meeting*, Annapolis, MD. (presented by Kuang Yu)

March 15, 2016 "Petascale orbital-free density functional theory enabled by small-box techniques," talk at the *2016 APS March Meeting*, Baltimore, MD. (presented by Mohan Chen)

Jan. 25, 2016 "How Do Surface Reconstructions Affect CO_2 Reduction over Semiconductor Photoelectrodes?," poster at the *AFOSR MURI Annual Review Meeting*, San Diego, CA. (presented by Tom Senftle)

Jan. 25, 2016 "Pyridine-catalyzed CO_2 reduction on p-GaP electrodes: new insights on the role of pyridinium from theoretical investigations," poster at the *AFOSR MURI Annual Review Meeting*, San Diego, CA. (presented by Martina Lessio)

Nov. 20, 2015 "Rock-Salt Structure Lithium Deuteride Formation in Liquid Lithium with High-Concentrations of Deuterium: A First-Principles Molecular Dynamics Study," poster at the *4th Annual Meeting of the Princeton E-ffiliates Partnership*, Princeton, NJ. (presented by Mohan Chen)

Nov. 20, 2015 "Pyridine-catalyzed CO_2 reduction on p-GaP electrodes: new insights on the role of pyridinium from theoretical investigations," poster at the *4th Annual Meeting of the Princeton E-ffiliates Partnership*, Princeton, NJ. (presented by Martina Lessio)

Nov. 12, 2015 "Predictive Power of Embedded-Atom Method (EAM) Force Fields for Lithium," talk at the *2015 AIChE Annual Meeting*, Salt Lake City, UT. (presented by Joseph R. Vella)

CURRENT EXTRAMURAL FUNDING SOURCES

Air Force Office of Scientific Research

Department of Defense Multidisciplinary University Research Initiative

Department of Energy, Basic Energy Sciences

Department of Energy, Advanced Scientific Computing Research

Department of Energy, Energy Efficiency & Renewable Energy