

# EMILY ANN CARTER

## PROFESSIONAL ADDRESS

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Princeton University  
 School of Engineering and Applied Science  
 C230 Engineering Quadrangle  
 Princeton, NJ 08544-5263  
 email: [eac@princeton.edu](mailto:eac@princeton.edu)  
 tel: (609) 258-5391  
 fax: (609) 258-6744  
 Web page: <http://carter.princeton.edu>

## EDUCATION

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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 ADDRESS

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2016-present	Dean of the School of Engineering and Applied Science, Princeton University
2011-present	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
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

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Development of efficient and accurate first principles quantum mechanics techniques for electron correlation, embedded correlated wavefunction, and orbital-free density functional theories. Applications are focused entirely on enabling discovery and design of molecules and materials for sustainable energy, including converting sunlight to electricity and fuels, providing clean electricity from solid oxide fuel cells, clean and efficient combustion of biofuels, optimizing lightweight metal alloys for fuel-efficient vehicles, and characterizing hydrogen isotope incorporation into plasma facing components of fusion reactors.

*ResearcherID:* P-4075-2014

*ORCID:* 0000-0001-7330-7554

## AWARDS AND HONORS

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- 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. Moscovitz 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 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* 80<sup>th</sup> 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 Lecture, 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

## MEMBERSHIPS IN PROFESSIONAL SOCIETIES

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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

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Member, Editorial Advisory Board, *Advanced Theory and Simulations*, 2017-  
Member, Editorial Advisory Board, *Journal of the American Chemical Society*, 2017-2020  
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*, 2010-2014  
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:* ACS Applied Materials & Interfaces, ChemCatChem, Small, ACS Sustainable Chemistry & Engineering, Nature Nanotechnology, Advanced Functional Materials, Advanced Energy Materials, RSC Advances, Energy & Fuels, Nature Chemistry, ACS Catalysis, Journal of Materials Chemistry A, Nanoscale, Energy & Environmental Science, Catalysis Today, Physical Chemistry Chemical Physics, Journal of Computational Chemistry, Journal of Physical Chemistry, Journal of Chemical Physics, Langmuir, Chemical Physics Letters, Chemical Physics, Journal of the American Chemical Society, Nature, Surface Science, Inorganic Chemistry, Molecular Physics, Journal of Organic Chemistry, American Chemical Society Symposium Series, Physical Review Letters, Physical Review B, Chemical Reviews, Canadian Journal of Chemistry, Applied Physics Letters, Journal of Applied Physics, Catalysis Letters, Physica A, IEEE Transactions on Plasma Science, THEOCHEM, John Wiley & Sons, Ltd., World Scientific Publishers, Chemical Communications, Accounts of Chemical Research, Angewandte Chemie, Surface and Coatings Technology, Accounts of Chemical Research, Spectrochimica Acta, Journal of Vacuum Science and Technology, Journal of Molecular Catalysis, International Journal for Multiscale Computational Engineering, Journal of Computational Physics, The European Physical Journal B.

## **PROFESSIONAL/COMMUNITY SERVICE**

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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).

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-

*Outreach activities:* October 4 – Invited Speaker, An Introduction to Engineering and Applied Science at Princeton, China Executive Summit 2018, Princeton University, Princeton, NJ  
September 19 – Interview with *ACS Energy Letters* Editor-in-Chief, Prashant V. Kamat, “A Conversation with Emily Carter,” *ACS Energy Lett.*, **3**, 2470 (2018). [doi: 10.1021/acseenergylett.8b01677](https://doi.org/10.1021/acseenergylett.8b01677)  
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, 253<sup>rd</sup> ACS Spring National Meeting, San Francisco, CA  
February 8 – Invited Speaker, 55<sup>th</sup> 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, 2016-2019  
Member, Secretary of Energy Advisory Board Task Force on CO<sub>2</sub> 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 *Outreach activities:* October 9 – Invited Speaker, Lead New Jersey Seminar on The Research Frontier in 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, 2014-2017

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 21<sup>st</sup> 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 21<sup>st</sup> 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
- June 2009 – Interview with NJNews television regarding EFRC on Combustion Science, aired on Channel 13 on June 12;  
[http://www.youtube.com/watch?v=dkMpor\\_q5\\_4](http://www.youtube.com/watch?v=dkMpor_q5_4)
- 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, 4<sup>th</sup> 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

70<sup>th</sup> 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 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, can be downloaded from [http://www.schoolinfosystem.org/archives/2005/02/more\\_on\\_women\\_i.php](http://www.schoolinfosystem.org/archives/2005/02/more_on_women_i.php).  
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 4<sup>th</sup> 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)  
Interview with German TV (Bayrischer Rundfunk) about research— August 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)

## LIST OF PUBLICATIONS

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388. G. S. Gautam, T. P. Senftle, N. Alidoust, and E. A. Carter, "Novel solar cell materials: Insights from first principles," *J. Phys. Chem. C*, in press (2018).  
[doi: 10.1021/acs.jpcc.8b08185](https://doi.org/10.1021/acs.jpcc.8b08185)
387. Z. Chen, J. M. P. Martirez, P. Zahl, E. A. Carter, and B. E. Koel, "Self-assembling of formic acid on the partially oxidized  $p(2\times 1)$  Cu(110) surface reconstruction at low coverages," *J. Chem. Phys.*, in press (2018).
386. Q. Ou and E. A. Carter, "Potential Functional Embedding Theory with an Improved Kohn-Sham Inversion Algorithm," *J. Chem. Theor. Comp.*, in press (2018).  
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5. E.A. Carter, "Coupling Quantum and Continuum Mechanics to Obtain Predictive Models of the Macroscopic Behavior of Materials," Multiscale Modeling of Materials II Conference, UCLA, Los Angeles, CA, 2-4 (2004).
4. R.L. Hayes, M. Fago, M. Ortiz and E.A. Carter, "Prediction of Initial Dislocation Nucleation in Metallic Systems via the Orbital-Free Density Functional Theory Local Quasicontinuum Method," Multiscale Modeling of Materials II Conference, UCLA, Los Angeles, CA, 64-66 (2004).
3. S. Serebrinsky, E.A. Carter, and M. Ortiz, "Combining Quantum and Continuum Mechanics to Model Hydrogen Embrittlement," Multiscale Modeling of Materials II Conference, UCLA, Los Angeles, CA, 141-143 (2004).
2. E.A.A. Jarvis and E.A. Carter, "The Effect of Oxide Ionicity in Thermal Barrier Coatings of Jet Engine Turbines," Dept. of Defense High Performance Computing Modernization Program, Users Group Conference, June 2002. Available: <http://www.hpcmo.hpc.mil/Htdocs/UGC/UGC02>.
1. E. A. Carter, "Orbital-Free Density Functional Theory Dynamics: Evolution of Thousands of Atoms with Quantum Forces," in *Advances in Computational Engineering and Sciences*, edited by S. N. Atluri and F. W. Brust, 1967 (Tech Science Press, Palmdale, 2000).

## NON-PEER REVIEWED ARTICLES

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10. E. A. Carter, "In era of cheap oil, our choices are clear: consume more or spark change," *Houston Chronicle*, 19 Jan. 2016.
9. K. A. Marino and E. A. Carter, "The effects of platinum on thermal barrier coating performance," *MHPCC Application Briefs*, 10 (2006).
8. B. Hinnemann and E. A. Carter, "Understanding aluminum oxide growth in thermal barrier coatings," *MHPCC Application Briefs*, 12 (2006).
7. D. E. Jiang and E. A. Carter, "Chemistry of Gun Tube Erosion from First Principles," *MHPCC Application Briefs*, 16 (2004).
6. K. M. Carling and E. A. Carter, "Improving Interface Adhesion of Jet Engine Thermal Barrier Coatings," *MHPCC Application Briefs*, 14 (2004).
5. Emily A. Jarvis and Emily A. Carter, "How Quantum Mechanics Can Impact Jet Engines: Improving Aircraft Design at the Nanoscale," *High Performance Computing contributions to DoD Mission Success: 2002*, March 2003.
4. E. A. A. Jarvis and E. A. Carter, "Use of Covalently-bonded Ceramics in Jet Engine Thermal Barrier Coatings," *MHPCC Application Briefs*, 4 (2002).
3. E. A. Jarvis and E. A. Carter, "Improving Jet Engine Turbine Thermal Barrier Coatings via Reactive Element Addition to the Bond Coat Alloy," *MHPCC Application Briefs*, 2 (2001).
2. E. A. Jarvis and E. A. Carter, "Jet Engine Turbine Thermal Barrier Coating Analysis," *MHPCC Application Briefs*, 8 (2000).
1. E. A. Asche and E. A. Carter, "Thermal Degradation of Ceramic Interfaces," *MHPCC Application Briefs*, 13 (1999).

## PATENTS

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Emily A. Carter and John Mark P. Martirez, *Plasmonic Haber-Bosch catalysts based on surface-doped Au nanoparticles*. Provisional Patent Application No.: 62/638,728 filed on March 5, 2018.

Emily A. Carter and Nima Alidoust, *Multi-Color Light Emitting Diode and Intermediate Band Solar Cells Based on Co-Ni Oxide*. Provisional Patent Application No.: 62210761 filed on August 27, 2015. Utility Patent re-filed as Emily A. Carter, Nima Alidoust, and Martina Lessio, *Multiple Band Gap Co-Ni Oxide Compositions and Applications Thereof*, Application No.: 15250633 filed on August 29, 2016.

Emily A. Carter, Peilin Liao, and John Andrew Keith, *Hematite-Based Photoanodes with Manganese, Cobalt, and Nickel Additives*. Provisional Patent Application No.: 61554287 filed on October 19, 2011. Utility Patent Application No.: 13666662 filed on November 1, 2012.

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)**

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### ***A. Invited Seminars***

- 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.
- July 6, 2015 "Quantum Mechanics Without Wavefunctions," Ecole Normale Superieure, Paris, France.
- Aug. 28, 2014 "(Photo)electrocatalysis: Theory and Mechanisms of Charge Transfer at Metal Surfaces," Malcolm Dole Distinguished Summer Lectures in Physical Chemistry, Northwestern University, Evanston, IL.
- Aug. 27, 2014 "Quantum Mechanics without Wavefunctions," Malcolm Dole Distinguished Summer Lectures in Physical Chemistry, Northwestern University, Evanston, IL.

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- Aug. 26, 2014 "Running Combustion Backwards: Fuels from Sunlight, From First Principles," Malcolm Dole Distinguished Summer Lectures in Physical Chemistry, Northwestern University, Evanston, IL.
- June 5, 2014 "Running Combustion Backwards: Fuels from Sunlight, From First Principles," Remsen Award Lecture, Johns Hopkins University, Baltimore, MD.
- March 10, 2014 "Running Combustion Backwards: Fuels from Sunlight, From First Principles," Stanford Chemical Engineering Student-Sponsored Colloquium, Stanford University, Stanford, CA.
- Feb. 17, 2014 "(Photo)electrocatalysis: Theory and Mechanisms of Charge Transfer at Metal Surfaces," The Linnett Lecture (General), Department of Chemistry, University of Cambridge, Cambridge, UK.
- Feb. 12, 2014 "Quantum Mechanics without Wavefunctions," The Linnett Lecture (Theory Seminar), Department of Chemistry, University of Cambridge, Cambridge, UK.
- Feb. 11, 2014 "Running Combustion Backwards: Fuels from Sunlight, From First Principles," The Linnett Lecture (General), Department of Chemistry, University of Cambridge, Cambridge, UK.
- Dec. 4, 2013 "How Quantum Mechanics Can Help Solve the World's Energy Problems," 2013 Hoyt C. Hottel Lecture in Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA.
- Nov. 26, 2013 "Quantum Mechanics without Wavefunctions," Kenneth S. Pitzer Lecture, Department of Chemistry, University of California, Berkeley, Berkeley, CA.

#### **B. Invited Lectures**

- Oct. 5, 2018 "Fuels from Sunlight," invited talk at the *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 *256<sup>th</sup> ACS Fall National Meeting*, Boston, MA.
- Aug. 19, 2018 "*Ab initio* potential energy surfaces and dynamics for sustainable chemistry," invited talk at the *256<sup>th</sup> ACS Fall National Meeting*, Boston, MA.
- Aug. 14, 2018 "Intricacies of Electrochemical Interfaces from First Principles," invited talk at the *2018 Gerischer Electrochemistry Today 2018 Meeting*, Boulder, CO.
- June 24, 2018 "Mechanisms for Sustainable Fuel and Chemical Production from First Principles," invited talk 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," invited talk at the *3rd International Conference on Proton Coupled Electron Transfer (PCET) 2018*, Blowing Rock, NC.

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- March 20, 2018 "Theoretical chemistry's role in providing sustainable energy," ACS Award in Theoretical Chemistry Lecture at the 255<sup>th</sup> 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 255<sup>th</sup> ACS Spring National Meeting, New Orleans, LA.
- March 19, 2018 "Advances in orbital-free density functional theory simulations of materials," at the 255<sup>th</sup> 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 5<sup>th</sup> 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 CO<sub>2</sub>," plenary lecture at the 2<sup>nd</sup> 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<sub>2</sub> Chemistry Solutions to Climate Change, Toronto, Ontario, Canada.
- April 3, 2017 "Understanding photoelectrocatalysis from first principles," keynote lecture at the 251<sup>st</sup> ACS Spring National Meeting, San Francisco, CA.
- April 2, 2017 "First principles optimization of novel solar cell materials," at the 251<sup>st</sup> 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.

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- 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<sub>2</sub> 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 *251<sup>st</sup> ACS Spring National Meeting*, San Diego, CA.
- Jan. 25, 2016 "Photoelectrochemical and electrochemical CO<sub>2</sub> 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 *Pacificchem 2015 Congress*, Honolulu, HI.
- Dec. 15, 2015 "Excited States in Condensed Matter from Embedded Correlation Wavefunction Theory," at the *Pacificchem 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 *250<sup>th</sup> ACS Fall National Meeting*, Boston, MA.

- July 7, 2015 "How Quantum Mechanics Can Help Provide a Sustainable Energy Future," plenary lecture at the *SCF'15 Conference on Chemistry and Energy Transition*, Lille, France.
- May 30, 2015 "Ab Initio Molecular Dynamics for Sustainable Energy: From Fuel Cells to Fusion," at the *Chemical Dynamics and the Rabinovitch Legacy: A Symposium in Memory of B. S. Rabinovitch*, University of Washington, Seattle, WA.
- April 27, 2015 "Embedded correlated wavefunction theory for semiconductors with applications to solar energy conversion," at the *BES-CTC PI Meeting*, Annapolis, MD.
- March 26, 2015 "Mechanisms of rhenium – and manganese-catalyzed electrochemical reduction of CO<sub>2</sub> from theory," at the *249<sup>th</sup> ACS Spring National Meeting*, Denver, CO.
- March 24, 2015 "What theory can reveal about carbon dioxide reduction and the role of molecular catalysts," at the *249<sup>th</sup> ACS Spring National Meeting*, Denver, CO.
- March 22, 2015 "Embedded correlated wavefunction theory: Advances and applications," at the *249<sup>th</sup> ACS Spring National Meeting*, Denver, CO.
- March 20, 2015 "Quantum Mechanical Simulations of Millions of Atoms and Its Application to Fusion Energy," at the *NAI Fellows Induction Ceremony*, Pasadena, CA.
- Feb. 14, 2015 "How Quantum Mechanics Can Help Solve the World's Energy Problems," at the *2015 AAAS Meeting*, San Jose, CA.
- Jan. 20, 2015 "Photoelectrochemical and electrochemical CO<sub>2</sub> reduction: Theoretical investigations," at the *AFOSR MURI Annual Review Meeting*, San Diego, CA.
- Dec. 3, 2014 "Quantum Mechanical Evaluation of Non-Silicon Inorganic Photovoltaic Materials," at the *2014 MRS Fall Meeting*, Boston, MA.
- Oct. 29, 2014 "Embedded Correlated Wavefunction Theory of Plasmon-Induced Chemistry," at the *AFOSR MURI Kickoff Meeting*, Rice University, Houston, TX.
- Oct. 24, 2014 "Building a Sustainable Energy and Environmental Future," at the *Dreyfus Teacher-Scholar Symposium*, New York Academy of Sciences, New York, NY.
- Oct. 7, 2014 "(Photo)Electrocatalysis: Theory and Mechanisms of Charge Transfer at Metal Surfaces," plenary lecture at the *10<sup>th</sup> Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC) 2014*, Santiago, Chile.
- Aug. 12, 2014 "Mechanisms for heterogeneous and homogeneous reduction of carbon dioxide from first principles," at the *248<sup>th</sup> ACS Fall National Meeting*, San Francisco, CA.
- Aug. 11, 2014 "Progress in (embedded) correlated wavefunction methods," at the *248<sup>th</sup> ACS Fall National Meeting*, San Francisco, CA.
- Aug. 10, 2014 "Pure density functional theory for most of the periodic table," at the *248<sup>th</sup> ACS Fall National Meeting*, San Francisco, CA.
- July 13, 2014 "First Principles Quantum Simulations of Renewable Energy Phenomena," at the *Gordon Research Conference on Atomic Molecular Interactions*, Easton, MA.
- May 20, 2014 "First Principles Quantum Simulations of the Essential Steps in (Photo)electrocatalysis," at the *AFOSR Molecular Dynamics and Theoretical Chemistry Program Review 2014*, Arlington, VA.

- Apr. 24, 2014 "Evaluation and Design of Photoelectrochemical Materials from First Principles," at the *2014 MRS Spring Meeting*, San Francisco, CA
- March 19, 2014 "First principles quantum simulations of (photo)electrocatalysis at semiconductor surfaces," at the *247th ACS Spring National Meeting*, Dallas, TX
- March 16, 2014 "First principles quantum mechanical evaluation of mixed electron-ion conductors and the oxygen reduction reaction," at the *247th ACS Spring National Meeting*, Dallas, TX
- Feb. 7, 2014 "At last: orbital-free DFT simulations of semiconductors and transition metals," at the *Royal Society Theo Murphy International Meeting on "Frontiers of Computer Simulation in Chemistry and Materials Science"*, Buckinghamshire, UK
- Dec. 9, 2013 "Photoelectrochemical CO<sub>2</sub> reduction: Theoretical investigations," at the *AFOSR MURI Annual Review Meeting*, La Jolla, CA

### **C. Invited Talks Given by Research Group Members**

- Oct. 24, 2018 "Ab initio modeling of light-driven catalysis on surface-doped plasmonic metals," invited talk at the *FACSS SciX 2018 Conference*, Atlanta, GA. (presented by Mark Martirez)
- Aug. 20, 2018 "Advances in nontraditional density-based electronic structure theories," invited talk 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," invited talk 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 CO<sub>2</sub> reduction on p-GaP photoelectrodes," invited talk 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," invited talk 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," invited talk 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," invited talk at the *254th ACS Fall National Meeting*, Washington, DC. (presented by Johannes Dieterich)
- May 9, 2017 "TigerCI: local multi-reference configuration interaction," invited talk 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," invited talk 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<sub>2</sub> capture, utilization, and storage strategy," invited poster at the *Accounts of Chemical Research Distinguished Scientists Poster Session, 251<sup>st</sup> ACS Spring National Meeting*, San Francisco, CA. (presented by Thomas Senftle)
- April 2, 2017 "Pyridine Co-catalysis impacting CO<sub>2</sub> reduction over semiconductor photoelectrodes," invited talk at the *251<sup>st</sup> ACS Spring National Meeting*, San Francisco, CA. (presented by Thomas Senftle)
- Feb. 28, 2017 "Computational Materials Discovery: From Reduced Pt Catalysts to Lightweight Alloys," invited talk at the *2017 TMS Annual Meeting & Exhibition*, San Diego, CA. (presented by Houlong Zhuang)
- Nov. 28, 2016 "Excited-State Heterogeneous Catalysis on Metallic Nanoparticles," invited talk 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 Heterogeneous Catalysis," invited talk 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," invited talk 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," talk at the *AFOSR MURI Meeting*, Rice University, Houston, TX. (presented by Caroline Krauter)
- May 16, 2016 "Excited State Dissociation Pathway for N<sub>2</sub> on Fe-substituted Plasmon-Active Au," talk at the *AFOSR MURI Meeting*, Rice University, Houston, TX. (presented by Mark Martirez)
- March 16, 2016 "How do surface reconstructions affect CO<sub>2</sub> reduction over GaP, CdTe, and CuInS<sub>2</sub> photoelectrodes?" invited talk at the *251<sup>st</sup> ACS Spring National Meeting*, San Diego, CA. (presented by Thomas Senftle)
- March 15, 2016 "Density functional embedding theory within the projector-augmented-wave formalism," invited talk at the *251<sup>st</sup> 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<sub>2</sub> dissociation catalysis," invited talk at the *251<sup>st</sup> ACS Spring National Meeting*, San Diego, CA. (presented by Mark Martirez)
- March 14, 2016 "Embedded correlated wavefunction methods for plasmon-induced photocatalysis," invited talk at the *251<sup>st</sup> 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<sub>2</sub> reduction on p-GaP photoelectrodes," talk at the 251<sup>st</sup> ACS Spring National Meeting, San Diego, CA. (presented by Martina Lessio)
- Jan. 22, 2015 "First-Principles-Derived Strategy to Stabilize Kesterite Phase CZTS for High Performance Solar Cells," invited talk at the *Electronic Materials and Applications 2015 Conference*, Orlando, FL. (presented by Kuang Yu)
- Feb. 17, 2014 "Angular-Momentum Dependent Orbital Free Density Functional Theory," invited talk at *The 54th Sanibel Symposium*, St. Simons' Island, GA. (presented by Florian Libisch)
- Jan. 9, 2014 "First-Principles Molecular Dynamics of Liquid Metals," invited talk at the "Where No Materials Dares To Go" Workshop, Leiden, the Netherlands (presented by Mohan Chen).

#### **D. Contributed Talks and Presentations**

- 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<sub>2</sub>ZnSnS<sub>4</sub> 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-affiliates Partnership 2018 Retreat*, New York, NY. (presented by Mark Martinez)
- 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 Martinez)
- 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)

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- 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  $\beta$ -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 CO<sub>2</sub> 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 *254<sup>th</sup> 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 *254<sup>th</sup> 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 *254<sup>th</sup> 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  $\beta$ -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<sub>4</sub> Dehydrogenation on Ru-functionalized Cu and N<sub>2</sub> 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<sub>2</sub> 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<sub>2</sub> 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  $\beta$ -Ni(OH)<sub>2</sub> and  $\beta$ -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<sub>2</sub> 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<sub>2</sub> 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<sub>2</sub> 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 4<sup>th</sup> Annual Meeting of the Princeton E-affiliates Partnership, Princeton, NJ. (presented by Mohan Chen)
- Nov. 20, 2015 "Pyridine-catalyzed CO<sub>2</sub> reduction on p-GaP electrodes: new insights on the role of pyridinium from theoretical investigations," poster at the 4<sup>th</sup> Annual Meeting of the Princeton E-affiliates 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)
- Aug. 10 & 11, 2015 "Dissociative Adsorption of Oxygen Molecule on Al(111)," poster at the Gordon Research Seminar on Dynamics at Surfaces, Newport, RI. (presented by Jin Cheng)
- July 30, 2015 "Implementation of Density Functional Embedding Theory with the Projector Augmented Wave Method," talk at the Penn Conference in Theoretical Chemistry 2015, Philadelphia, PA. (presented by Kuang Yu)
- May 11, 2015 "TigerCI: A parallel implementation of local configuration interaction methods for quantum chemistry," poster at the Princeton-Industry Symposium on High Performance Computing, Princeton, NJ. (presented by Caroline Krauter)
- March 26, 2015 "Pyridine-catalyzed CO<sub>2</sub> reduction on p-GaP photoelectrodes: First-principles investigation of possible reaction mechanisms," talk at the 249<sup>th</sup> ACS Spring National Meeting, Denver, CO. (presented by Martina Lessio)
- March 16, 2015 "Py-catalyzed CO<sub>2</sub> Reduction on GaP Electrodes: Can Surface Hydrogen Atoms Play a Role?," poster at the Third Biennial CO<sub>2</sub> Workshop, Princeton, NJ. (presented by Martina Lessio)
- March 16, 2015 "Observation of surface-bound negatively charged hydride and hydroxide on GaP(110) in H<sub>2</sub>O environments," poster at the Third Biennial CO<sub>2</sub> Workshop, Princeton, NJ. (presented by Coleman Kronawitter)
- March 16, 2015 "Hydrogen-bonded cyclic water clusters nucleated on an oxide surface," poster at the Third Biennial CO<sub>2</sub> Workshop, Princeton, NJ. (presented by Coleman Kronawitter)
- March 4, 2015 "First-principles molecular dynamics simulations of high-concentration deuterium implantation in liquid lithium," talk at the APS March Meeting 2015, San Antonio, TX. (presented by Mohan Chen)
- Feb. 5, 2015 "Ab Initio Reaction Kinetics of Hydrogen Abstraction from Methyl Propanoate and Subsequent Unimolecular Decomposition and Isomerization Reactions of Radicals," poster at the Princeton E-affiliates Partnership Student/Postdoc/Faculty/Industry Retreat, Princeton, NJ. (presented by Ting Tan)
- Jan. 29, 2015 "Efficient orbital-free density functional simulations of a million atoms," talk at Lawrence Berkeley National Laboratory, Berkeley, CA. (presented by Mohan Chen)

- Jan. 20, 2015 "Py-catalyzed CO<sub>2</sub> Reduction on GaP Electrodes: Can Surface Hydrogen Atoms Play a Role?," poster at the *AFOSR MURI Annual Review Meeting*, San Diego, CA. (presented by Martina Lessio)
- Dec. 16, 2014 "Pyridine-catalyzed CO<sub>2</sub> Reduction on p-GaP Electrodes: New Mechanistic Insights from Theoretical Investigations," talk at the *Tokyo Tech ACEEES Forum: 3<sup>rd</sup> International Education Forum on Environment and Energy Science*, Perth, Australia. (presented by Martina Lessio)
- Nov. 14, 2014 "Understanding the Differences between Rhenium- and Manganese-Catalyzed Electrochemical Reduction of CO<sub>2</sub>," poster at the *3<sup>rd</sup> Annual Meeting of the Princeton E-affiliates Partnership*, Princeton, NJ. (presented by Christoph Riplinger)
- Nov. 14, 2014 "New insights into the mechanism of Py-catalyzed CO<sub>2</sub> reduction on GaP electrodes," poster at the *3<sup>rd</sup> Annual Meeting of the Princeton E-affiliates Partnership*, Princeton, NJ. (presented by Martina Lessio)
- July 23, 2014 "Strategies to Improve CZTS Efficiency: A Computational Study," poster at the *American Conference on Theoretical Chemistry (ACTC) 2014*, Telluride, CO. (presented by Kuang Yu)
- July 23, 2014 "Ab Initio Reaction Kinetics of Hydrogen Abstraction from Methyl Acetate and Subsequent Unimolecular Decomposition Reactions of Radicals," poster at the *American Conference on Theoretical Chemistry (ACTC) 2014*, Telluride, CO. (presented by Ting Tan)
- July 22, 2014 "Embedded correlated wavefunction theory: development and application," poster at the *American Conference on Theoretical Chemistry (ACTC) 2014*, Telluride, CO. (presented by Jin Cheng)
- July 22, 2014 "New insights into the mechanism of Py-catalyzed CO<sub>2</sub> reduction on GaP electrodes," poster at the *American Conference on Theoretical Chemistry (ACTC) 2014*, Telluride, CO. (presented by Martina Lessio)
- July 16 & 17, 2014 "Understanding the Differences between Rhenium- and Manganese-Catalyzed Electrochemical Reduction of CO<sub>2</sub>," poster at the *Gordon Research Conference on Atomic Molecular Interactions*, Easton, MA. (presented by Christoph Riplinger)
- Apr. 23, 2014 "Oxygen Diffusion in SOFC Cathodes: Insight from First Principles," poster at the *HeteroFoam EFRC Annual Advisory Board Meeting*, Washington, DC. (presented by Andrew Ritzmann)
- March 16, 2014 "First-principles descriptors for molecular heterocycles that promote CO<sub>2</sub> reduction," invited talk at the *247<sup>th</sup> ACS Spring National Meeting*, Dallas, TX. (presented by John A. Keith)
- March 16, 2014 "Ab initio study of the oxygen reduction reaction at SOFC cathodes: State-of-the-art La(1-x)SrxMnO<sub>3</sub> vs. the new SrFe(1+x)MoxO(6-δ) mixed ion-electron conductor," talk at the *247<sup>th</sup> ACS Spring National Meeting*, Dallas, TX. (presented by Ana B. Muñoz-García)
- March 5, 2014 "Density-Decomposed Orbital-Free Density Functional Theory for Covalent Systems and Application to Li-Si alloys," talk at the *American Physical Society (APS) March Meeting 2014*, Denver, CO. (presented by Steven Xia)

- March 3, 2014 "Optimized Gaussian Basis Sets for Plane-Wave Compatible Calculations," talk at the *American Physical Society (APS) March Meeting 2014*, Denver, CO. (presented by Jin Cheng)
- March 3, 2014 "Implementation of the Small Box Fast Fourier Transformation Method within Orbital-Free Density Functional Theory (OFDFT)," talk at the *American Physical Society (APS) March Meeting 2014*, Denver, CO. (presented by Mohan Chen)
- Feb. 19, 2014 "Density-Decomposed Orbital-Free Density Functional Theory for Covalent Systems and Application to Li-Si alloys," poster at *The 54th Sanibel Symposium*, St. Simons' Island, GA. (presented by Junchao Xia)
- Dec. 9, 2013 "Towards understanding pyridine-catalyzed photocatalytic reduction of CO<sub>2</sub> on GaP electrodes," poster at the *AFOSR MURI Annual Review Meeting*, La Jolla, CA. (presented by Martina Lessio)
- Dec. 9, 2013 "Understanding the Differences between Rhenium- and Manganese-Catalyzed Electrochemical Reduction of CO<sub>2</sub>," poster at the *AFOSR MURI Annual Review Meeting*, La Jolla, CA. (presented by Christoph Riplinger)
- Nov. 15, 2013 "Towards Si Anodes for Next-Generation Li-Ion Batteries: An Orbital-Free Density Functional Theory Study of Li-Si Alloys," poster at the *2<sup>nd</sup> Annual Meeting of the Princeton E-affiliates Partnership*, Princeton, NJ. (presented by Junchao Xia)
- Nov. 15, 2013 Ab Initio Reaction Kinetics of Hydrogen Abstraction from Small Methyl Esters and Subsequent Unimolecular Decomposition Reactions of Radicals," poster at the *2<sup>nd</sup> Annual Meeting of the Princeton E-affiliates Partnership*, Princeton, NJ. (presented by Ting Tan)
- Nov. 15, 2013 "Towards Understanding the Differences Between Rhenium- and Manganese-Catalyzed Electrochemical Reduction of CO<sub>2</sub>," poster at the *2<sup>nd</sup> Annual Meeting of the Princeton E-affiliates Partnership*, Princeton, NJ. (presented by Christoph Riplinger)
- Nov. 15, 2013 "Pyridine-Catalyzed Photocatalytic Reduction of CO<sub>2</sub> on GaP Electrodes," poster at the *2<sup>nd</sup> Annual Meeting of the Princeton E-affiliates Partnership*, Princeton, NJ. (presented by Martina Lessio)
- Nov. 15, 2013 "Towards a Better Understanding of Plasma-Surface Interactions in a Fusion Reactor: an Orbital-Free First-Principles Molecular Dynamics Study of Liquid Lithium," poster at the *2<sup>nd</sup> Annual Meeting of the Princeton E-affiliates Partnership*, Princeton, NJ. (presented by Mohan Chen)

## **CURRENT EXTRAMURAL FUNDING SOURCES**

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Air Force Office of Scientific Research

Office of Naval Research

Department of Energy, Basic Energy Sciences

Department of Energy, Energy Efficiency & Renewable Energy

Department of Energy, Advanced Scientific Computing Research

Department of Defense Multidisciplinary University Research Initiative