CURRICULUM VITAE

EMILY ANN CARTER

BIRTHDATE

November 28, 1960

BIRTHPLACE

Los Gatos, California, U. S. A.

PROFESSIONAL ADDRESS

Princeton University
School of Engineering and Applied Science
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EDUCATION

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

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

PROFESSIONAL POSITIONS

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

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.

AWARDS AND HONORS

2017	2017 Albert J. Moscowitz Memorial Lecture, University of Minnesota
2017	Distinguished Lecture 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 Lecture, Lehigh University
2016	2016 Pitzer Lecture 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* 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 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

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, *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-

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: 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

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).

2017 Febuary 8 – Invited Speaker, 55th Reunion Reception and Dinner with Princeton Class of 1962, New York Yacht Club, New York, NY

Outreach activities:

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-

Member, Lawrence Berkeley National Laboratory (LBNL) Advisory Board, 2016-2019

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 Martime 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-present

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

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

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 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.

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)

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

357. J. M. Dieterich, W. C. Witt, E. A. Carter, "libKEDF: an accelerated library of kinetic energy density functionals," *J. Comput. Chem.*, in press (2017). doi: 10.1002/jcc.24806

356. J. M. Dieterich and E. A. Carter, "Quantum Solutions for a Sustainable Energy Future," *Nat. Rev. Chem.*, in press (2017).

354. K. Yu, C. M. Krauter, J. M. Dieterich, and E. A. Carter, "Density and Potential Functional Embedding: Theory and Practice," in "Fragmentation: Toward Accurate Calculations on Complex Molecular Systems," Mark Gordon, Ed. (John Wiley & Sons), ISBN: 978-1-119-12924-0, in press (2016). http://www.wiley.com/WileyCDA/WileyTitle/productCd-1119129249.html

354. J. M. P. Martirez and E. A. Carter, "Excited-State N_2 Dissociation Pathway on Fe-Functionalized Au," *J. Am. Chem. Soc.*, 139, 4390 (2017). doi: 10.1021/jacs.6b12301

353. T. Senftle and E. A. Carter, "The Holy Grail: Chemistry enabling an economically viable CO_2 capture, utilization, and storage strategy," *Acc. Chem. Res.*, 50, 472 (2017). doi: 10.1021/acs.accounts.6b00479

352. J. Cheng, K. Yu, F. Libisch, J. M. Dieterich, and E. A. Carter, "Potential Functional Embedding Theory at the Correlated Wave Function Level, Part II: Error Sources and Performance Tests," *J. Chem. Theor. Comp.*, 13, 1081 (2017). doi: 10.1021/acs.jctc.6b01011

351. J. Cheng, F. Libisch, K. Yu, M. Chen, J. M. Dieterich, and E. A. Carter, "Potential Functional Embedding Theory at the Correlated Wavefunction Level, Part I: Mixed Basis Set Embedding," *J. Chem. Theor. Comp.*, 13, 1067 (2017). doi: 10.1021/acs.jctc.6b01010

350. D. Felsmann, H. Zhao, Q. Wang, I. Graf, T. Tan, X. Yang, E. A. Carter, Y. Ju, and K. Kohse-Hoeinghaus, "Contributions to improving small ester combustion chemistry: theory, model and experiments," *Proceedings of the Combustion Institute*, 36, 543 (2017). doi: 10.1016/j.proci.2016.05.012

349. J. R. Vella, M. Chen, F. H. Stillinger, E. A. Carter, P. G. Debenedetti, and A. Z. Panagiotopoulos, "Structural and Dynamic Properties of Liquid Tin From a New Modified Embedded-Atom Method Force Field," *Phys. Rev. B*, 95, 064202 (2017). doi: 10.1103/PhysRevB.95.064202

348. H. Zhuang, A. J. Tkalych, and E. A. Carter, "The Surface Energy as a Descriptor of Catalytic Activity," *J. Phys. Chem. C*, 120, 23698 (2016). doi: 10.1021/acs.jpcc.6b09687

347. A. M. Ritzmann, J. M. Dieterich, and E. A. Carter, "Density Functional Theory Investigation of the Electronic Structure and Defect Chemistry of $Sr_{1-x}K_xFeO_3$," *MRS Communications*, 6, 145 (2016). doi: 10.1557/mrc.2016.23

346. M. Lessio, C. Riplinger, and E. A. Carter, "Stability of surface protons in pyridine-catalyzed CO_2 reduction at p-GaP photoelectrodes," *Phys. Chem. Chem. Phys.*, 18, 26434 (2016). doi: 10.1039/c6cp04272d

345. T. P. Senftle, M. Lessio, E. A. Carter, "Implications of Surface Reconstructions for Py-catalyzed CO_2 Reduction on GaP(111) and CdTe(111) Photo-electrodes," *Chem. Mater.*, 28, 5799 (2016). doi: 10.1021/acs.chemmater.6b02084

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CONFERENCE PROCEEDINGS

6. D.F. Johnson, E.A. Carter, "Structure, Bonding and Adhesion of Materials Interfaces with Density Functional Theory: Cr/Fe, SiC/Fe, $MoSi_2$/Ni," 25th Army Science Conference, Orlando, Florida, November 2006.
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

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

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 and Nima Alidoust, *Three Dimensional Hole Transport in Nickel Oxide by Alloying with MgO or ZnO for Use as p-Type Transparent Conducting Oxides*. Provisional Patent Application No.: 62195906 filed on July 23, 2015; Provisional Patent Application No.: 62347157 filed on June 8, 2016.

Emily A. Carter and Maytal C. Toroker, *Wustite-Based Photoelectrodes with Lithium, Hydrogen, Sodium, Magnesium, Manganese, Zinc, and Nickel Additives.* Provisional Patents: Application No.: 61578342 filed on December 21, 2011; Application No.: 61578600 filed on December 21, 2011; Application No.: 61649601 filed on May 22, 2012. Utility Patent Application No.: 13/899,049 filed on May 21, 2013.

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 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

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

Oct. 22, 2013 "Running Combustion Backwards: Fuels from Sunlight, from First Principles," Lord Chemistry Lecture, Department of Chemistry, Allegheny College, Meadville, PA.

Oct. 21, 2013 "How Quantum Mechanics Can Help Solve the World's Energy Problems," Lord Public Lecture, Department of Chemistry, Allegheny College, Meadville, PA.

Oct. 7, 2013 "First Principles Solid State Quantum Mechanics Methods for Sustainable Energy: From Fuel Cells to Fusion," Vienna Computational Material Laboratory, Vienna University of Technology, Vienna, Austria.

May 2, 2013 "Quantum Mechanics without Wavefunctions," Francis Clifford Phillips Lectures, Xi Chapter of the Phi Lambda Upsilon National Honorary Chemical Society and the Department of Chemistry, University of Pittsburgh, Pittsburgh, PA.

May 1, 2013 "A Quantum Search for Fuels from Sunlight," Francis Clifford Phillips Lectures, Xi Chapter of the Phi Lambda Upsilon National Honorary Chemical Society and the Department of Chemistry, University of Pittsburgh, Pittsburgh, PA.

April 25, 2013 "Quantum Mechanics and the Future of the Planet," Tedori-Callinan Lecture, Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania, Philadelphia, PA.

March 28, 2013 "Quantum Mechanical Evaluation of Energy Conversion Materials for Generating Electricity and Fuels," Chemistry Colloquium Speaker, Columbia University, New York, NY.

March 14, 2013 "Quantum Mechanical Evaluation of Electron and Ion Transport in Metal Oxides," Distinguished Lecture, Naval Research Laboratory Chemistry Division Colloquium, Washington, DC.

March 1, 2013 "The Role of Science in Moving the Planet to Green Energy and a Sustainable Future," W. Allan Powell Lecture, Virginia Section of the American Chemical Society and the University of Richmond, Richmond, VA.

Oct. 5, 2012 "Quantum Mechanical Evaluation of Energy Conversion Materials for Generating Electricity and Fuels," Institute of Mechanical Engineering Seminar, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland.

Sept. 13, 2012 "The Role of Science in Solving Our Planet's Energy Problems," Rutgers Energy Institute and Bloustein School of Planning and Public Policy Energy Policy Seminar, Rutgers University, New Brunswick, NJ.

B. Invited Lectures

April 3, 2017 "Understanding photoelectrocatalysis from first principles," 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.

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_2 from theory," at the *249th 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 *249th ACS Spring National Meeting*, Denver, CO.

March 22, 2015 "Embedded correlated wavefunction theory: Advances and applications," at the *249th 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_2 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 *10th 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 *248th ACS Fall National Meeting*, San Francisco, CA.

Aug. 11, 2014 "Progress in (embedded) correlated wavefunction methods," at the *248th ACS Fall National Meeting*, San Francisco, CA.

Aug. 10, 2014 "Pure density functional theory for most of the periodic table," at the *248th 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_2 reduction: Theoretical investigations," at the *AFOSR MURI Annual Review Meeting*, La Jolla, CA

Nov. 5, 2013 "First Principles Quantum Mechanics Methods for Simulating Fundamental Phenomena in Batteries and Fuel Cells," at the *Institute of Pure and Applied Mathematics Workshop III: Batteries and Fuel Cells*, Los Angeles, CA

Nov. 4, 2013 "Quantum Mechanics and the Future of the Planet," *Mathematics of Planet Earth 2013 Simons Public Lecture at the Institute for Pure and Applied Mathematics*, Los Angeles, CA

Oct. 28, 2013 "Mechanisms of (Photo)Electrochemical Reduction of Carbon Dioxide From First Principles," keynote lecture at the *224th Electrochemical Society Meeting*, San Francisco, CA

Oct. 3, 2013 "Charge Transfer Excited States from First Principles Theories," at the *18th European Theoretical Spectroscopy Facility (ETSF) Workshop on Electronic Excitations*, Luxembourg

Sept. 27, 2013 "Mechanisms of Photoelectrochemical Reduction of Carbon Dioxide and Water Splitting from First Principles," at the *Avogadro Colloquia (second edition) on Challenges for theoretical and computational chemistry in Horizon2020*, Pisa, Italy

Aug. 27, 2013 "How Quantum Mechanics Can Help Solve the World's Energy Problems," plenary lecture at the *Applied Mathematics, Modeling and Computational Science (AMMCS) 2013 International Conference*, Waterloo, ON, Canada

Aug. 14, 2013 "First Principles Quantum Predictions of Charge Transfer at Surfaces," at the *Gordon Research Conference on Dynamics at Surfaces*, Newport, RI

Feb. 27, 2013 "Quantum Mechanics Without Wavefunctions," plenary lecture at the *Society for Industrial and Applied Mathematics (SIAM) Conference on Computational Science and Engineering (CSE13)*, Boston, MA.

Dec. 13, 2012 "Materials Genome Initiative: Hard Condensed Matter for Energy Applications," at the *NSF Materials Genome Initiative Workshop*, Arlington, VA.

Dec. 7, 2012 "Photoelectrochemical CO_2 Reduction: Theoretical Investigations," at the *2012 MURI Review Meeting*, San Diego, CA.

Aug. 20, 2012 "Advances in Quantum Embedding Theory and Applications," at the *224th American Chemical Society National Meeting and Exposition*, Philadelphia, PA.

Aug. 14, 2012 "Quantum Mechanical Design and Evaluation of New Solar Energy Conversion Materials," keynote lecture at the *SPIE Optics & Photonics 2012*, San Diego, CA.

July 23, 2012 "Accurate Ab Initio Potential Energy Surfaces for Molecules – Metal Surface Dynamics Including Charge Transfer from an Exact Embedding Theory," at the *Gordon Research Conference on Computational Chemistry*, Mount Snow, VT.

June 8, 2012 "The Role of Science in Moving the Planet to Green Energy and a Sustainable Future," keynote address at the *2012 Midwest Theoretical Chemistry Conference*, Madison, WI.

May 25, 2012 "Quantum Mechanical Evaluation of Photoelectrochemical and Solid Oxide Fuel Cells," keynote lecture at the *11th Spring Meeting of the International Society of Electrochemistry*, Washington, DC.

May 23, 2012 "Novel Catalytic Mechanisms for the Chemical Reduction of Carbon Dioxide to Energy-Dense Liquids (MURI)," at *the AFOSR Molecular Dynamics Contractor's Meeting*, Arlington, VA.

May 9, 2012 "Status and Challenges for Quantum Simulations of Materials at the Mesoscale," at the *PICSciE Conference: Research Computing at Princeton*, Princeton, NJ.

April 12, 2012 "Quantum Mechanical Evaluation of Solid Oxide Fuel Cell Materials," at the *2012 MRS Spring Meeting & Exhibit*, San Francisco, CA.

C. Invited Talks Given by Research Group Members

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_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," invited talk 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," 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 HeterogeneousCatalysis," 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_2 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_2 reduction over GaP, CdTe, and $CuInS_2$ photoelectrodes?" talk 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," invited talk 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," talk 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," invited talk 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," talk at the *251st 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).

Sept. 9, 2013 "Quantum mechanical insights into photoelectrochemical CO_2 reduction processes," invited talk at the *246th ACS National Meeting Physical Chemistry of Solar Energy Conversion*, Indianapolis, IN. (presented by John A. Keith)

June 25, 2013 "Quantum Mechanical Insights into Photoelectrochemical Reduction of CO_2 with Pyridinium Catalysts," invited talk at the *12th International Conference on Carbon Dioxide Utilization (ICCDU)*, Alexandria, VA. (presented by John A. Keith)

May 15, 2013 "First-Principles Insights into Oxygen Transport in Solid Oxide Fuel Cell Cathode Materials," talk at the *223rd ECS Meeting 2013*, Toronto, Ontario, Canada. (presented by Andrew Ritzmann)

Nov. 27, 2012 "Tackling Molecule-Surface Interactions Using High-Level Embedded Correlated Wavefunction Methods," invited talk at the *Dynamical Phenomena at Surfaces: The Role of Complexity Workshop*, Leiden, Netherlands. (presented by Florian Libisch)

Oct. 12, 2012 "Quantum Mechanical Insights Into Photoelectrochemical Reduction of CO_2 with Pyridinium Catalysts," invited talk at the *CECAM Workshop on Future Challenges in CO_2-Reduction*, Bremen, Germany. (presented by John Keith)

Sept. 5, 2012 "Orbital-Free Density Functional Theory of Molecules and Semiconductors," invited talk at the *CECAM Workshop on Orbital Free Methods*, Paris, France. (presented by Junchao Xia)

D. Contributed Talks and Presentations

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)

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_2 reduction on p-GaP photoelectrodes: First-principles investigation of possible reaction mechanisms," talk at the *249th ACS Spring National Meeting*, Denver, CO. (presented by Martina Lessio)

March 16, 2015 "Py-catalyzed CO_2 Reduction on GaP Electrodes: Can Surface Hydrogen Atoms Play a Role?," poster at the *Third Biennial CO_2 Workshop*, Princeton, NJ. (presented by Martina Lessio)

March 16, 2015 "Observation of surface-bound negatively charged hydride and hydroxide on GaP(110) in H2O environments," poster at the *Third Biennial CO_2 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_2 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-ffiliates 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_2 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_2 Reduction on p-GaP Electrodes: New Mechanistic Insights from Theoretical Investigations," talk at the *Tokyo Tech ACEEES Forum: 3rd 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_2," poster at the *3rd Annual Meeting of the Princeton E-ffiliates Partnership*, Princeton, NJ. (presented by Christoph Riplinger)

Nov. 14, 2014 "New insights into the mechanism of Py-catalyzed CO_2 reduction on GaP electrodes," poster at the *3rdAnnual Meeting of the Princeton E-ffiliates 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 CO2 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 CO2," 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 CO2 reduction," invited talk at the *247th 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)SrxMnO3 vs. the new SrFe(1+x)MoxO(6-δ) mixed ion-electron conductor," talk at the *247th ACS Spring National Meeting*, Dallas, TX. (presented by Ana B. Muñoz-Garcia)

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_2 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_2," 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 *2nd Annual Meeting of the Princeton E-ffiliates 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 *2nd Annual Meeting of the Princeton E-ffiliates Partnership*, Princeton, NJ. (presented by Ting Tan)

Nov. 15, 2013 "Towards Understanding the Differences Between Rhenium- and Manganese-Catalyzed Electrochemical Reduction of CO_2," poster at the *2nd Annual Meeting of the Princeton E-ffiliates Partnership*, Princeton, NJ. (presented by Christoph Riplinger)

Nov. 15, 2013 "Pyridine-Catalyzed Photocatalytic Reduction of CO_2 on GaP Electrodes," poster at the *2nd Annual Meeting of the Princeton E-ffiliates 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 *2nd Annual Meeting of the Princeton E-ffiliates Partnership*, Princeton, NJ. (presented by Mohan Chen)

Nov. 5, 2013 "Modeling Photoelectrochemical Water Oxidation and CO_2 Reduction With DFT+U, DFT+D, and Heterogeneous Solvation," talk at the *2013 AIChE Annual Meeting*, San Francisco, CA. (presented by John A. Keith)

Nov. 5, 2013 "Insights Into the Performance of Cu_2O in Photocatalytic CO_2 Conversion," talk at the *2013 AIChE Annual Meeting*, San Francisco, CA. (presented by Leah Isseroff Bendavid)

Oct. 3, 2013 "The melting point of lithium: an orbital-free first-principles molecular dynamics study," poster at the *66th Gaseous Electronics Conference*, Princeton, NJ. (presented by Mohan Chen)

April 10, 2013 "*Ab initio* Reaction Kinetics of Methyl Formate Hydrogen Abstraction and Subsequent β-scission," talk at the *ACS National Meeting & Exposition*, New Orleans, LA. (presented by Ting Tan)

April 10, 2013 "Band Gap Engineering of Nickel(II) Oxide via Degenerate Alloying with Li_2O for Solar Energy Conversion: A Theoretical Study," talk at the *ACS National Meeting & Exposition*, New Orleans, LA. (presented by Nima Alidoust)

April 10, 2013 "Biodiesel Thermochemistry from Multi-Reference Correlated Wavefunction Calculations," talk at the *ACS National Meeting & Exposition*, New Orleans, LA. (presented by Victor Oyeyemi)

March 22, 2013 "Embedding Methods: Application and Development," talk at the *2013 American Physical Society (APS) March Meeting*, Baltimore, MD. (presented by Jin Cheng)

March 21, 2013 "Efficient Optimal Effective Potential Approach for Periodic Plane-Wave Density Functional Theory," talk at the *2013 American Physical Society (APS) March Meeting*, Baltimore, MD. (presented by Florian Libisch)

March 21, 2013 "Angular Momentum Dependent Orbital Free Density Functional Theory," talk at the *2013 American Physical Society (APS) March Meeting*, Baltimore, MD. (presented by Youqi Ke)

March 21, 2013 "Ab Initio Molecular Dynamics Study of Liquid Li Surfaces Exposed to Deuterium," talk at the *2013 American Physical Society (APS) March Meeting*, Baltimore, MD. (presented by Mohan Chen)

Dec. 7, 2012 "Quantum Mechanical Insights into Photoelectrochemical Reduction of CO2 with Pyridinium Catalysts," poster at the *2012 MURI Review Meeting*, San Diego, CA. (presented by John Keith)

Dec. 6, 2012 "New Solar Energy Conversion Materials," talk at the *New Jersey Technology Council 2012 Regional Commercialization Conference*, Wilmington, DE. (presented by Leah Isseroff)

Nov. 29, 2012 "New Solar Energy Conversion Materials," talk at *Celebrate Princeton Invention 2012*, Princeton, NJ. (presented by Nima Alidoust, Leah Isseroff, and John Keith)

Nov. 12, 2012 "Band Gap Engineering of Nickel Oxide for Solar Energy Applications," poster at the *Synergize 2012 Inaugural Annual Meeting of the Princeton Energy & Environmental Corporate Affiliates Program*, Princeton, NJ. (presented by Nima Alidoust)

Nov. 12, 2012 "First-Principles Quantum Mechanics Analysis of Oxygen Diffusion in $La_{1x}Sr_xFeO_3$ and $La_{1-x}Sr_xCoO_3$," poster at the *Synergize 2012 Inaugural Annual Meeting of the Princeton Energy & Environmental Corporate Affiliates Program*, Princeton, NJ. (presented by Andrew Ritzmann)

Nov. 9, 2012 "Quantum Mechanical Insights into Photoelectrochemical Reduction of CO2 with Pyridinium Catalysts," poster at the *Second Biennial CO_2 Workshop*, Princeton, NJ. (presented by John Keith)

Aug. 21, 2012 "Band Gap Engineering of Nickel Oxide for Solar Energy Applications," poster at the *Summer School on Inorganic Materials for Energy Conversion and Storage*, Santa Barbara, CA. (presented by Nima Alidoust)

July 23 & 25, 2012 "Electronic Structure of Pure and Doped Cuprous Oxide with Copper Vacancies: Suppression of Trap States," poster at the *Gordon Research Conference on Computational Chemistry*, Mount Snow, VT. (presented by Leah Isseroff)

June 27, 2012 "Ab Initio Reaction Pathways for Dissociative Adsorption of Dioxygen on Al (111)," poster at the *International Conference of Quantum Chemistry (ICQC)*, Boulder, CO. (presented by Florian Libisch)

June 21, 2012 "First-Principles Study of $Sr_2Fe_{2-x}Mo_xO_{6-d}$ (SFMO) for Solid Oxide Fuel Cell Applications," poster at the *GEI-ERA 2012*, Santa Marina Salina, Italy. (presented by Ana Belen Muñoz-García)

June 19, 2012 "Effects of A- and B-site doping on {La,Sr}MnO_3 (LSM)-based cathode materials for solid oxide fuel cells," talk at the *GEI-ERA 2012*, Santa Marina Salina, Italy. (presented by Michele Pavone)

May 22, 2012 "First Principles Evaluation of Optical, Transport, and Catalytic Properties of Pure and Doped Hematite for Photocatalytic Water Splitting," poster at the *AFOSR Molecular Dynamics Contractor's Meeting*, Arlington, VA. (presented by Peilin Liao)

May 15, 2012 "Origin of the Barrier to Reactions of O2 on Al(111): Charger Transfer," invited seminar talk at the *Institute for Theoretical Chemistry, Technische Universität München*, Munich, Germany. (presented by Florian Libisch)

CURRENT EXTRAMURAL FUNDING SOURCES

National Science Foundation

Air Force Office of Scientific Research

Office of Naval Research

Department of Energy, Basic Energy Sciences

Department of Defense Multidisciplinary University Research Initiative