

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
C230 Engineering Quadrangle
Princeton, NJ 08544-5263
email: eac@princeton.edu
tel: (609) 258-5391
fax: (609) 258-6744
Web page: <http://carter.princeton.edu>

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 Coblenz 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 *Outreach activities:* February 8 – Invited Speaker, 55th Reunion Reception and Dinner with Princeton Class of 1962, New York Yacht Club, New York, NY
- January 19 – IdeasLab panelist, Responding to Climate Change with Princeton University, World Economic Forum Annual Meeting 2017, Davos, Switzerland
- January 18 – Panelist, Princeton's Breakfast Panel: Income Inequality and Opportunities to Improve the Human Condition, World Economic Forum Annual Meeting 2017, Davos, Switzerland
- 2016 Member, Molecular Sciences Software Institute (MolSSI) Advisory Board, 2016-2019
- Member, Lawrence Berkeley National Laboratory (LBNL) Advisory Board, 2016-2019
- Member, Secretary of Energy Advisory Board Task Force on CO₂ 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 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](https://doi.org/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 N₂ Dissociation Pathway on Fe-Functionalized Au," *J. Am. Chem. Soc.*, 139, 4390 (2017).
[doi: 10.1021/jacs.6b12301](https://doi.org/10.1021/jacs.6b12301)
353. T. Senftle and E. A. Carter, "The Holy Grail: Chemistry enabling an economically viable CO₂ capture, utilization, and storage strategy," *Acc. Chem. Res.*, 50, 472 (2017). [doi: 10.1021/acs.accounts.6b00479](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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 $\text{Sr}_{1-x}\text{K}_x\text{FeO}_3$," *MRS Communications*, 6, 145 (2016). doi: [10.1557/mrc.2016.23](https://doi.org/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](https://doi.org/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](https://doi.org/10.1021/acs.chemmater.6b02084)
344. D. F. Swearer, H. Zhao, L. Zhou, C. Zhang, H. Robotjazi, J. M. P. Martirez, C. M. Krauter, S. Yazdi, M. J. McClain, E. Ringe, E. A. Carter, P. Nordlander, N. J. Halas, "Heterometallic antenna-reactor complexes for photocatalysis," *Proc. Natl. Acad. Sci. U.S.A.*, 113, 8916 (2016). doi: [10.1073/pnas.1609769113](https://doi.org/10.1073/pnas.1609769113)
343. M. Lessio, T. P. Senftle, and E.A. Carter, "Is the Surface Playing a Role during Pyridine-Catalyzed CO_2 Reduction on p-GaP Photoelectrodes?," *ACS Energy Lett.*, 1, 464 (2016). doi: [10.1021/acsenergylett.6b00233](https://doi.org/10.1021/acsenergylett.6b00233)
342. L. B. Roskop, E. F. Valeev, E. A. Carter, M. S. Gordon, and T. S. Windus, "A Spin-free $[2]_{\text{R}12}$ Basis Set Incompleteness Correction to the Local Multi-Reference Configuration Interaction and the Local Multi-Reference Average Coupled Pair Functional Methods," *J. Chem. Theor. Comp.*, 12, 3176 (2016). doi: [10.1021/acs.jctc.6b00315](https://doi.org/10.1021/acs.jctc.6b00315)
341. H. Zhuang, M. Chen, and E. A. Carter, "Elastic and thermodynamic properties of complex Mg-Al intermetallic compounds via orbital-free density functional theory," *Phys. Rev. Appl.*, 5, 064021 (2016). doi: [10.1103/PhysRevApplied.5.064021](https://doi.org/10.1103/PhysRevApplied.5.064021)
340. M. Chen, J. Roszell, E. V. Scoullous, C. Riplinger, B. E. Koel, and E. A. Carter, "Effect of temperature on the desorption of lithium from molybdenum (110) surfaces: implications for fusion reactor first wall materials," *J. Phys. Chem. B*, 120, 6110 (2016). doi: [10.1021/acs.jpcc.6b02092](https://doi.org/10.1021/acs.jpcc.6b02092)
339. K. Yu and E. A. Carter, "Determining and Controlling the Stoichiometry of $\text{Cu}_2\text{ZnSnS}_4$ Photovoltaics: the Physics and Its Implications," *Chem. Mater.*, 28, 4415 (2016). doi: [10.1021/acs.chemmater.6b01612](https://doi.org/10.1021/acs.chemmater.6b01612)
338. M. Chen, X. Jiang, H. Zhuang, L. Wang, and E. A. Carter, "Petascale Orbital-Free Density Functional Theory Enabled by Small-Box Algorithms," *J. Chem. Theor. Comp.*, 12, 2950 (2016). doi: [10.1021/acs.jctc.6b00326](https://doi.org/10.1021/acs.jctc.6b00326)

337. A. M. Ritzmann, J. M. Dieterich, and E. A. Carter, "Density Functional Theory +U Analysis of the Electronic Structure and Defect Chemistry of LSCF ($\text{La}_{0.5}\text{Sr}_{0.5}\text{Co}_{0.25}\text{Fe}_{0.75}\text{O}_{3-\delta}$)," *Phys. Chem. Chem. Phys.*, 18, 12260 (2016). [doi: 10.1039/C6CP01720G](https://doi.org/10.1039/C6CP01720G)
336. H. Zhuang, A. J. Tkalych, and E. A. Carter, "Understanding and Tuning the Hydrogen Evolution Reaction on Pt-Covered Tungsten Carbide Cathodes," *J. Electrochem. Soc.*, 163, F629 (2016). [doi: 10.1149/2.0481607jes](https://doi.org/10.1149/2.0481607jes)
335. J. Xia and E. A. Carter, "Orbital-Free Density Functional Theory Study of Amorphous Li-Si Alloys and Introduction of a Simple Density Decomposition Formalism," *Modell. Simul. Mater. Sci. Eng.*, 24, 035014 (2016). [doi: 10.1088/0965-0393/24/3/035014](https://doi.org/10.1088/0965-0393/24/3/035014)
334. T. Tan, X. Yang, Y. Ju, and E. A. Carter, "Ab Initio Reaction Kinetics of $\text{CH}_3\text{OC}(=\text{O})$ and $\text{CH}_2\text{OC}(=\text{O})\text{H}$ Radicals," *J. Phys. Chem. B*, 120, 1590 (2016). [doi: 10.1021/acs.jpccb.5b07959](https://doi.org/10.1021/acs.jpccb.5b07959)
333. J. M. P. Martirez and E. A. Carter, "Thermodynamic Constraints in Using AuM (M= Fe, Co, Ni and Mo) alloys as N_2 Dissociation Catalysts: Functionalizing a Plasmon-Active Metal," *ACS Nano*, 10, 2940 (2016). [doi: 10.1021/acsnano.6b00085](https://doi.org/10.1021/acsnano.6b00085)
332. L. Zhou, C. Zhang, M. McClain, A. Manjavacas, C. Krauter, S. Tian, F. Berg, H. Everitt, E. A. Carter, P. Nordlander, and N. Halas, "Aluminum Nanocrystal as a Plasmonic Photocatalyst for Hydrogen Dissociation," *Nano Lett.*, 16, 1478 (2016). [doi: 10.1021/acs.nanolett.5b05149](https://doi.org/10.1021/acs.nanolett.5b05149)
331. K. Yu and E. A. Carter, "Elucidating Structural Disorder and the Effects of Cu Vacancies on the Electronic Properties of $\text{Cu}_2\text{ZnSnS}_4$ Photovoltaics," *Chem. Mater.*, 28, 864 (2016). [doi: 10.1021/acs.chemmater.5b04351](https://doi.org/10.1021/acs.chemmater.5b04351)
330. T. Tan, X. Yang, Y. Ju, and E. A. Carter, "Ab Initio Kinetics Studies of Hydrogen Atom Abstraction from Methyl Propanoate," *Phys. Chem. Chem. Phys.*, 18, 4594 (2016). [doi: 10.1039/C5CP07282D](https://doi.org/10.1039/C5CP07282D)
329. N. Alidoust, M. Lessio, and E. A. Carter, "Cobalt (II) oxide and nickel (II) oxide alloys as potential intermediate-band semiconductors: A theoretical study," *J. Appl. Phys.*, 119, 025102 (2016). [doi: 10.1063/1.4939286](https://doi.org/10.1063/1.4939286)
328. T. Abrams, M. A. Jaworski, M. Chen, E. A. Carter, R. Kaita, D. P. Stotler, G. De Temmerman, T. W. Morgan, M. A. van den Berg, and H. J. van der Meiden, "Suppressed gross erosion of high-temperature lithium via rapid deuterium implantation," *Nucl. Fusion*, 56, 016022 (2016). [doi: 10.1088/0029-5515/56/1/016022](https://doi.org/10.1088/0029-5515/56/1/016022)
327. M. Chen, T. Abrams, M. Jaworski, and E. A. Carter, "Rock-Salt Structure Lithium Deuteride Formation in Liquid Lithium with High-Concentrations of Deuterium: A First-Principles Molecular Dynamics Study," *Nucl. Fusion*, 56, 016020 (2016). [doi: 10.1088/0029-5515/56/1/016020](https://doi.org/10.1088/0029-5515/56/1/016020)
326. C. X. Kronawitter, M. Lessio, P. Zahl, A. B. Muñoz-García, P. Sutter, E. A. Carter, and B. E. Koel, "Orbital-resolved imaging of the adsorbed state of pyridine on a III-V semiconductor identifies atomic sites susceptible to nucleophilic attack," *J. Phys. Chem. C*, 119, 28917 (2015). [doi: 10.1021/acs.jpcc.5b08659](https://doi.org/10.1021/acs.jpcc.5b08659)

325. T. Tan, X. Yang, Y. Ju, and E. A. Carter, "Ab Initio Pressure-Dependent Reaction Kinetics of Methyl Propanoate Radicals," *Phys. Chem. Chem. Phys.*, 17, 31061 (2015). doi: [10.1039/C5CP06004D](https://doi.org/10.1039/C5CP06004D)
324. N. Alidoust and E. A. Carter, "Three-Dimensional Hole Transport in Nickel Oxide by Alloying with MgO or ZnO," *J. Appl. Phys.*, 118, 185102 (2015). doi: [10.1063/1.4935478](https://doi.org/10.1063/1.4935478)
323. D. B. Krisiloff, C. M. Krauter, F. J. Ricci, and E. A. Carter, "Density fitting and Cholesky decomposition of the two-electron integrals in local multireference configuration interaction theory," *J. Chem. Theor. Comp.*, 11, 5242 (2015). doi: [10.1021/acs.jctc.5b00762](https://doi.org/10.1021/acs.jctc.5b00762)
322. A. Tkalych, K. Yu, and E. A. Carter, "Structural and electronic features of β -Ni(OH)₂ and β -NiOOH from first principles," *J. Phys. Chem. C*, 43, 24315 (2015). doi: [10.1021/acs.jpcc.5b08481](https://doi.org/10.1021/acs.jpcc.5b08481)
321. T. Tan, X. Yang, Y. Ju, and E. A. Carter, "Ab Initio Unimolecular Reaction Kinetics of CH₂C(=O)OCH₃ and CH₃C(=O)OCH₂ Radicals," *J. Phys. Chem. A*, 119, 10553 (2015). doi: [10.1021/acs.jpca.5b08331](https://doi.org/10.1021/acs.jpca.5b08331)
320. M. Lessio and E. A. Carter, "What is the Role of Pyridinium in Pyridine-Catalyzed CO₂ Reduction on p-GaP Photocathodes?," *J. Am. Chem. Soc.*, 137, 13248 (2015). doi: [10.1021/jacs.5b08639](https://doi.org/10.1021/jacs.5b08639)
319. J. Xia and E. A. Carter, "Reply to Comment on 'Single-point kinetic energy density functionals: a pointwise kinetic energy density analysis and numerical convergence investigation,'" *Phys. Rev. B*, 91, 045124 (2015), *Phys. Rev. B*, 92, 117102 (2015). doi: [10.1103/PhysRevB.92.117102](https://doi.org/10.1103/PhysRevB.92.117102)
318. C. X. Kronawitter, M. Lessio, P. Zhao, C. Riplinger, J. A. Boscoboinik, D. Starr, P. Sutter, E. A. Carter, and B. E. Koel, "Observation of surface-bound negatively charged hydride and hydroxide on GaP(110) in H₂O environments," *J. Phys. Chem. C*, 119, 17762 (2015). doi: [10.1021/acs.jpcc.5b05361](https://doi.org/10.1021/acs.jpcc.5b05361)
317. M. Chen, J. R. Vella, F. H. Stillinger, E. A. Carter, A. Z. Panagiotopoulos, and P. G. Debenedetti, "Liquid Li Structure and Dynamics: A Comparison Between OFDFT and Second Nearest-Neighbor Embedded-Atom Method," *AIChE Journal*, 6, 2841 (2015). doi: [10.1002/aic.14795](https://doi.org/10.1002/aic.14795)
316. N. Alidoust and E. A. Carter, "First-principles assessment of hole transport in pure and Li-doped NiO," *Phys. Chem. Chem. Phys.*, 17, 18098 (2015). doi: [10.1039/C5CP03429A](https://doi.org/10.1039/C5CP03429A)
315. K. Yu, F. Libisch, and E. A. Carter, "Implementation of density functional embedding theory within the projector-augmented-wave method and applications to semiconductor defect states," *J. Chem. Phys.*, 143, 102806 (2015). doi: [10.1063/1.4922260](https://doi.org/10.1063/1.4922260)
314. T. Tan, X. Yang, C. M. Krauter, Y. Ju, and E. A. Carter, "Ab Initio Kinetics of Hydrogen Abstraction from Methyl Acetate by Hydrogen, Methyl, Oxygen, Hydroxyl, and Hydroperoxy Radicals," *J. Phys. Chem. A*, 119, 6377 (2015). doi: [10.1021/acs.jpca.5b03506](https://doi.org/10.1021/acs.jpca.5b03506)

313. M. C. Toroker and E. A. Carter, "Strategies to suppress cation vacancies in metal oxide alloys: consequences for solar energy conversion," *J. Mat. Sci.*, 50, 5715 (2015). doi: [10.1007/s10853-015-9113-y](https://doi.org/10.1007/s10853-015-9113-y)
312. D. B. Krisiloff, J. M. Dieterich, F. Libisch, and E. A. Carter, "Numerical Challenges in a Cholesky-Decomposed Local Correlation Quantum Chemistry Framework," in "Mathematical and Computational Modeling: With Applications in the Natural and Social Sciences, Engineering, and the Arts," pp. 59-91, R. Melnick, Ed. (John Wiley & Sons, Inc.), ISBN: 978-1118853986 (2015). <http://www.wiley.com/WileyCDA/WileyTitle/productCd-1118853989.html>
311. C. Riplinger and E. A. Carter, "Cooperative effects in water binding to cuprous oxide surfaces," *J. Phys. Chem. C*, 119, 9311 (2015). doi: [10.1021/acs.jpcc.5b00383](https://doi.org/10.1021/acs.jpcc.5b00383)
310. K. Yu and E. A. Carter, "A Strategy to Stabilize Kesterite CZTS for High-Performance Solar Cells," *Chem. Mater.*, 27, 2920 (2015). doi: [10.1021/acs.chemmater.5b00172](https://doi.org/10.1021/acs.chemmater.5b00172)
309. J. Cheng, F. Libisch, and E. A. Carter, "Dissociative Adsorption of O₂ on Al(111): the Role of Orientational Degrees of Freedom," *J. Phys. Chem. Lett.*, 6, 1661 (2015). doi: [10.1021/acs.jpcclett.5b00597](https://doi.org/10.1021/acs.jpcclett.5b00597)
308. V. B. Oyeyemi, J. M. Dieterich, D. B. Krisiloff, T. Tan, and E. A. Carter, "Bond dissociation energies of C10 and C18 methyl esters from local multireference averaged-coupled pair functional theory," *J. Phys. Chem. A*, 119, 3429 (2015). doi: [10.1021/jp512974k](https://doi.org/10.1021/jp512974k)
307. M. Chen, J. Xia, C. Huang, J. M. Dieterich, L. Hung, I. Shin, and E. A. Carter, "Introducing PROFESS 3.0: An advanced program for orbital-free density functional theory molecular dynamics simulations," *Comp. Phys. Comm.*, 190, 228 (2015). doi: [10.1016/j.cpc.2014.12.021](https://doi.org/10.1016/j.cpc.2014.12.021)
306. C. Riplinger and E. A. Carter, "Influence of Weak Brønsted Acids on Electrocatalytic CO₂ Reduction by Manganese and Rhenium Bipyridine Catalysts," *ACS Catal.*, 5, 900 (2015). doi: [10.1021/cs501687n](https://doi.org/10.1021/cs501687n)
305. J. A. Keith, A. B. Muñoz-García, M. Lessio, and E. A. Carter, "Cluster Models for Studying CO₂ Reduction on Semiconductor Photoelectrodes," *Top. Catal.*, 58, 46 (2015). doi: [10.1007/s11244-014-0341-1](https://doi.org/10.1007/s11244-014-0341-1)
304. J. Xia and E. A. Carter, "Single-Point Kinetic Energy Density Functionals Based on a Pointwise Kinetic Energy Density Analysis," *Phys. Rev. B*, 91, 045124, (2015). doi: [10.1103/PhysRevB.91.045124](https://doi.org/10.1103/PhysRevB.91.045124)
303. X. Yang, D. Felsmann, N. Kurimoto, J. Krüger, T. Wada, T. Tan, E. A. Carter, K. Kohse-Höinghaus, and Y. Ju, "Kinetic studies of methyl acetate pyrolysis and oxidation in a flow reactor and a low-pressure flat flame using molecular-beam mass spectrometry," *Proceedings of the Combustion Institute*, 35, 491 (2015). doi: [10.1016/j.proci.2014.05.058](https://doi.org/10.1016/j.proci.2014.05.058)
302. J. M. Dieterich and E. A. Carter, "Assessment of a semi integral-direct local multi-reference configuration interaction implementation employing shared-memory parallelization," *Comp. Theor. Chem.*, 1051, 47 (2015). (Editor's Choice) doi: [10.1016/j.comptc.2014.10.030](https://doi.org/10.1016/j.comptc.2014.10.030)

301. C. Riplinger, M. D. Sampson, A. M. Ritzmann, C. P. Kubiak, and E. A. Carter, "Mechanistic Contrasts between Manganese and Rhenium Bipyridine Electrocatalysts for the Reduction of Carbon Dioxide," *J. Am. Chem. Soc.*, 136, 16285 (2014). [doi: 10.1021/ja508192y](https://doi.org/10.1021/ja508192y)
300. A. B. Muñoz-García, A. M. Ritzmann, M. Pavone, J. A. Keith, and E. A. Carter, "Oxygen transport in perovskite-type solid oxide fuel cell materials: insights from quantum mechanics," *Acc. Chem. Res.*, 47, 3340 (2014). [doi: 10.1021/ar4003174](https://doi.org/10.1021/ar4003174)
299. J. M. Dieterich, D. B. Krisiloff, A. Gaenko, F. Libisch, T. Windus, M. S. Gordon, and E. A. Carter, "Shared-memory parallelization of a local correlation multi-reference CI program," *Comput. Phys. Commun.*, 185, 3175 (2014). [doi: 10.1016/j.cpc.2014.08.016](https://doi.org/10.1016/j.cpc.2014.08.016)
298. C. X. Kronawitter, C. Riplinger, X. He, P. Zahl, E. A. Carter, P. Sutter, and B. E. Koel, "Hydrogen-bonded cyclic water clusters nucleated on an oxide surface," *J. Am. Chem. Soc.*, 136, 13283 (2014). [doi: 10.1021/ja5056214](https://doi.org/10.1021/ja5056214)
297. F. Libisch, C. Huang, and E. A. Carter, "Embedded Correlated Wavefunction Schemes: Theory and Applications," *Acc. Chem. Res.*, 47, 2768 (2014). (Cover Article) [doi: 10.1021/ar500086h](https://doi.org/10.1021/ar500086h)
296. C. X. Kronawitter, I. Zegkinoglou, S.-H. Shen, P. Liao, I. S. Cho, O. Zandi, K. Lashgari, G. Westin, J.-H. Guo, F. J. Himpsel, E. A. Carter, X. L. Zheng, T. W. Hamann, B. E. Koel, S. S. Mao, and L. Vayssieres, "Titanium Incorporation into Hematite Photoelectrodes: Theoretical Considerations and Experimental Observations," *Energy Environ. Sci.*, 7, 3100 (2014). [doi: 10.1039/C4EE01066C](https://doi.org/10.1039/C4EE01066C)
295. V. B. Oyeyemi, J. A. Keith, and E. A. Carter, "Accurate bond energies of biodiesel methyl esters from multireference averaged coupled-pair functional calculations," *J. Phys. Chem. A*, 118, 7392 (2014). [doi: 10.1021/jp412727w](https://doi.org/10.1021/jp412727w)
294. S. Suthirakun, S. Cheetu Ammal, A. B. Muñoz-García, G. Xiao, F. Chen, H.-C. zur Loye, E. A. Carter, and A. Heyden, "Theoretical Investigation of H₂ Oxidation on the Sr₂Fe_{1.5}Mo_{0.5}O₆ (001) Perovskite Surface under Anodic Solid Oxide Fuel Cell Conditions," *J. Am. Chem. Soc.*, 136 8374 (2014). [doi: 10.1021/ja502629j](https://doi.org/10.1021/ja502629j)
293. N. Alidoust, M. C. Toroker, and E. A. Carter, "Revisiting photoemission and inverse photoemission spectra of nickel oxide from first principles: implications for solar energy conversion," *J. Phys. Chem. B*, 118, 7963 (2014). [doi: 10.1021/jp500878s](https://doi.org/10.1021/jp500878s)
292. M. Pavone, A. B. Muñoz-García, A. M. Ritzmann, and E. A. Carter, "First-Principles Study of Lanthanum Strontium Manganite: Insights into Electronic Structure and Oxygen Vacancy Formation," *J. Phys. Chem. C*, 118, 13346 (2014). [doi: 10.1021/jp500352h](https://doi.org/10.1021/jp500352h)
291. I. Shin and E. A. Carter, "Simulations of Dislocation Mobility in Magnesium from First Principles," *Int. J. Plasticity*, 60, 58 (2014). [doi: 10.1016/j.ijplas.2014.04.002](https://doi.org/10.1016/j.ijplas.2014.04.002)
290. V. B. Oyeyemi, J. A. Keith, and E. A. Carter, "Trends in Bond Dissociation Energies of Alcohols and Aldehydes Computed with Multireference Averaged Coupled-Pair Functional Theory," *J. Phys. Chem. A*, 118, 3039 (2014). [doi: 10.1021/jp501636r](https://doi.org/10.1021/jp501636r)

289. A. M. Ritzmann, M. Pavone, A. B. Muñoz-García, J. A. Keith, and E. A. Carter, "Ab Initio DFT+U Analysis of Oxygen Transport in LaCoO₃: The Effect of Co³⁺ Magnetic States," *J. Mater. Chem. A*, 2, 8060 (2014). doi: [10.1039/C4TA00801D](https://doi.org/10.1039/C4TA00801D)
288. I. Shin and E. A. Carter, "Enhanced von Weizsäcker Wang-Govind-Carter Kinetic Energy Density Functional for Semiconductors," *J. Chem. Phys.*, 140, 18A531 (2014). doi: [10.1063/1.4869867](https://doi.org/10.1063/1.4869867)
287. Y. Ke, F. Libisch, J. Xia, and E. A. Carter, "Angular Momentum Dependent Orbital Free Density Functional Theory: Formulation and Implementation," *Phys. Rev. B*, 89, 155112 (2014). doi: [10.1103/PhysRevB.89.155112](https://doi.org/10.1103/PhysRevB.89.155112)
286. C. Huang, F. Libisch, Q. Peng, and E. A. Carter, "Time-dependent potential-functional embedding theory," *J. Chem. Phys.*, 140, 124113 (2014). doi: [10.1063/1.4869538](https://doi.org/10.1063/1.4869538)
285. K. Yu and E. A. Carter, "Communication: Comparing *Ab initio* Methods of Obtaining Effective U Parameters for Closed-Shell Materials," *J. Chem. Phys.*, 140, 121105 (2014). doi: [10.1063/1.4869718](https://doi.org/10.1063/1.4869718)
284. D. K. Kanan, J. A. Keith, and E. A. Carter, "First Principles Modeling of Electrochemical Water Oxidation on MnO:ZnO(001)," *ChemElectroChem*, 1, 407 (2014). doi: [10.1002/celec.201300089](https://doi.org/10.1002/celec.201300089)
283. L. Isseroff Bendavid and E. A. Carter, "Status in Calculating Electronic Excited States in Transition Metal Oxides from First Principles," in *Topics in Current Chemistry*, Vol. 347, pp. 47-98, C. Di Valentin, S. Botti, and M. Cococcioni, Eds. (Springer, Germany), ISBN: 978-3-642-55067-6 (2014). doi: [10.1007/128_2013_503](https://doi.org/10.1007/128_2013_503)
282. V. B. Oyeyemi, D. B. Krisiloff, J. A. Keith, F. Libisch, M. Pavone, and E. A. Carter, "Size-extensivity-corrected multireference configuration interaction schemes to accurately predict bond dissociation energies of oxygenated hydrocarbons," *J. Chem. Phys.*, 140, 044317 (2014). doi: [10.1063/1.4862159](https://doi.org/10.1063/1.4862159)
281. N. Alidoust, M. C. Toroker, J. A. Keith, and E. A. Carter, "Significant Reduction in Nickel(II) Oxide Band Gap Upon Alloying with Lithium Oxide: Applications to Solar Energy Conversion," *ChemSusChem*, 7, 195 (2014). doi: [10.1002/cssc.201300595](https://doi.org/10.1002/cssc.201300595)
280. J. Xia and E. A. Carter, "Orbital-Free Density Functional Theory Study of Crystalline Li-Si Alloys," *J. Power Sources*, 254, 62 (2014). doi: [10.1016/j.jpowsour.2013.12.097](https://doi.org/10.1016/j.jpowsour.2013.12.097)
279. D. B. Krisiloff, V. B. Oyeyemi, F. Libisch, and E. A. Carter, "Analysis of and remedies for unphysical ground states of the Multireference Averaged Coupled-Pair Functional," *J. Chem. Phys.*, 140, 024102 (2014). doi: [10.1063/1.4861035](https://doi.org/10.1063/1.4861035)
278. I. Shin and E. A. Carter, "First-Principles Simulations of Plasticity in BCC Magnesium-Lithium Alloys," *Acta Materialia*, 64, 198 (2014). doi: [10.1016/j.actamat.2013.10.030](https://doi.org/10.1016/j.actamat.2013.10.030)
277. L. Isseroff Bendavid and E. A. Carter, "CO₂ Adsorption on Cu₂O(111): A DFT+U and DFT-D study," *J. Phys. Chem. C*, 117, 26048 (2013). doi: [10.1021/jp407468t](https://doi.org/10.1021/jp407468t)

276. L. Isseroff Bendavid and E. A. Carter, "First Principles Predictions of the Structure, Stability, and Photocatalytic Potential of Cu₂O Surfaces," *J. Phys. Chem. B*, 117, 15750 (2013). doi: [10.1021/jp406454c](https://doi.org/10.1021/jp406454c)
275. M. Chen, L. Hung, C. Huang, J. Xia, and E. A. Carter, "The Melting Point of Lithium: An Orbital-Free First-Principles Molecular Dynamics Study," *Molecular Physics*, 111, 3448 (2013). doi: [10.1080/00268976.2013.828379](https://doi.org/10.1080/00268976.2013.828379)
274. J. A. Keith and E. A. Carter, "Theoretical Insights into Electrochemical CO₂ Reduction Mechanisms Catalyzed by Surface Bound Nitrogen Heterocycles," *J. Phys. Chem. Lett.*, 4, 4058 (2013). doi: [10.1021/jz4021519](https://doi.org/10.1021/jz4021519); Correction: *J. Phys. Chem. Lett.*, 6, 568 (2015). doi: [10.1021/acs.jpcclett.5b00170](https://doi.org/10.1021/acs.jpcclett.5b00170)
273. F. Libisch, J. Cheng, and E. A. Carter, "Electron-Transfer-Induced Dissociation of H₂ on Gold Nanoparticles: Excited-State Potential Energy Surfaces via Embedded Correlated Wavefunction Theory," *Z. Phys. Chem.*, 227, 1455 (2013). doi: [10.1524/zpch.2013.0406](https://doi.org/10.1524/zpch.2013.0406)
272. J. A. Keith, K. A. Grice, C. P. Kubiak, and E. A. Carter, "Elucidation of the Selectivity of Proton-Dependent Electrocatalytic CO₂ Reduction by *fac*-Re(bpy)(CO)₃Cl," *J. Am. Chem. Soc.*, 135, 15823 (2013). doi: [10.1021/ja406456g](https://doi.org/10.1021/ja406456g)
271. L. Isseroff Bendavid and E. A. Carter, "First Principles Study of Bonding, Adhesion, and Electronic Structure at the Cu₂O(111)/ZnO(1010) Interface," *Surf. Sci.*, 618, 62 (2013). doi: [10.1016/j.susc.2013.07.027](https://doi.org/10.1016/j.susc.2013.07.027)
270. A. M. Ritzmann, A. B. Muñoz-García, M. Pavone, J. A. Keith, and E. A. Carter, "Ab Initio Evaluation of Oxygen Diffusivity in LaFeO₃: The Role of Lanthanum Vacancies," *MRS Communications*, 3, 161 (2013). doi: [10.1557/mrc.2013.28](https://doi.org/10.1557/mrc.2013.28)
269. D. K. Kanan, J. A. Keith, and E. A. Carter, "Water Adsorption on MnO:ZnO(001) – From Single Molecules to Bilayer Coverage," *Surf. Sci.*, 617, 218 (2013). doi: [10.1016/j.susc.2013.07.023](https://doi.org/10.1016/j.susc.2013.07.023)
268. I. Shin and E. A. Carter, "Possible Origin of the Discrepancy in the Peierls Stresses of FCC Metals: First-Principles Simulations of Dislocation Mobility in Aluminum," *Phys. Rev. B*, 88, 064106 (2013). doi: [10.1103/PhysRevB.88.064106](https://doi.org/10.1103/PhysRevB.88.064106)
267. Y. Ke, F. Libisch, J. Xia, L.-W. Wang, and E. A. Carter, "Angular Momentum Dependent Orbital Free Density Functional Theory," *Phys. Rev. Lett.*, 111, 066402 (2013). doi: [10.1103/PhysRevLett.111.066402](https://doi.org/10.1103/PhysRevLett.111.066402)
266. A. M. Ritzmann, A. B. Muñoz-García, M. Pavone, J. A. Keith, and E. A. Carter, "Ab initio DFT+U Analysis of Oxygen Vacancy Formation and Migration in La_{1-x}Sr_xFeO_{3-δ} (x=0, 0.25, 0.50)," *Chem. Mater.*, 25, 3011 (2013). doi: [10.1021/cm401052w](https://doi.org/10.1021/cm401052w)
265. D. K. Kanan and E. A. Carter, "Optical Excitations in MnO and MnO:ZnO via Embedded CASPT2 Theory and their Implications for Solar Energy Conversion," *J. Phys. Chem. C*, 117, 13816 (2013). doi: [10.1021/jp4024475](https://doi.org/10.1021/jp4024475)
264. D. K. Kanan and E. A. Carter, "Ab Initio Study of Electron and Hole Transport in Pure and Doped MnO and MnO:ZnO Alloy," *J. Mater. Chem. A*, 1, 9246 (2013). doi: [10.1039/C3TA11265A](https://doi.org/10.1039/C3TA11265A)

263. E. E. Benson, M. D. Sampson, K. A. Grice, J. M. Smieja, J. D. Froehlich, D. Friebe, J. A. Keith, E. A. Carter, A. Nilsson, and C. P. Kubiak, "The Electronic States of Rhenium Bipyridyl Electrocatalysts for CO₂ Reduction as Revealed by X-Ray Absorption Spectroscopy and Computational Quantum Chemistry," *Angew. Chem. Int. Ed.*, 52, 4841 (2013). doi: [10.1002/anie.201209911](https://doi.org/10.1002/anie.201209911)
262. A. B. Muñoz-García, M. Pavone, A. M. Ritzmann, and E. A. Carter, "Oxide Ion Transport in Sr₂Fe_{1.5}Mo_{0.5}O_{6.8}, a Mixed Ion-Electron Conductor: New Insights from First Principles Modeling," *Phys. Chem. Chem. Phys.*, 15, 6250 (2013). doi: [10.1039/C3CP50995H](https://doi.org/10.1039/C3CP50995H)
261. J. A. Keith and E. A. Carter, "Electrochemical Reactivities of Pyridinium in Solution: Consequences for CO₂ Reduction Mechanisms," *Chem. Sci.*, 4, 1490 (2013). doi: [10.1063/1.454099](https://doi.org/10.1063/1.454099)
260. P. Liao and E. A. Carter, "New Concepts and Modeling Strategies to Design and Evaluate Photo-electro-catalysts Based on Transition Metal Oxides," *Chem. Soc. Rev.*, 42, 2401 (2013). doi: [10.1039/C2CS35267B](https://doi.org/10.1039/C2CS35267B)
259. L. Y. Isseroff and E. A. Carter, "Electronic Structure of Pure and Doped Cuprous Oxide with Copper Vacancies: Suppression of Trap States," *Chem. Mater.*, 25, 253 (2013). doi: [10.1021/cm3040278](https://doi.org/10.1021/cm3040278)
258. M. C. Toroker and E. A. Carter, "Transition Metal Oxide Alloys as Potential Solar Energy Conversion Materials," *J. Mater. Chem. A*, 1, 2474 (2013). ("Hot Article") doi: [10.1039/C2TA00816E](https://doi.org/10.1039/C2TA00816E)
257. S. Mukherjee, F. Libisch, N. Large, O. Neumann, L. V. Brown, J. Cheng, J. B. Lassiter, E. A. Carter, P. Nordlander, and N. J. Halas, "Hot Electrons Do the Impossible: Plasmon-Induced Dissociation of H₂ on Au," *Nano Letters*, 13, 240 (2013). doi: [10.1021/nl303940z](https://doi.org/10.1021/nl303940z)
256. J. Xia and E. A. Carter, "Density-Decomposed Orbital-Free Density Functional Theory for Covalently Bonded Molecules and Materials," *Phys. Rev. B*, 86, 235109 (2012). doi: [10.1103/PhysRevB.86.235109](https://doi.org/10.1103/PhysRevB.86.235109)
255. F. Libisch, C. Huang, P. Liao, M. Pavone, and E. A. Carter, "Origin of the Energy Barrier to Chemical Reactions of O₂ on Al(111): Evidence for Charge Transfer, Not Spin Selection," *Phys. Rev. Lett.*, 109, 198303 (2012). doi: [10.1103/PhysRevLett.109.198303](https://doi.org/10.1103/PhysRevLett.109.198303)
254. J. A. Keith and E. A. Carter, "Quantum Chemical Benchmarking, Validation, and Prediction of Acidity Constants for Substituted Pyridinium Ions and Pyridinyl Radicals," *J. Chem. Theor. Comp.*, 8, 3187 (2012). doi: [10.1021/ct300295g](https://doi.org/10.1021/ct300295g)
253. A. B. Muñoz-García and E. A. Carter, "Non-innocent Dissociation of H₂O on GaP(110): Implications for Electrochemical Reduction of CO₂," *J. Am. Chem. Soc.*, 134, 13600 (2012). (Highlighted Article) doi: [10.1021/ja3063106](https://doi.org/10.1021/ja3063106)
252. T. Tan, M. Pavone, D. B. Krisiloff, and E. A. Carter, "Ab Initio Reaction Kinetics of Hydrogen Abstraction from Methyl Formate by Hydrogen, Methyl, Oxygen, Hydroxyl, and Hydroperoxy Radicals," *J. Phys. Chem. A*, 116, 8431 (2012). doi: [10.1021/jp304811z](https://doi.org/10.1021/jp304811z); Correction: *J. Phys. Chem. A*, 119, 2186 (2015). doi: [10.1021/acs.jpca.5b01185](https://doi.org/10.1021/acs.jpca.5b01185)

251. M. C. Toroker and E. A. Carter, "Hole Transport in Non-Stoichiometric and Doped Wüstite," *J. Phys. Chem. C*, 116, 17403 (2012). doi: [10.1021/ja301567f](https://doi.org/10.1021/ja301567f)
250. P. Liao, J. A. Keith, and E. A. Carter, "Water Oxidation on Pure and Doped Hematite (0001) Surfaces: Prediction of Co and Ni as Effective Dopants for Photocatalysis," *J. Am. Chem. Soc.*, 134, 13296 (2012). doi: [10.1021/ja301567f](https://doi.org/10.1021/ja301567f)
249. P. Liao and E. A. Carter, "Hole Transport in Pure and Doped Hematite," *J. Appl. Phys.*, 112, 013701 (2012). doi: [10.1063/1.4730634](https://doi.org/10.1063/1.4730634)
248. L. Y. Isseroff and E. A. Carter, "Importance of Reference Hamiltonians Containing Exact Exchange for Accurate One-Shot GW Calculations of Cu_2O ," *Phys. Rev. B*, 85, 235142 (2012). doi: [10.1103/PhysRevB.85.235142](https://doi.org/10.1103/PhysRevB.85.235142)
247. J. A. Keith and E. A. Carter, "Theoretical Insights into Pyridinium-Based Photoelectrocatalytic Reduction of CO_2 ," *J. Am. Chem. Soc.*, 134, 7580 (2012). doi: [10.1021/ja300128e](https://doi.org/10.1021/ja300128e); Erratum: *J. Am. Chem. Soc.*, 135, 7386 (2013). doi: [10.1021/ja402838u](https://doi.org/10.1021/ja402838u)
246. D. K. Kanan and E. A. Carter, "Band Gap Engineering of MnO via ZnO Alloying: A Potential New Visible-Light Photocatalyst," *J. Phys. Chem. C*, 116, 9876 (2012). doi: [10.1021/jp300590d](https://doi.org/10.1021/jp300590d)
245. D. B. Krisiloff and E. A. Carter, "Approximately Size Extensive Local Multireference Singles and Doubles Configuration Interaction," *Phys. Chem. Chem. Phys.*, 14, 7710 (2012). doi: [10.1039/C2CP23757A](https://doi.org/10.1039/C2CP23757A)
244. A. B. Muñoz-García, D. E. Bugaris, M. Pavone, J. P. Hodges, A. Huq, F. Chen, H.-C. zur Loye, and E. A. Carter, "Unveiling Structure-Property Relationships in $\text{Sr}_2\text{Fe}_{1.5}\text{Mo}_{0.5}\text{O}_{6-\delta}$, an Electrode Material for Symmetric Solid Oxide Fuel Cells," *J. Am. Chem. Soc.*, 134, 6826 (2012). doi: [10.1021/ja300831k](https://doi.org/10.1021/ja300831k)
243. J. Xia, C. Huang, I. Shin and E. A. Carter, "Can Orbital-Free Density Functional Theory Simulate Molecules?" *J. Chem. Phys.*, 136, 084102 (2012). (Cover Article) doi: [10.1063/1.3685604](https://doi.org/10.1063/1.3685604)
242. C. Huang and E. A. Carter, "Toward an Orbital-free Density Functional Theory of Transition Metals Based on an Electron Density Decomposition," *Phys. Rev. B*, 85, 045126 (2012). doi: [10.1103/PhysRevB.85.045126](https://doi.org/10.1103/PhysRevB.85.045126)
241. L. Hung, C. Huang, and E. A. Carter, "Preconditioners and Electron Density Optimization in Orbital-Free Density Functional Theory," *Comm. Comp. Phys.*, 12, 135 (2012). doi: [10.4208/cicp.190111.090911a](https://doi.org/10.4208/cicp.190111.090911a)
240. V. Oyeyemi, J. A. Keith, M. Pavone and E. A. Carter, "Insufficient Hartree-Fock Exchange in Hybrid DFT Functionals Produces Bent Alkynyl Radical Structures," *J. Phys. Chem. Lett.*, 3, 289 (2012). doi: [10.1021/jz201564g](https://doi.org/10.1021/jz201564g)
239. D. K. Kanan, S. Sharifzadeh and E. A. Carter, "Quantum Mechanical Modeling of Electronic Excitations in Metal Oxides: Magnesia as a Prototype," *Chem. Phys. Lett.*, 519, 18 (2012). (Editor's Choice) doi: [10.1016/j.cplett.2011.11.003](https://doi.org/10.1016/j.cplett.2011.11.003)
238. I. Shin and E. A. Carter, "Orbital-Free Density Functional Theory Simulations of Dislocations in Magnesium," *Modell. Simul. Mater. Sci. Eng.*, 20, 015006 (2012). (Cover Article) doi: [10.1088/0965-0393/20/1/015006](https://doi.org/10.1088/0965-0393/20/1/015006)

237. V. B. Oyeyemi, M. Pavone and E. A. Carter, "Accurate Bond Energies of Hydrocarbons from Complete Basis Set Extrapolated Multi-Reference Singles and Doubles Configuration Interaction," *ChemPhysChem*, 12, 3354 (2011).
[doi: 10.1002/cphc.201100447](https://doi.org/10.1002/cphc.201100447)
236. M. Pavone, A. M. Ritzmann and E. A. Carter, "Quantum-Mechanics-Based Design Principles for Solid Oxide Fuel Cell Cathode Materials," *Energy Environ. Sci.*, 4, 4933 (2011). [doi: 10.1039/C1EE02377B](https://doi.org/10.1039/C1EE02377B)
235. P. Liao and E. A. Carter, "Optical Excitations in Hematite (α -Fe₂O₃) Via Embedded Cluster Models: A CASPT2 Study," *J. Phys. Chem. C*, 115, 20795 (2011). [doi: 10.1021/jp206991v](https://doi.org/10.1021/jp206991v)
234. C. Huang and E. A. Carter, "Direct Minimization of the Optimized Effective Problem Based on Efficient Finite Differences," *Phys. Rev. B*, 84, 165122 (2011).
[doi: 10.1103/PhysRevB.84.165122](https://doi.org/10.1103/PhysRevB.84.165122)
233. C. Huang and E. A. Carter, "Potential-Functional Embedding Theory for Molecules and Materials," *J. Chem. Phys.*, 135, 194104 (2011). (Editor's Choice, Highlighted Article "Journal of Chemical Physics 80th Anniversary Collection")
[doi: 10.1063/1.3659293](https://doi.org/10.1063/1.3659293)
232. A. B. Muñoz-García, M. Pavone and E. A. Carter, "Effect of Antisite Defects on the Formation of Oxygen Vacancies in Sr₂FeMoO₆: Implications for Ion and Electron Transport," *Chem. Mater.*, 23, 4525 (2011). [doi: 10.1021/cm201799c](https://doi.org/10.1021/cm201799c)
231. M. Caspary Toroker, D. K. Kanan, N. Alidoust, L. Y. Isseroff, P. Liao and E. A. Carter, "First Principles Scheme to Evaluate Band Edge Positions in Potential Transition Metal Oxide Photocatalysts and Photoelectrodes," *Phys. Chem. Chem. Phys.*, 13, 16644 (2011). [doi: 10.1039/c1cp22128k](https://doi.org/10.1039/c1cp22128k)
230. P. Liao and E. A. Carter, "Testing Variations of the GW Approximation on Strongly Correlated Transition Metal Oxides: Hematite (α -Fe₂O₃) as a Benchmark," *Phys. Chem. Chem. Phys.*, 13, 15189 (2011). [doi: 10.1039/c1cp20829b](https://doi.org/10.1039/c1cp20829b)
229. L. Hung and E. A. Carter, "Ductile Processes at Aluminum Crack Tips: Comparison of Orbital-Free Density Functional Theory with Classical Potential Predictions," *Modell. Simul. Mater. Sci. Eng.*, 19, 045002 (2011).
[doi: 10.1088/0965-0393/19/4/045002](https://doi.org/10.1088/0965-0393/19/4/045002)
228. C. Huang, M. Pavone, and E. A. Carter, "Quantum Mechanical Embedding Theory Based on a Unique Embedding Potential," *J. Chem. Phys.*, 134, 154110 (2011).
[doi: 10.1063/1.3577516](https://doi.org/10.1063/1.3577516)
227. K. A. Marino, B. Hinnemann, and E. A. Carter, "Atomic-scale Insight and Design Principles For Turbine Engine Thermal Barrier Coatings From Theory," *Proc. Natl. Acad. Sci. U.S.A.*, 108, 5480 (2011). (Highlighted Article "From the Cover")
[doi: 10.1073/pnas.1102426108](https://doi.org/10.1073/pnas.1102426108)
226. P. Liao, M. Caspary Toroker, and E. A. Carter, "Electron Transport in Pure and Doped Hematite," *Nano Letters*, 11, 1775 (2011). [doi: 10.1149/1.2127253](https://doi.org/10.1149/1.2127253)
225. L. Hung and E. A. Carter, "Orbital-Free DFT Simulations of Elastic Response and Tensile Yielding of Ultrathin [111] Al Nanowires," *J. Phys. Chem. C*, 115, 6269 (2011). [doi: 10.1021/jp112196t](https://doi.org/10.1021/jp112196t)

224. I. Milas, B. Hinnemann, and E. A. Carter, "Diffusion of Al, O, Pt, Hf, and Y atoms on α -Al₂O₃(0001): Implications for the role of alloying elements in thermal barrier coatings," *J. Mater. Chem.*, 21, 1447 (2011). doi: [10.1039/C0JM02212H](https://doi.org/10.1039/C0JM02212H)
223. T. S. Chwee and E. A. Carter, "Valence Excited States in Large Molecules via Local Multireference Singles and Doubles Configuration Interaction," *J. Chem. Theory Comput.*, 7, 103 (2011). doi: [10.1021/ct100486q](https://doi.org/10.1021/ct100486q)
222. T. S. Chwee and E. A. Carter, "Density Fitting of Two-Electron Integrals in Local Multireference Single and Double Excitation Configuration Interaction Calculations," *Molecular Physics*, 108, 2519 (2010). doi: [10.1080/00268976.2010.508052](https://doi.org/10.1080/00268976.2010.508052)
221. L. Hung, C. Huang, I. Shin, G. Ho, V. L. Ligneres, and E. A. Carter, "Introducing PROFESS 2.0: a parallelized, fully linear scaling program for orbital-free density functional theory calculations," *Comput. Phys. Commun.*, 181, 2208 (2010). doi: [10.1016/j.cpc.2010.09.001](https://doi.org/10.1016/j.cpc.2010.09.001)
220. P. Liao and E. A. Carter, "Ab initio DFT+U predictions of the shear response of iron oxides," *Acta Materialia*, 58, 5912 (2010). doi: [10.1016/j.actamat.2010.07.007](https://doi.org/10.1016/j.actamat.2010.07.007)
219. Q. Peng, X. Zhang, C. Huang, E. A. Carter, and G. Lu, "Quantum Mechanical Study of Solid Solution Effects on Dislocation Nucleation During Nanoindentation," *Modell. Simul. Mater. Sci. Eng.*, 18, 075003 (2010). doi: [10.1088/0965-0393/18/7/075003](https://doi.org/10.1088/0965-0393/18/7/075003)
218. P. Liao and E. A. Carter, "Ab initio DFT+U predictions of tensile properties of iron oxides," *J. Mater. Chem.*, 20, 6703 (2010). doi: [10.1039/C0JM01199A](https://doi.org/10.1039/C0JM01199A)
217. K. A. Marino and E. A. Carter, "Ni and Al diffusion in Ni-rich NiAl and the effect of Pt additions," *Intermetallics*, 18, 1470 (2010). doi: [10.1016/j.intermet.2010.03.044](https://doi.org/10.1016/j.intermet.2010.03.044)
216. D. F. Johnson and E. A. Carter, "First Principles Assessment of Carbon Absorption into FeAl and Fe₃Si: Toward Prevention of Cementite Formation and Metal Dusting of Steels," *J. Phys. Chem. C*, 114, 4436 (2010). doi: [10.1021/jp907883h](https://doi.org/10.1021/jp907883h)
215. K. A. Marino and E. A. Carter, "The effect of platinum on Al diffusion kinetics in beta-NiAl: Implications for thermal barrier coating lifetime," *Acta Materialia*, 58, 2726 (2010). doi: [10.1016/j.actamat.2010.01.008](https://doi.org/10.1016/j.actamat.2010.01.008)
214. T. S. Chwee and E. A. Carter, "Cholesky Decomposition within Local Multireference Singles and Doubles Configuration Interaction," *J. Chem. Phys.*, 132, 074104 (2010). doi: [10.1063/1.3315419](https://doi.org/10.1063/1.3315419)
213. D. F. Johnson and E. A. Carter, "Hydrogen in Tungsten: Absorption, Diffusion, Vacancy Trapping, and Decohesion," *J. Mater. Res.*, 25, 315 (2010). doi: [10.1557/JMR.2010.0036](https://doi.org/10.1557/JMR.2010.0036)
212. C. Huang and E. A. Carter, "Nonlocal orbital-free kinetic energy density functional for semiconductors," *Phys. Rev. B*, 81, 045206 (2010). (Editor's Suggestion) doi: [10.1103/PhysRevB.81.045206](https://doi.org/10.1103/PhysRevB.81.045206)

211. D. F. Johnson and E. A. Carter, "First Principles Assessment of Hydrogen Absorption into FeAl and Fe₃Si: Towards Prevention of Steel Embrittlement," *Acta Materialia*, 58, 638 (2010). doi: [10.1016/j.actamat.2009.09.042](https://doi.org/10.1016/j.actamat.2009.09.042)
210. I. Shin, A. Ramasubramaniam, C. Huang, L. Hung, and E. A. Carter, "Orbital-Free Density Functional Theory Simulations of Dislocations in Aluminum," *Philos. Mag.*, 89, 3195 (2009). doi: [10.1080/14786430903246353](https://doi.org/10.1080/14786430903246353)
209. S. Sharifzadeh, P. Huang, and E. A. Carter, "Origin of Tunneling Lineshape Trends for Kondo States of Co Adatoms on Coinage Metal Surfaces," *J. Phys.: Condens. Matter*, 21, 355501 (2009). doi: [10.1088/0953-8984/21/35/355501](https://doi.org/10.1088/0953-8984/21/35/355501)
208. L. Hung and E. A. Carter, "Accurate Simulations of Metals at the Mesoscale: Explicit Treatment of 1 Million Atoms with Quantum Mechanics," *Chem. Phys. Lett.*, 475, 163 (2009). (Cover Article) doi: [10.1016/j.cplett.2009.04.059](https://doi.org/10.1016/j.cplett.2009.04.059)
207. J. Chai, V. L. Ligneres, G. Ho, E. A. Carter, and J. D. Weeks, "Orbital-Free Density Functional Theory: Linear Scaling Methods for Kinetic Potentials, and Applications to Solid Al and Si," *Chem. Phys. Lett.*, 473, 263 (2009). doi: [10.1016/j.cplett.2009.03.064](https://doi.org/10.1016/j.cplett.2009.03.064)
206. G. Ho and E. A. Carter, "Mechanical Response of Aluminum Nanowires via Orbital-Free Density Functional Theory," *J. Comput. Theor. Nanos.*, 6, 1236 (2009). (Cover Article) doi: [10.1166/jctn.2009.1172](https://doi.org/10.1166/jctn.2009.1172)
205. N. J. Mosey and E. A. Carter, "Shear Strength of Chromia across Multiple Length Scales from First Principles," *Acta Materialia*, 57, 2933 (2009). doi: [10.1016/j.actamat.2009.03.001](https://doi.org/10.1016/j.actamat.2009.03.001)
204. A. Ramasubramaniam, M. Itakura, and E. A. Carter, "Interatomic potentials for hydrogen in α -iron based on density functional theory," *Phys. Rev. B*, 79, 174101 (2009). doi: [10.1103/PhysRevB.79.174101](https://doi.org/10.1103/PhysRevB.79.174101); Erratum: *Phys. Rev. B*, 81, 099902(E), (2010). doi: [10.1103/PhysRevB.81.099902](https://doi.org/10.1103/PhysRevB.81.099902)
203. D. F. Johnson and E. A. Carter, "Structure and Adhesion of MoSi₂/Ni Interfaces: Evaluation of MoSi₂ as an Alternative Bond Coat Alloy," *Surf. Sci.*, 603, 1276 (2009). doi: [10.1016/j.susc.2009.03.018](https://doi.org/10.1016/j.susc.2009.03.018)
202. D. F. Johnson and E. A. Carter, "Bonding and Adhesion at the SiC/Fe Interface," *J. Phys. Chem. A*, 113, 4367 (2009). doi: [10.1021/jp8110259](https://doi.org/10.1021/jp8110259)
201. I. Milas and E. A. Carter, "Effect of Dopants on Alumina Grain Boundary Sliding: Implications for Creep Inhibition," *J. Mater. Sci.*, 44, 1741 (2009). doi: [10.1007/s10853-008-3191-z](https://doi.org/10.1007/s10853-008-3191-z)
200. S. Sharifzadeh, P. Huang, and E. A. Carter, "All-Electron Embedded Correlated Wavefunction Theory for Condensed Matter Electronic Structure," *Chem. Phys. Lett.*, 470, 347 (2009). doi: [10.1016/j.cplett.2009.01.072](https://doi.org/10.1016/j.cplett.2009.01.072)
199. K. A. Marino and E. A. Carter, "The effect of platinum on diffusion kinetics in β -NiAl: implications for thermal barrier coating lifetimes," *ChemPhysChem*, 10, 226 (2009). doi: [10.1002/cphc.200800528](https://doi.org/10.1002/cphc.200800528) Corrigendum: *ChemPhysChem*, 10, 2367 (2009). doi: [10.1002/cphc.200990058](https://doi.org/10.1002/cphc.200990058)

198. N. J. Mosey and E. A. Carter, "Ab initio LDA+U Prediction of the Tensile Properties of Chromia across Multiple Length Scales," *J. Mech. Phys. Solids*, 57, 287 (2009). [doi: 10.1016/j.jmps.2008.10.009](https://doi.org/10.1016/j.jmps.2008.10.009)
197. C. Huang and E. A. Carter, "Transferable local pseudopotentials for magnesium, aluminum and silicon," *Phys. Chem. Chem. Phys.*, 10, 7109 (2008). [doi: 10.1039/b810407g](https://doi.org/10.1039/b810407g)
196. K. A. Marino and E. A. Carter, "First-Principles Characterization of Ni Diffusion Kinetics in β -NiAl," *Phys. Rev. B*, 78, 184105 (2008). [doi: 10.1103/PhysRevB.78.184105](https://doi.org/10.1103/PhysRevB.78.184105); Erratum: *Phys. Rev. B*, 80, 069901(E), (2009). [doi: 10.1103/PhysRevB.80.069901](https://doi.org/10.1103/PhysRevB.80.069901)
195. G. Ho, V. L. Lignères, and E. A. Carter, "Introducing PROFESS: a new program for orbital-free density functional theory calculations," *Comput. Phys. Commun.*, 179, 839 (2008). [doi: 10.1016/j.cpc.2008.07.002](https://doi.org/10.1016/j.cpc.2008.07.002)
194. A. Ramasubramaniam, M. Itakura, M. Ortiz, and E. A. Carter, "The effect of atomic scale plasticity on hydrogen diffusion in iron: quantum mechanically informed and on-the-fly kinetic Monte Carlo simulations," *J. Mater. Res.*, 23, 2757 (2008). [doi: 10.1557/JMR.2008.0340](https://doi.org/10.1557/JMR.2008.0340)
193. G. Ho, C. Huang, and E. A. Carter, "Describing Metal Surfaces and Nanostructures with Orbital-Free Density Functional Theory," *Curr. Opin. Solid State Mater. Sci.*, 11, 57 (2008). [doi: 10.1016/j.cossms.2008.06.005](https://doi.org/10.1016/j.cossms.2008.06.005)
192. Q. Peng, X. Zhang, L. Hung, E. A. Carter, and G. Lu, "Quantum Simulation of Materials at Micron Scales and Beyond," *Phys. Rev. B*, 78, 054118 (2008). [doi: 10.1103/PhysRevB.78.054118](https://doi.org/10.1103/PhysRevB.78.054118)
191. E. A. Carter, "Challenges in Modeling Materials Properties without Experimental Input," *Science*, 321, 800 (2008). [doi: 10.1126/science.1158009](https://doi.org/10.1126/science.1158009)
190. K. A. Marino and E. A. Carter, "The effect of platinum on defect formation energies in β -NiAl," *Acta Materialia*, 56, 3502 (2008). [doi: 10.1016/j.actamat.2008.03.029](https://doi.org/10.1016/j.actamat.2008.03.029)
189. G. Ho, V. L. Lignères, and E. A. Carter, "Analytic form for a non-local kinetic energy functional with a density-dependent kernel for orbital-free density functional theory under periodic and Dirichlet boundary conditions," *Phys. Rev. B*, 78, 045105 (2008). [doi: 10.1103/PhysRevB.78.045105](https://doi.org/10.1103/PhysRevB.78.045105)
188. N. J. Mosey, P. Liao, and E. A. Carter, "Rotationally-Invariant ab initio Evaluation of Coulomb and Exchange Parameters for DFT + U Calculations," *J. Chem. Phys.*, 129, 014103 (2008). [doi: 10.1063/1.2943142](https://doi.org/10.1063/1.2943142)
187. T. S. Chwee, A. B. Szilva, R. Lindh, and E. A. Carter, "Linear Scaling Multireference Singles and Doubles Configuration Interaction," *J. Chem. Phys.*, 128, 224106 (2008). [doi: 10.1063/1.2937443](https://doi.org/10.1063/1.2937443)
186. I. Milas, B. Hinnemann, and E. A. Carter, "Structure of and Ion Segregation to an Alumina Grain Boundary: Implications for Growth and Creep," *J. Mater. Res.*, 23, 1494 (2008). [doi: 10.1557/JMR.2008.0188](https://doi.org/10.1557/JMR.2008.0188)

185. P. Huang and E. A. Carter, "Ab initio explanation of tunneling lineshapes for the Kondo impurity state," *Nano Letters*, 8, 1265 (2008). doi: [10.1021/nl0804203](https://doi.org/10.1021/nl0804203)
184. S. Sharifzadeh, P. Huang, and E. A. Carter, "Embedded configuration interaction description of CO on Cu(111): Resolution of the site preference conundrum," *J. Phys. Chem. C*, 112, 4649 (2008). doi: [10.1021/jp710890a](https://doi.org/10.1021/jp710890a)
183. A. Andersen and E. A. Carter, "First-Principles-Derived Kinetics of the Reactions Involved in Low-Temperature Dimethyl Ether Oxidation," *Molecular Physics*, 106, 367 (2008). doi: [10.1080/00268970701837008](https://doi.org/10.1080/00268970701837008); Erratum: *Molecular Physics*, 106, 963 (2008). doi: [10.1080/00268970802201211](https://doi.org/10.1080/00268970802201211)
182. P. Huang and E. A. Carter, "Advances in Correlated Electronic Structure Methods for Solids, Surfaces, and Nanostructures," *Ann. Rev. Phys. Chem.*, 59, 261 (2008). doi: [10.1146/annurev.physchem.59.032607.093528](https://doi.org/10.1146/annurev.physchem.59.032607.093528)
181. D. F. Johnson and E. A. Carter, "Nonadiabaticity in the iron bcc to hcp phase transformation," *J. Chem. Phys.*, 128, 104703 (2008). doi: [10.1063/1.2883592](https://doi.org/10.1063/1.2883592)
180. A. Ramasubramaniam and E. A. Carter, "Coupled quantum-atomistic and quantum-continuum mechanics methods in materials research," *Materials Research Society Bulletin*, 32, 913 (2007). doi: [10.1557/mrs2007.188](https://doi.org/10.1557/mrs2007.188)
179. N. J. Mosey and E. A. Carter, "Ab initio Evaluation of Coulomb and Exchange Parameters for DFT+U Calculations," *Phys. Rev. B*, 76, 155123 (2007). doi: [10.1103/PhysRevB.76.155123](https://doi.org/10.1103/PhysRevB.76.155123)
178. G. Ho, M.T. Ong, K.J. Caspersen, and E. A. Carter, "Energetics and Kinetics of Vacancy Diffusion and Aggregation in Shocked Aluminum via Orbital-Free Density Functional Theory," *PhysChemChemPhys*, 9, 4951 (2007). (Cover Article) doi: [10.1039/B705455F](https://doi.org/10.1039/B705455F)
177. B. Hinnemann and E. A. Carter, "Adsorption of Al, O, Hf, Y, Pt, and S atoms on α -Al₂O₃(0001)," *J. Phys. Chem. C*, 111, 7105 (2007). (Cover Article) doi: [10.1021/jp068869c](https://doi.org/10.1021/jp068869c)
176. K. M. Carling and E. A. Carter, "Effects of segregating elements on the adhesive strength and structure of the α -Al₂O₃/ β -NiAl interface," *Acta Materialia*, 55, 2791 (2007). doi: [10.1016/j.actamat.2006.12.020](https://doi.org/10.1016/j.actamat.2006.12.020)
175. K. Niedfeldt, P. Nordlander, and E. A. Carter, "Prediction of structure-dependent charge transfer rates for a Li atom outside a Si (001) surface," *Surf. Sci. Letters*, 601, L29 (2007). doi: [10.1016/j.susc.2006.12.085](https://doi.org/10.1016/j.susc.2006.12.085)
174. D. F. Johnson, D. E. Jiang, and E. A. Carter, "Structure, Magnetism, and Adhesion at Cr/Fe Interfaces from Density Functional Theory," *Surf. Sci.*, 601, 699 (2007). doi: [10.1016/j.susc.2006.10.034](https://doi.org/10.1016/j.susc.2006.10.034)
173. D. E. Jiang and E. A. Carter, "Prediction of a Highly Activated State of CO Adsorbed on an Al/Fe(100) Bimetallic Surface," *J. Phys. Chem. B*, 110, 22213 (2006). doi: [10.1021/jp056123t](https://doi.org/10.1021/jp056123t)
172. K. Niedfeldt, E. A. Carter, and P. Nordlander, "Influence of surface band gaps on the lifetimes of charge transfer states," *Surf. Sci.*, 600, 291 (2006). doi: [10.1016/j.susc.2006.08.005](https://doi.org/10.1016/j.susc.2006.08.005)

171. P. Huang and E. A. Carter, "Self-consistent embedding theory for locally correlated configuration interaction wave functions in condensed matter," *J. Chem. Phys.*, 125, 084102 (2006). doi: [10.1063/1.2336428](https://doi.org/10.1063/1.2336428)
170. K. Niedfeldt, P. Nordlander, and E. A. Carter, "Mechanism of enhanced broadening of the ionization level of Li outside transition metal surfaces," *Phys. Rev. B*, 74, 115109 (2006). doi: [10.1103/PhysRevB.74.115109](https://doi.org/10.1103/PhysRevB.74.115109)
169. P. Huang and E. A. Carter, "Local electronic structure around a single Kondo impurity," *Nano Letters*, 6, 1146 (2006). (Cover Article) doi: [10.1021/nl0602847](https://doi.org/10.1021/nl0602847)
168. R. L. Hayes, G. S. Ho, M. Ortiz, and E. A. Carter, "Prediction of dislocation nucleation during nanoindentation of Al₃Mg by the orbital-free density functional theory local quasicontinuum method," *Phil. Mag.*, 86, 2343 (2006). doi: [10.1080/14786430500525829](https://doi.org/10.1080/14786430500525829)
167. K. M. Carling, W. Glover, H. Gunaydin, T. Mitchell, and E. A. Carter, "Comparison of S, Pt, and Hf Adsorption on NiAl(110)," *Surf. Sci.*, 600, 2079 (2006). doi: [10.1016/j.susc.2006.02.047](https://doi.org/10.1016/j.susc.2006.02.047)
166. E. A. A. Jarvis and E. A. Carter, "A Nanoscale Mechanism of Fatigue in Ionic Solids," *Nano Letters*, 6, 505 (2006). doi: [10.1021/nl0525655](https://doi.org/10.1021/nl0525655)
165. A. Lew, K. Caspersen, E. A. Carter, and M. Ortiz, "Quantum Mechanics Based Multiscale Modeling of Stress-Induced Phase Transformations in Iron," *J. Mech. Phys. Solids*, 54, 1276 (2006). doi: [10.1016/j.jmps.2005.11.009](https://doi.org/10.1016/j.jmps.2005.11.009)
164. A. Andersen and E. A. Carter, "Insight into Selected Reactions in Low-Temperature Dimethyl Ether Combustion from Born-Oppenheimer Molecular Dynamics," *J. Phys. Chem. A*, 110, 1393 (2006). doi: [10.1021/jp054509y](https://doi.org/10.1021/jp054509y)
163. E. A. Carter and P. J. Rossky, "Editorial on Theoretical Chemistry," *Acc. Chem. Res.*, 39, 71 (2006). doi: [10.1021/ar050190o](https://doi.org/10.1021/ar050190o)
162. R.L. Hayes and E.A. Carter, "Atomic Origin of Hysteresis During Cyclic Loading of Si Due to Bond Rearrangements at the Crack Surfaces," *J. Chem. Phys.*, 123, 244704 (2005). doi: [10.1063/1.2137692](https://doi.org/10.1063/1.2137692)
161. V. Cocula, C. J. Pickard, and E. A. Carter, "Ultrasoft Spin-Dependent Pseudopotentials," *J. Chem. Phys.*, 123, 214101 (2005). doi: [10.1063/1.2121547](https://doi.org/10.1063/1.2121547)
160. D. E. Jiang and E. A. Carter, "Effects of Alloying on the Chemistry of CO and H₂S on Fe Surfaces," *J. Phys. Chem. B*, 109, 20469-20478 (2005). doi: [10.1021/jp052656q](https://doi.org/10.1021/jp052656q)
159. D. E. Jiang and E. A. Carter, "First Principles Study of the Interfacial Adhesion between SiO₂ and MoSi₂," *Phys. Rev. B*, 72, 165410 (2005). doi: [10.1103/PhysRevB.72.165410](https://doi.org/10.1103/PhysRevB.72.165410)
158. D. E. Jiang and E. A. Carter, "Prediction of Strong Adhesion at the MoSi₂/Fe Interface," *Acta Materialia*, 53, 4489 (2005). doi: [10.1016/j.actamat.2005.06.001](https://doi.org/10.1016/j.actamat.2005.06.001)
157. B. Zhou and E. A. Carter, "First Principles Local Pseudopotential for Silver: Towards Orbital-Free Density Functional Theory for Transition Metals," *J. Chem. Phys.*, 122, 184108 (2005). doi: [10.1063/1.1897379](https://doi.org/10.1063/1.1897379)

156. R. L. Hayes, M. Fago, M. Ortiz, and E. A. Carter, "Prediction of Dislocation Nucleation During Nanoindentation by the Orbital-Free Density Functional Theory Local Quasicontinuum Method," *Multiscale Modeling and Simulation*, 4, 359(2005). doi: [10.1137/040615869](https://doi.org/10.1137/040615869); Erratum: *Multiscale Modeling and Simulation*, 7, 1003 (2008). doi: [10.1137/080727531](https://doi.org/10.1137/080727531)
155. V. Lignères and E. A. Carter, "Introduction to Orbital-Free Density Functional Theory," in *Handbook of Materials Modeling*, S.Yip (Ed.), 137-148 (2005). doi: [10.1007/978-1-4020-3286-8_9](https://doi.org/10.1007/978-1-4020-3286-8_9)
154. D. E. Jiang and E. A. Carter, "First principles study of H₂S adsorption and dissociation on Fe(110)," *Surf. Sci.*, 583, 60 (2005). doi: [10.1016/j.susc.2005.03.023](https://doi.org/10.1016/j.susc.2005.03.023)
153. K. J. Caspersen and E. A. Carter, "Finding Transition States for Crystalline Solid-Solid Phase Transformations," *Proc. Natl. Acad. Sci.*, 102, 6738 (2005). doi: [10.1073/pnas.0408127102](https://doi.org/10.1073/pnas.0408127102)
152. D. E. Jiang and E. A. Carter, "Carbon atom adsorption on and diffusion into Fe(110) and Fe(100) from first principles," *Phys. Rev. B*, 71, 045402 (2005). doi: [10.1103/PhysRevB.71.045402](https://doi.org/10.1103/PhysRevB.71.045402)
151. B. Zhou, V. Lignerés, and E. A. Carter, "Improving the Orbital-Free Density Functional Theory Description of Covalent Materials," *J. Chem. Phys.* 122, 044103 (2005). doi: [10.1063/1.1834563](https://doi.org/10.1063/1.1834563)
150. D. E. Jiang and E. A. Carter, "Adsorption, Diffusion, and Dissociation of H₂S on Fe(100) from First Principles," *J. Phys. Chem. B*, 108, 19140 (2004). doi: [10.1021/jp046475k](https://doi.org/10.1021/jp046475k)
149. S. Serebrinsky, E. A. Carter, and M. Ortiz, "A quantum-mechanically informed model of hydrogen embrittlement," *J. Mech. Phys. Sol.*, 52, 2403 (2004). doi: [10.1016/j.jmps.2004.02.010](https://doi.org/10.1016/j.jmps.2004.02.010)
148. D. E. Jiang and E. A. Carter, "Adsorption and Dissociation of CO on Fe(110) from First Principles," *Surf. Sci.*, 570, 167-177 (2004). doi: [10.1016/j.susc.2004.07.035](https://doi.org/10.1016/j.susc.2004.07.035)
147. M. Fago, R. L. Hayes, E. A. Carter, and M. Ortiz, "Density Functional Theory Based Local Quasicontinuum Method: Prediction of Dislocation Nucleation," *Phys. Rev. B*, 70, 100102(R) (2004). doi: [10.1103/PhysRevB.70.100102](https://doi.org/10.1103/PhysRevB.70.100102)
146. K. J. Caspersen, A. Lew, M. Ortiz, and E. A. Carter, "Importance of Shear in the bcc-to-hcp Transformation in Iron," *Phys. Rev. Lett.*, 93,115501 (2004). doi: [10.1103/PhysRevLett.93.115501](https://doi.org/10.1103/PhysRevLett.93.115501)
145. D. E. Jiang and E. A. Carter, "First Principles Assessment of Ideal Fracture Energies of Materials with Mobile Impurities: Implications for Hydrogen Embrittlement of Metals," *Acta Materialia*, 52, 4801 (2004). doi: [10.1016/j.actamat.2004.06.037](https://doi.org/10.1016/j.actamat.2004.06.037)
144. E. Aprà, E. A. Carter, and A. Fortunelli, "On the Separability Between Valence and Conduction Bands in Transition Metal Clusters," *Int. J. Quant. Chem.*, 100, 277 (2004). doi: [10.1002/qua.20192](https://doi.org/10.1002/qua.20192)

143. K. Niedfeldt, E. A. Carter, and P. Nordlander, "First principles resonance widths for Li near an Al(001) surface: Predictions of scattered ion neutralization probabilities," *J. Chem. Phys.*, 121, 3751 (2004). doi: [10.1063/1.1777218](https://doi.org/10.1063/1.1777218)
142. D. E. Jiang and E. A. Carter, "Diffusion of interstitial hydrogen into and through bcc Fe from first principles," *Phys. Rev. B*, 70, 064102 (2004). doi: [10.1103/PhysRevB.70.064102](https://doi.org/10.1103/PhysRevB.70.064102)
141. M. Bendikov, H. M. Duong, K. Starkey, K. N. Houk, E. A. Carter, and F. Wudl, "Oligoacenes. Theoretical Prediction of an Open Shell Singlet Ground State and a Constant, Semiconductor Type HOMO-LUMO Gap," *J. Am. Chem. Soc.*, 126, 7416 (2004). doi: [10.1021/ja048919w](https://doi.org/10.1021/ja048919w); Erratum: *J. Am. Chem. Soc.*, 126, 10493 (2004). doi: [10.1021/ja045878v](https://doi.org/10.1021/ja045878v)
140. A. Arya and E. A. Carter, "Structure, bonding, and adhesion at the ZrC(100)/Fe(110) interface from first principles," *Surf. Sci.*, 560, 103 (2004). doi: [10.1016/j.susc.2004.04.022](https://doi.org/10.1016/j.susc.2004.04.022)
139. R. L. Hayes, M. Ortiz, and E. A. Carter, "Universal binding-energy relation for crystals that accounts for surface relaxation," *Phys. Rev. B*, 69, 172104 (2004). doi: [10.1103/PhysRevB.69.172104](https://doi.org/10.1103/PhysRevB.69.172104)
138. R. Puthenkovilakam, E. A. Carter, and J. P. Chang, "First-principles exploration of alternative gate dielectrics: Electronic structure of ZrO₂/Si and ZrSiO₄/Si interfaces," *Phys. Rev. B*, 69, 155329 (2004). doi: [10.1103/PhysRevB.69.155329](https://doi.org/10.1103/PhysRevB.69.155329)
137. E. A. Carter and D. Walter, "Reduced scaling electron correlation methods," In von Ragué Schleyer P, Allinger NL, Clark T, Gasteiger J, Kollman PA, Schaefer III HF, Schreiner PR, editors, *Encyclopedia of Computational Chemistry* (online edition). John Wiley & Sons, Ltd, Chichester, UK. Article online posting date: (15th April 2004). doi: [10.1002/0470845015.cu0024](https://doi.org/10.1002/0470845015.cu0024)
136. B. Zhou, Y.A. Wang, and E. A. Carter, "Transferable Local Pseudopotentials Derived via Inversion of the Kohn-Sham Equations in a Bulk Environment," *Phys. Rev. B*, 69 125109 (2004). doi: [10.1103/PhysRevB.69.125109](https://doi.org/10.1103/PhysRevB.69.125109)
135. V. Cocula and E. A. Carter, "Breakdown of the pseudopotential approximation for magnetic systems: Predicting magnetic quenching at the V(001) surface with spin-dependent pseudopotentials," *Phys. Rev. B*, 69, 052404 (2004). doi: [10.1103/PhysRevB.69.052404](https://doi.org/10.1103/PhysRevB.69.052404)
134. A. Venkatnathan, A. B. Szilva, D. Walter, R. J. Gdanitz, and E. A. Carter, "Size Extensive Modification of Local Multireference Configuration Interaction," *J. Chem. Phys.*, 120, 1693 (2004). doi: [10.1063/1.1635796](https://doi.org/10.1063/1.1635796)
133. D. E. Jiang and E. A. Carter, "Adsorption and Diffusion Energetics of Hydrogen Atoms on Fe(110) from First Principles," *Surf. Sci.*, 547, 85 (2003). doi: [10.1016/j.susc.2003.10.007](https://doi.org/10.1016/j.susc.2003.10.007)
132. A. Andersen and E. A. Carter, "Hybrid Density Functional Theory Predictions of Low-Temperature Dimethyl Ether Combustion Pathways. II. Chain-Branching Energetics and Possible Role of the Criegee Intermediate," *J. Phys. Chem. A*, 107, 9463 (2003). doi: [10.1021/jp035423c](https://doi.org/10.1021/jp035423c)

131. V. Cocula, F. Starrost, S. C. Watson, and E. A. Carter, "Spin-Dependent Pseudopotentials in the Solid State Environment: Applications to Ferromagnetic and Antiferromagnetic Metals," *J. Chem. Phys.*, 119, 7659 (2003).
[doi: 10.1063/1.1609399](https://doi.org/10.1063/1.1609399)
130. D. E. Jiang and E. A. Carter, "Carbon Dissolution and Diffusion in Ferrite and Austenite from First Principles," *Phys. Rev. B*, 67, 214103 (2003).
[doi: 10.1103/PhysRevB.67.214103](https://doi.org/10.1103/PhysRevB.67.214103)
129. A. Andersen and E. A. Carter, "A Hybrid Density Functional Theory Study of the Low-Temperature Dimethyl Ether Combustion Pathways I: Chain-propagation," *Israel J. of Chem*, 42, 245 (2003). [doi: 10.1560/YQM7-5E5M-523Q-AQG2](https://doi.org/10.1560/YQM7-5E5M-523Q-AQG2)
128. A. Arya and E. A. Carter, "Structure, bonding, and adhesion at the TiC(100)/Fe(110) interface from first principles," *J. Chem. Phys.*, 118, 8982 (2003). [doi: 10.1063/1.1565323](https://doi.org/10.1063/1.1565323); Erratum: *J. Chem. Phys.* 120, 1142 (2004).
[doi: 10.1063/1.1631815](https://doi.org/10.1063/1.1631815)
127. D. Walter, A. Venkatnathan, and E. A. Carter, "Local Correlation in the Virtual Space in Multireference Singles and Doubles Configuration Interaction," *J. Chem. Phys.*, 118, 8127 (2003). [doi: 10.1063/1.1565314](https://doi.org/10.1063/1.1565314)
126. K. M. Carling and E. A. Carter, "Orbital-free density functional theory calculations of the properties of Al, Mg and Al-Mg crystalline phases," *Mod. Sim. Mat. Sci. Eng.*, 11, 339 (2003). [doi: 10.1088/0965-0393/11/3/307](https://doi.org/10.1088/0965-0393/11/3/307)
125. W. C. Chiou, Jr. and E. A. Carter, "Structure and stability of Fe₃C-cementite surfaces from first principles," *Surf. Sci.*, 530, 87 (2003). [doi: 10.1016/S0039-6028\(03\)00352-2](https://doi.org/10.1016/S0039-6028(03)00352-2)
124. E. A. A. Jarvis and E. A. Carter, "Exploiting Covalency to Enhance Metal-Oxide and Oxide-Oxide Adhesion at Heterogeneous Interfaces," *J. of the Am. Ceramic Society*, 86, 373 (2003). [doi: 10.1111/j.1151-2916.2003.tb03309.x](https://doi.org/10.1111/j.1151-2916.2003.tb03309.x)
123. A. Andersen and E. A. Carter, "First-Principles Dynamics Study along the Reaction Path of C₂H₅ + O₂ → C₂H₄ + HO₂ : Evidence for Vibronic State Mixing," *J. Phys. Chem. A.*, 106, 9672 (2002). [doi: 10.1021/jp0206267](https://doi.org/10.1021/jp0206267)
122. E. A. A. Jarvis and E. A. Carter, "An Atomic Perspective of a Doped Metal-Oxide Interface," *J. Phys. Chem. B*, 106, 7995 (2002). [doi: 10.1021/jp0257348](https://doi.org/10.1021/jp0257348)
121. E. A. Jarvis and E. A. Carter, "Importance of Open-Shell Effects in Adhesion at Metal-Ceramic Interfaces," *Phys. Rev. B*, 66, 100103 (2002).
[doi: 10.1103/PhysRevB.66.100103](https://doi.org/10.1103/PhysRevB.66.100103)
120. D. Walter, A. Szilva, K. Niedfeldt, and E. A. Carter, "Local Weak Pairs Pseudospectral Multireference Configuration Interaction," *J. Chem. Phys.*, 117, 1982 (2002). [doi: 10.1063/1.1487816](https://doi.org/10.1063/1.1487816)
119. T. Klüner, N. Govind, Y. A. Wang, and E. A. Carter, "Reply to the Comment on 'Prediction of Electronic Excited States of Adsorbates on Metal Surfaces from First Principles', *Phys. Rev. Lett.*, 86, 5954 (2001) by Klüner et al." *Phys. Rev. Lett.*, 88, 209702 (2002). [doi: 10.1103/PhysRevLett.88.209702](https://doi.org/10.1103/PhysRevLett.88.209702)

118. F. Starrost and E. A. Carter, "Modeling the Full Monty: Baring the Nature of Surfaces Across Time and Space," *Surf. Sci. Millenium Issue*, 500, 323 (2002). doi: [10.1016/S0039-6028\(01\)01546-1](https://doi.org/10.1016/S0039-6028(01)01546-1)
117. E. A. Jarvis and E. A. Carter, "The Role of Reactive Elements in the Bond Coat for Thermal Barrier Coatings," *Comp. Sci. Eng.*, 4, 33 (2002). doi: [10.1109/5992.988645](https://doi.org/10.1109/5992.988645)
116. T. Klüner, N. Govind, Y. A. Wang, and E. A. Carter, "Periodic Density Functional Embedding Theory for Complete Active Space Self-Consistent Field and Configuration Interaction Calculations: Ground and Excited States," *J. Chem. Phys.* 116, 42 (2002). doi: [10.1063/1.1420748](https://doi.org/10.1063/1.1420748)
115. F. Starrost, H. Kim, S. C. Watson, E. Kaxiras, and E. A. Carter, "Density Functional Theory Modeling of Bulk Magnetism with Spin-Dependent Pseudopotentials," *Phys. Rev. B*, 64, 235105 (2001). doi: [10.1103/PhysRevB.64.235105](https://doi.org/10.1103/PhysRevB.64.235105)
114. D. Walter and E. A. Carter, "Multireference Weak Pairs Local Configuration Interaction: Efficient Calculations of Bond Breaking," *Chem. Phys. Lett.*, 346, 177 (2001). doi: [10.1016/S0009-2614\(01\)00966-6](https://doi.org/10.1016/S0009-2614(01)00966-6)
113. F. Starrost and E. A. Carter, "Quantum Structural Methods for the Solid State and Surfaces," in the *Encyclopedia of Chemical Physics and Physical Chemistry*, J. H. Moore and N. Spencer, Eds. (Institute of Physics), 2, 1947 (2001).
112. E. A. A. Jarvis, A. Christensen, and E. A. Carter, "Weak Bonding of Alumina Coatings on Ni(111)," *Surf. Sci.*, 487, 55 (2001). doi: [10.1016/S0039-6028\(01\)01071-8](https://doi.org/10.1016/S0039-6028(01)01071-8)
111. T. Klüner, N. Govind, Y. A. Wang, and E. A. Carter, "Prediction of Electronic Excited States of Adsorbates on Metal Surfaces from First Principles," *Phys. Rev. Lett.*, 86, 5954 (2001). doi: [10.1103/PhysRevLett.86.5954](https://doi.org/10.1103/PhysRevLett.86.5954)
110. E. A. A. Jarvis and E. A. Carter, "Metallic Character of the $\text{Al}_2\text{O}_3(0001)-(\sqrt{31}\times\sqrt{31})R\pm 9^\circ$ Surface Reconstruction," *J. Phys. Chem. B*, 105, 4045 (2001). doi: [10.1021/jp003587c](https://doi.org/10.1021/jp003587c)
109. A. Christensen and E. A. Carter, "Adhesion of Ultrathin $\text{ZrO}_2(111)$ Films on Ni(111) from First Principles," *J. Chem. Phys.*, 114, 5816 (2001). doi: [10.1063/1.1352079](https://doi.org/10.1063/1.1352079)
108. A. Christensen, E. A. A. Jarvis, and E. A. Carter, "Atomic-Level Properties of Thermal Barrier Coatings: Characterization of Metal-Ceramic Interfaces," in *Chemical Dynamics in Extreme Environments*, edited by R. A. Dressler, *Advanced Series in Physical Chemistry*, 11, Series Editor: C. Y. Ng (World Scientific, Singapore, 2001), pp 490-546.
107. R. L. Hayes, E. Fattal, N. Govind, and E. A. Carter, "Long Live Vinylidene! A New View of the $\text{H}_2\text{C}=\text{C} \rightarrow \text{HCCH}$ Rearrangement from Ab Initio Molecular Dynamics," *J. Am. Chem. Soc.*, 123, 641 (2001). doi: [10.1021/ja000907x](https://doi.org/10.1021/ja000907x)
106. E. A. A. Jarvis, R. L. Hayes, and E. A. Carter, "Effects of Oxidation on the Nanoscale Mechanisms of Crack Formation in Aluminum," *ChemPhysChem*, 2, 55 (2001). doi: [10.1002/1439-7641\(20010119\)2:1<55::AID-CPHC55>3.0.CO;2-S](https://doi.org/10.1002/1439-7641(20010119)2:1<55::AID-CPHC55>3.0.CO;2-S)

105. A. Christensen and E. A. Carter, "First Principles Characterization of a Hetero-Ceramic Interface: $\text{ZrO}_2(001)$ Deposited on an $\alpha\text{-Al}_2\text{O}_3(1102)$ Substrate," *Phys. Rev. B*, 62, 16968 (2000). doi: [10.1103/PhysRevB.62.16968](https://doi.org/10.1103/PhysRevB.62.16968)
104. Y. A. Wang and E. A. Carter, "Orbital-Free Kinetic Energy Density Functional Theory," in "Theoretical Methods in Condensed Phase Chemistry," S. D. Schwartz, Ed., within the series "Progress in Theoretical Chemistry and Physics," Kluwer, 117-84 (2000).
103. S. C. Watson and E. A. Carter, "Linear Scaling Parallel Algorithms for the First Principles Treatment of Metals," *Comp. Phys. Comm.*, 128, 67 (2000). doi: [10.1016/S0010-4655\(00\)00064-3](https://doi.org/10.1016/S0010-4655(00)00064-3)
102. E. A. A. Jarvis, E. Fattal, A. J. R. da Silva, and E. A. Carter, "Characterization of Photoionization Intermediates via Ab Initio Molecular Dynamics," *J. Phys. Chem. A*, 104, 2333 (2000). doi: [10.1021/jp9919866](https://doi.org/10.1021/jp9919866)
101. E. Fattal and E. A. Carter, "Ab Initio Reaction Energetics of Phosgene Decomposition by Zn^{2+} and Ni Atoms: Implications for Gas Mask Filters," *J. Phys. Chem. A*, 104, 2248 (2000). (Cover Article) doi: [10.1021/jp992964m](https://doi.org/10.1021/jp992964m)
100. E. A. Carter and E. B. Stechel, "Tribute to William Andrew Goddard III," *J. Phys. Chem. A*, 104, 2145 (2000). doi: [10.1021/jp000180z](https://doi.org/10.1021/jp000180z)
99. Y. A. Wang, N. Govind, and E. A. Carter, "Orbital-Free Kinetic-Energy Density Functionals with a Density-Dependent Kernel," *Phys. Rev. B*, 60, 16350 (1999). doi: [10.1103/PhysRevB.60.16350](https://doi.org/10.1103/PhysRevB.60.16350); Erratum: *Phys. Rev. B*, 64, 089903-1 (2001). doi: [10.1103/PhysRevB.64.089903](https://doi.org/10.1103/PhysRevB.64.089903)
98. Y. A. Wang and E. A. Carter, "Improved Lower Bounds for Uncertainty-like Relationships in Many-Body Systems," *Phys. Rev. A*, 60, 4153 (1999). doi: [10.1103/PhysRevA.60.4153](https://doi.org/10.1103/PhysRevA.60.4153)
97. F. Terstegen, E. A. Carter, and V. Buss, "Interconversion Pathways of the Protonated β -Ionone Schiff Base - An Ab Initio Molecular Dynamics Study," *Int. J. Quant. Chem.*, 75, 141 (1999). doi: [10.1002/\(SICI\)1097-461X\(1999\)75:3<141::AID-QUA4>3.0.CO;2-9](https://doi.org/10.1002/(SICI)1097-461X(1999)75:3<141::AID-QUA4>3.0.CO;2-9)
96. N. Govind, Y. A. Wang, and E. A. Carter, "Electronic Structure Calculations by First Principles Density-Based Embedding of Explicitly Correlated Systems," *J. Chem. Phys.*, 110, 7677 (1999). doi: [10.1063/1.478679](https://doi.org/10.1063/1.478679)
95. H. H. Wadleigh III, I. V. Ionova, and E. A. Carter, "Generalized Symmetric Rayleigh-Ritz Procedure Applied to the Closed Shell Hartree-Fock Problem," *J. Chem. Phys.*, 110, 4152 (1999). doi: [10.1063/1.478299](https://doi.org/10.1063/1.478299)
94. N. Rom, E. Fattal, A. K. Gupta, E. A. Carter, and D. Neuhauser, "Shifted-Contour Auxiliary-Field Monte Carlo for Molecular Electronic Structure," *J. Chem. Phys.*, 109, 8241 (1998). doi: [10.1063/1.477486](https://doi.org/10.1063/1.477486)
93. S. C. Watson and E. A. Carter, "Spin-Dependent Pseudopotentials," *Phys. Rev. B*, 58, R13309 (1998). doi: [10.1103/PhysRevB.58.R13309](https://doi.org/10.1103/PhysRevB.58.R13309)

92. Y. A. Wang, N. Govind, and E. A. Carter, "Orbital-Free Kinetic Energy Functionals for the Nearly-Free Electron Gas," *Phys. Rev. B*, 58, 13465 (1998). [doi: 10.1103/PhysRevB.58.13465](https://doi.org/10.1103/PhysRevB.58.13465); Erratum: *Phys. Rev. B*, 64, 129901-1 (2001). [doi: 10.1103/PhysRevB.60.17162](https://doi.org/10.1103/PhysRevB.60.17162)
91. N. Govind, Y. A. Wang, A. J. R. da Silva, and E. A. Carter, "Accurate Ab Initio Energetics of Extended Systems via Explicit Correlation Embedded in a Density Functional Environment," *Chem. Phys. Lett.*, 295, 129 (1998). [doi: 10.1016/S0009-2614\(98\)00939-7](https://doi.org/10.1016/S0009-2614(98)00939-7)
90. A. Christensen and E. A. Carter, "First Principles Study of the Surfaces of Zirconia," *Phys. Rev. B*, 58, 8050 (1998). [doi: 10.1103/PhysRevB.58.8050](https://doi.org/10.1103/PhysRevB.58.8050)
89. C. C. Tzartas, C. R. Anderson, and E. A. Carter, "Automated Selection of Optimal Gaussian Fits to Arbitrary Functions in Electronic Structure Theory," *J. Comp.Chem.*, 19, 1300 (1998). [doi: 10.1002/\(SICI\)1096-987X\(199808\)19:11<1300::AID-JCC10>3.0.CO;2-P](https://doi.org/10.1002/(SICI)1096-987X(199808)19:11<1300::AID-JCC10>3.0.CO;2-P)
88. B. E. Koel, D. A. Blank, and E. A. Carter, "Thermochemistry of the Selective Dehydrogenation of Cyclohexane to Benzene on Pt Surfaces," *J. Mol. Catal A: Chemical.*, 131, 39 (1998). [doi: 10.1016/S1381-1169\(97\)00255-0](https://doi.org/10.1016/S1381-1169(97)00255-0)
87. A. J. R. da Silva, J. W. Pang, E. A. Carter, and D. Neuhauser, "Anharmonic Vibrations via Filter Diagonalization of Ab Initio Dynamics Trajectories," *J. Phys. Chem. A.*, 102, 881 (1998). [doi: 10.1021/jp9727198](https://doi.org/10.1021/jp9727198)
86. S. Watson, B. J. Jesson, E. A. Carter, and P. A. Madden, "Ab Initio Pseudopotentials for Orbital-Free Density Functionals," *Europhys. Lett.*, 41, 37 (1998). [doi: 10.1209/epl/i1998-00112-5](https://doi.org/10.1209/epl/i1998-00112-5)
85. E. Fattal, M. R. Radeke, G. Reynolds, and E. A. Carter, "Ab Initio Structure and Energetics for the Molecular and Dissociative Adsorption of NH₃ on Si(100)-2x1," *J. Phys. Chem. B*, 101, 8658 (1997). [doi: 10.1021/jp9712967](https://doi.org/10.1021/jp9712967)
84. M. R. Radeke and E. A. Carter, "Ab Initio Dynamics of Surface Chemistry," *Ann. Rev. Phys. Chem.*, 48, 243 (1997). [doi: 10.1146/annurev.physchem.48.1.243](https://doi.org/10.1146/annurev.physchem.48.1.243)
83. A. J. R. da Silva, H.-Y. Cheng, D. A. Gibson, K. L. Sorge, Z. Liu, and E. A. Carter, "Limitations of Ab Initio Molecular Dynamics Simulations of Simple Reactions: F+ H₂ as a Prototype," *Spectrochimica Acta Part A*, 53, 1285 (1997). [doi: 10.1016/S1386-1425\(97\)89474-7](https://doi.org/10.1016/S1386-1425(97)89474-7)
82. D. A. Gibson and E. A. Carter, "Ab Initio Molecular Dynamics of Pseudorotating Li₅," *Chem. Phys. Lett.*, 271, 266 (1997). [doi: 10.1016/S0009-2614\(97\)00484-3](https://doi.org/10.1016/S0009-2614(97)00484-3)
81. A. J. R. da Silva, M. R. Radeke, and E. A. Carter, "Ab Initio Molecular Dynamics of H₂ Desorption from Si(100)-2x1," *Surf. Sci. Lett.*, 381, L628 (1997). [doi: 10.1016/S0039-6028\(97\)00124-6](https://doi.org/10.1016/S0039-6028(97)00124-6)
80. G. Reynolds and E. A. Carter, "Removal of the Bottleneck in Local Correlation Methods," *Chem. Phys. Lett.*, 265, 660 (1997). [doi: 10.1016/S0009-2614\(96\)01491-1](https://doi.org/10.1016/S0009-2614(96)01491-1)

79. M. R. Radeke and E. A. Carter, "An Ab Initio-Derived Kinetic Monte Carlo Model of H₂ Desorption from Si(100)-2x1," *Phys. Rev. B*, 55, 4649 (1997).
[doi: 10.1103/PhysRevB.55.4649](https://doi.org/10.1103/PhysRevB.55.4649)
78. D. A. Gibson and E. A. Carter, "Generalized Valence Bond Molecular Dynamics at Constant Temperature," *Mol. Phys.*, 89, 1265 (1996).
[doi: 10.1080/002689796173165](https://doi.org/10.1080/002689796173165)
77. I. V. Ionova and E. A. Carter, "Error Vector Choice in the Direct Inversion in the Iterative Subspace Method," *J. Comp. Chem.*, 17, 1836 (1996).
[doi: 10.1002/\(SICI\)1096-987X\(199612\)17:16<1836::AID-JCC4>3.0.CO;2-O](https://doi.org/10.1002/(SICI)1096-987X(199612)17:16<1836::AID-JCC4>3.0.CO;2-O)
76. G. Reynolds, T. J. Martinez, and E. A. Carter, "Local Weak Pairs Spectral and Pseudospectral Singles and Doubles Configuration Interaction," *J. Chem. Phys.*, 105, 6455 (1996). [doi: 10.1063/1.472495](https://doi.org/10.1063/1.472495)
75. M. R. Radeke and E. A. Carter, "A Dynamically and Kinetically Consistent Mechanism for H₂ Adsorption/Desorption from Si(100)-2x1," *Phys. Rev. B*, 54, 11803 (1996). [doi: 10.1103/PhysRevB.54.11803](https://doi.org/10.1103/PhysRevB.54.11803)
74. L. E. Carter and E. A. Carter, "Simulated Reaction Dynamics of F Atoms on Partially Fluorinated Si(100) Surfaces," *Surf. Sci.*, 360, 200 (1996).
[doi: 10.1016/0039-6028\(96\)00620-6](https://doi.org/10.1016/0039-6028(96)00620-6)
73. M. R. Radeke and E. A. Carter, "Ab Initio Explanation of the Apparent Violation of Detailed Balance for H₂ Adsorption/Desorption from Si(100)," *Surf. Sci.*, 355, L289 (1996). [doi: 10.1016/0039-6028\(96\)00607-3](https://doi.org/10.1016/0039-6028(96)00607-3)
72. L. E. Carter and E. A. Carter, "Ab Initio-Derived Dynamics for F₂ Reactions with Partially Fluorinated Si(100) Surfaces: Translational Activation as a Possible Etching Tool," *J. Chem. Phys.*, 100, 873 (1996). [doi: 10.1021/jp952905i](https://doi.org/10.1021/jp952905i)
71. T. J. Martinez and E. A. Carter, "Pseudospectral Methods Applied to the Electron Correlation Problem," in *Modern Electronic Structure Theory Part II*, D. R. Yarkony, editor, Advanced Series in Physical Chemistry, Vol. 2, pp 1132-1165 (World Scientific, Singapore, 1995). [doi: 10.1142/9789812832115_0006](https://doi.org/10.1142/9789812832115_0006)
70. I. V. Ionova and E. A. Carter, "DIIS-Induced Acceleration of the Ridge Method for Finding Transition States," *J. Chem. Phys.*, 103, 5437 (1995).
[doi: 10.1063/1.470579](https://doi.org/10.1063/1.470579)
69. T. J. Martinez and E. A. Carter, "Pseudospectral Correlation Methods on Distributed Memory Parallel Architectures," *Chem. Phys. Lett.*, 241, 490 (1995).
[doi: 10.1016/0009-2614\(95\)00654-M](https://doi.org/10.1016/0009-2614(95)00654-M)
68. D. A. Gibson, I. V. Ionova, and E. A. Carter, "Comparison of Car-Parrinello and Born-Oppenheimer Generalized Valence Bond Molecular Dynamics," *Chem. Phys. Lett.*, 240, 261 (1995). [doi: 10.1016/0009-2614\(95\)00537-E](https://doi.org/10.1016/0009-2614(95)00537-E)
67. T. J. Martinez and E. A. Carter, "Pseudospectral Multi-Reference Single and Double Excitation Configuration Interaction," *J. Chem. Phys.*, 102, 7564 (1995).
[doi: 10.1063/1.469088](https://doi.org/10.1063/1.469088)

66. T.-M. Chang and E. A. Carter, "Structures and Growth Mechanisms for Heteroepitaxial Fcc(111) Thin Metal Films," *J. Phys. Chem.*, 99, 7637 (1995).
[doi: 10.1021/j100019a051](https://doi.org/10.1021/j100019a051)
65. Z. Liu, L. E. Carter, and E. A. Carter, "Full Configuration Interaction Molecular Dynamics of Na₂ and Na₃," *J. Phys. Chem.*, 99, 4355 (1995).
[doi: 10.1021/j100013a001](https://doi.org/10.1021/j100013a001)
64. M. R. Radeke and E. A. Carter, "Interfacial Strain-Enhanced Reconstruction of Au Multilayer Films on Rh(100)," *Phys. Rev. B*, 51, 4388 (1995).
[doi: 10.1103/PhysRevB.51.4388](https://doi.org/10.1103/PhysRevB.51.4388)
63. I. V. Ionova and E. A. Carter, "Orbital-Based Direct Inversion in the Iterative Subspace for the Generalized Valence Bond Method," *J. Chem. Phys.*, 102, 1251 (1995). [doi: 10.1063/1.468912](https://doi.org/10.1063/1.468912)
62. L. E. Carter and E. A. Carter, "F₂ Reaction Dynamics with Defective Si(100): Defect-Insensitive Surface Chemistry," *Surf. Sci.*, 323, 39 (1995).
[doi: 10.1016/0039-6028\(94\)00622-9](https://doi.org/10.1016/0039-6028(94)00622-9)
61. T.-M. Chang and E. A. Carter, "Mean Field Theory of Heteroepitaxial Thin Metal Film Morphologies," *Surf. Sci.*, 318, 187 (1994). [doi: 10.1016/0039-6028\(94\)90354-9](https://doi.org/10.1016/0039-6028(94)90354-9)
60. G. G. Reynolds and E. A. Carter, "Bimetallic Thermochemistry: Perturbations in M-H and M-C Bond Strengths Due to the Presence of M'," *J. Phys. Chem.*, 98, 8144 (1994). [doi: 10.1021/j100084a037](https://doi.org/10.1021/j100084a037)
59. L. E. Carter and E. A. Carter, "The Influence of Single Atomic Height Steps on F₂ Reactions with Si(100)-2x1," *J. Vac. Sci. Tech. A*, 12, 2235 (1994).
[doi: 10.1116/1.579121](https://doi.org/10.1116/1.579121)
58. C. J. Wu, I. V. Ionova, and E. A. Carter, "First Principles-Derived Rate Constants for H Adatom Surface Diffusion on Si(100)-2x1," *Phys. Rev. B*, 49, 13488 (1994).
[doi: 10.1103/PhysRevB.49.13488](https://doi.org/10.1103/PhysRevB.49.13488)
57. I. V. Ionova and E. A. Carter, "O(N³) Scaling of Two-Electron Integrals During Molecular Geometry Optimization," *J. Chem. Phys.*, 100, 6562 (1994).
[doi: 10.1063/1.467065](https://doi.org/10.1063/1.467065)
56. T. J. Martinez and E. A. Carter, "Pseudospectral Møller-Plesset Perturbation Theory Through Third Order," *J. Chem. Phys.*, 100, 3631 (1994).
[doi: 10.1063/1.466350](https://doi.org/10.1063/1.466350)
55. L. E. Carter, S. Khodabandeh, P. C. Weakliem, and E. A. Carter, "First Principles-Derived Dynamics of F₂ Reactive Scattering on Si(100)-2x1," *J. Chem. Phys.*, 100, 2277 (1994). [doi: 10.1063/1.466526](https://doi.org/10.1063/1.466526)
54. B. Hartke and E. A. Carter, "Ab Initio Molecular Dynamics Simulated Annealing at the Generalized Valence Bond Level: Application to a Small Nickel Cluster," *Chem. Phys. Lett.*, 216, 324 (1993). [doi: 10.1016/0009-2614\(93\)90103-8](https://doi.org/10.1016/0009-2614(93)90103-8)
53. D. A. Gibson and E. A. Carter, "Time-Reversible Multiple Time Scale Ab Initio Molecular Dynamics," *J. Phys. Chem.*, 97, 13429 (1993). [doi: 10.1021/j100153a002](https://doi.org/10.1021/j100153a002)

52. C. J. Wu, I. V. Ionova, and E. A. Carter, "Ab Initio H₂ Desorption Pathways for H/Si(100): The Role of SiH₂(a)," *Surf. Sci.*, 295, 64 (1993). doi: [10.1016/0039-6028\(93\)90185-M](https://doi.org/10.1016/0039-6028(93)90185-M)
51. L. E. Carter, P. C. Weakliem, and E. A. Carter, "Temperature and Composition Dependent Structures of Si_xGe_{1-x}/Si and Si_xGe_{1-x}/Ge Superlattices," *J. Vac. Sci. Tech. A*, 11, 2059 (1993). doi: [10.1116/1.578410](https://doi.org/10.1116/1.578410)
50. T. J. Martinez and E. A. Carter, "Pseudospectral Double Excitation Configuration Interaction," *J. Chem. Phys.*, 98, 7081 (1993). doi: [10.1063/1.464751](https://doi.org/10.1063/1.464751)
49. S. Khodabandeh and E. A. Carter, "Methyl Substitution in Carbenes: Lack of Steric or Hyperconjugative Stabilization Effects on the CH₃CH Singlet-Triplet Splitting," *J. Phys. Chem.*, 97, 4360 (1993). doi: [10.1021/j100119a018](https://doi.org/10.1021/j100119a018)
48. B. C. Bolding and E. A. Carter, "Two-dimensional Metallic Adlayers: Dispersion versus Island Formation," in "On Clusters and Clustering, From Atoms to Fractals," P. J. Reynolds, ed.; in the series "Random Processes and Materials," (Elsevier, Amsterdam, 1993), 167.
47. I. V. Ionova and E. A. Carter, "Ridge Method for Finding Saddle Points on Potential Energy Surfaces," *J. Chem. Phys.*, 98, 6377 (1993). doi: [10.1063/1.465100](https://doi.org/10.1063/1.465100)
46. H. Wang and E. A. Carter, "Metal-Metal Bonding in Engel-Brewer Intermetallics: Anomalous Charge Transfer in ZrPt₃," *J. Am. Chem. Soc.*, 115, 2357 (1993). doi: [10.1021/ja00059a034](https://doi.org/10.1021/ja00059a034)
45. P. C. Weakliem and E. A. Carter, "Surface Chemical Reactions Studied via Ab Initio-Derived Molecular Dynamics Simulations: Fluorine Etching of Si(100)," *J. Chem. Phys.*, 98, 737 (1993). doi: [10.1063/1.464620](https://doi.org/10.1063/1.464620)
44. B. Hartke, D. A. Gibson, and E. A. Carter, "Multiple Time Scale Hartree-Fock Molecular Dynamics," *Int. J. Quantum Chem.*, 45, 59 (1993). doi: [10.1002/qua.560450109](https://doi.org/10.1002/qua.560450109)
43. B. C. Bolding and E. A. Carter, "Minimization of Periodic Boundary-Induced Strain in Interface Simulations," *Molecular Simulation*, 9, 269 (1992). doi: [10.1080/08927029208047433](https://doi.org/10.1080/08927029208047433)
42. B. Hartke and E. A. Carter, "Ab Initio Molecular Dynamics with Correlated Molecular Wavefunctions: Generalized Valence Bond Molecular Dynamics and Simulated Annealing," *J. Chem. Phys.*, 97, 6569 (1992). doi: [10.1063/1.463660](https://doi.org/10.1063/1.463660)
41. C. J. Wu and E. A. Carter, "Anisotropic Diffusion of Hydrogen Atoms on the Si(100)-2x1 Surface," *Phys. Rev. B*, 46, 4651 (1992). doi: [10.1103/PhysRevB.46.4651](https://doi.org/10.1103/PhysRevB.46.4651)
40. T. J. Martinez, A. Mehta, and E. A. Carter, "Pseudospectral Full Configuration Interaction," *J. Chem. Phys.*, 97, 1876 (1992). doi: [10.1063/1.463176](https://doi.org/10.1063/1.463176); Erratum: 99, 4238 (1993). doi: [10.1063/1.466235](https://doi.org/10.1063/1.466235)

39. P. C. Weakliem, C. J. Wu, and E. A. Carter, "First Principles-Derived Dynamics of a Surface Reaction: Fluorine Etching of Si(100)," *Phys. Rev. Lett.*, 69, 200 (1992). [doi: 10.1103/PhysRevLett.69.200](https://doi.org/10.1103/PhysRevLett.69.200); Erratum: 69, 1475 (1992). [doi: 10.1103/PhysRevLett.69.1475](https://doi.org/10.1103/PhysRevLett.69.1475)
38. P. C. Weakliem and E. A. Carter, "Surface and Bulk Equilibrium Structures of Silicon-Germanium Alloys from Monte Carlo Simulations," *Phys. Rev. B*, 45, 13458 (1992). [doi: 10.1103/PhysRevB.45.13458](https://doi.org/10.1103/PhysRevB.45.13458)
37. C. J. Wu and E. A. Carter, "Structures and Adsorption Energetics of Chemisorbed Fluorine Atoms on Si(100)-2x1," *Phys. Rev. B*, 45, 9065 (1992). [doi: 10.1103/PhysRevB.45.9065](https://doi.org/10.1103/PhysRevB.45.9065)
36. B. C. Bolding and E. A. Carter, "Effect of Strain on Thin Film Growth: Deposition of Ni on Ag(100)," *Surface Sci.*, 268, 142 (1992). [doi: 10.1016/0039-6028\(92\)90957-8](https://doi.org/10.1016/0039-6028(92)90957-8)
35. P. C. Weakliem and E. A. Carter, "Constant Temperature Molecular Dynamics Simulations of Si(100) and Ge(100): Equilibrium Structures and Short-Time Behaviour," *J. Chem. Phys.*, 96, 3240 (1992). [doi: 10.1063/1.461968](https://doi.org/10.1063/1.461968)
34. B. Hartke and E. A. Carter, "Spin Eigenstate-Dependent Hartree-Fock Molecular Dynamics," *Chem. Phys. Lett.*, 189, 358 (1992). [doi: 10.1016/0009-2614\(92\)85215-V](https://doi.org/10.1016/0009-2614(92)85215-V)
33. H. Wang and E. A. Carter, "Metal-Metal Bonding in Transition Metal Clusters with Open d-Shells: Pt₃," *J. Phys. Chem.*, 96, 1197 (1992). [doi: 10.1021/j100182a033](https://doi.org/10.1021/j100182a033)
32. C. J. Wu and E. A. Carter, "Mechanistic Predictions for Fluorine Etching of Si(100)," *J. Am. Chem. Soc.*, 113, 9061 (1991). [doi: 10.1021/ja00024a005](https://doi.org/10.1021/ja00024a005)
31. C. J. Wu and E. A. Carter, "Adsorption of Hydrogen Atoms on the Si(100)-2x1 Surface: Implications for the H₂ Desorption Mechanism," *Chem. Phys. Lett.*, 185, 172 (1991). [doi: 10.1016/0009-2614\(91\)80159-U](https://doi.org/10.1016/0009-2614(91)80159-U)
30. C. J. Wu and E. A. Carter, "Ab Initio Thermochemistry for Unsaturated C₂ Hydrocarbons," *J. Phys. Chem.*, 95, 8352 (1991). [doi: 10.1021/j100174a058](https://doi.org/10.1021/j100174a058)
29. B. C. Bolding and E. A. Carter, "Temperature Dependence of the Morphology of Strained Overlayers: Deposition of Pd on a bcc(110) Substrate," *Phys. Rev. B*, 44, 3251 (1991). [doi: 10.1103/PhysRevB.44.3251](https://doi.org/10.1103/PhysRevB.44.3251)
28. E. A. Carter and J. T. Hynes, "Solvation Dynamics for an Ion Pair in a Polar Solvent: Time Dependent Fluorescence and Photochemical Charge Transfer", *J. Chem. Phys.*, 94, 5961 (1991). [doi: 10.1063/1.460431](https://doi.org/10.1063/1.460431)
27. G. W. Smith and E. A. Carter, "Interactions of NO and CO with Pd and Pt Atoms," *J. Phys. Chem.*, 95, 2327 (1991). [doi: 10.1021/j100159a040](https://doi.org/10.1021/j100159a040); Erratum: 95, 10828 (1991). [doi: 10.1021/j100179a056](https://doi.org/10.1021/j100179a056)
26. B. C. Bolding and E. A. Carter, "Simulation of Lattice-Strain Driven Bcc→Fcc Phase Transitions in Pd Thin Films," *Phys. Rev. B*, 42, 11380 (1990). [doi: 10.1103/PhysRevB.42.11380](https://doi.org/10.1103/PhysRevB.42.11380)

25. P. C. Weakliem, G. W. Smith, and E. A. Carter, "Subpicosecond Interconversion of Buckled and Symmetric Dimers on Si(100)," *Surface Sci. Lett.*, 232, L219 (1990). doi: [10.1016/0039-6028\(90\)90112-L](https://doi.org/10.1016/0039-6028(90)90112-L)
24. C. J. Wu and E. A. Carter, "Ab Initio Bond Strengths in Ethylene and Acetylene," *J. Am. Chem. Soc.*, 112, 5893 (1990). doi: [10.1021/ja00171a047](https://doi.org/10.1021/ja00171a047)
23. E. A. Carter, "Linking Chemical Physics and Surface Science: Thermochemistry of Adsorbates from Purely Gas Phase Data," *Chem. Phys. Lett.*, 169, 218 (1990). doi: [10.1016/0009-2614\(90\)85191-E](https://doi.org/10.1016/0009-2614(90)85191-E)
22. E. A. Carter and B. E. Koel, "A Method for Estimating Surface Reaction Energetics: Application to the Mechanism of Ethylene Decomposition on Pt(111)," *Surf. Sci.*, 226, 339 (1990). doi: [10.1016/0039-6028\(90\)90498-W](https://doi.org/10.1016/0039-6028(90)90498-W)
21. J. T. Hynes, E. A. Carter, G. Ciccotti, H. J. Kim, D. A. Zichi, M. Ferrario, and R. Kapral, "Environmental Dynamics and Electron Transfer Reactions," in *Perspectives in Photosynthesis*, J. Jortner, and B. Pullman, Eds. (Kluwer, Netherlands, 1990) 133-148. doi: [10.1007/978-94-009-0489-7_12](https://doi.org/10.1007/978-94-009-0489-7_12)
20. M. E. Bartram, B. E. Koel, and E. A. Carter, "Electronic Effects of Surface Oxygen on the Bonding of NO to Pt(111)," *Surf. Sci.*, 219, 467 (1989). doi: [10.1016/0039-6028\(89\)90522-0](https://doi.org/10.1016/0039-6028(89)90522-0)
19. E. A. Carter, G. Ciccotti, J. T. Hynes, and R. Kapral, "Constrained Reaction Coordinate Dynamics for the Simulation of Rare Events," *Chem. Phys. Lett.*, 156, 472 (1989). doi: [10.1016/S0009-2614\(89\)87314-2](https://doi.org/10.1016/S0009-2614(89)87314-2)
18. E. A. Carter and J. T. Hynes, "Solute-Dependent Solvent Force Constants for Ion Pairs and Neutral Pairs in a Polar Solvent," *J. Phys. Chem.*, 93, 2184 (1989). doi: [10.1021/j100343a002](https://doi.org/10.1021/j100343a002)
17. E. A. Carter and W. A. Goddard III, "Chemisorption of Oxygen, Chlorine, Hydrogen, Hydroxide, and Ethylene on Silver Clusters: A Model for the Olefin Epoxidation Reaction," *Surf. Sci.*, 209, 243 (1989). doi: [10.1016/0039-6028\(89\)90071-X](https://doi.org/10.1016/0039-6028(89)90071-X)
16. E. A. Carter and W. A. Goddard III, "Relationships between Bond Energies in Coordinatively Unsaturated and Coordinatively Saturated Transition-Metal Complexes: A Quantitative Guide for Single, Double, and Triple Bonds," *J. Phys. Chem.*, 92, 5679 (1988). doi: [10.1021/j100331a026](https://doi.org/10.1021/j100331a026)
15. E. A. Carter and W. A. Goddard III, "The Surface Atomic Oxyradical Mechanism for Ag-Catalyzed Olefin Epoxidation," *J. Catal.*, 112, 80 (1988). doi: [10.1016/0021-9517\(88\)90122-4](https://doi.org/10.1016/0021-9517(88)90122-4)
14. E. A. Carter and W. A. Goddard III, "The C=C Double Bond of Tetrafluoroethylene," *J. Am. Chem. Soc.*, 110, 4077 (1988). doi: [10.1021/ja00220a079](https://doi.org/10.1021/ja00220a079)
13. E. A. Carter and W. A. Goddard III, "Early versus Late Transition Metal-Oxo Bonds: the Electronic Structure of VO⁺ and RuO⁺," *J. Phys. Chem.*, 92, 2109 (1988). doi: [10.1021/j100319a005](https://doi.org/10.1021/j100319a005)

12. E. A. Carter and W. A. Goddard III, "Correlation-Consistent Configuration Interaction: Accurate Bond Dissociation Energies from Simple Wave Functions," *J. Chem. Phys.*, 88, 3132 (1988). doi: [10.1063/1.453957](https://doi.org/10.1063/1.453957)
11. E. A. Carter and W. A. Goddard III, "Modeling Fischer-Tropsch Chemistry: the Thermochemistry and Insertion Kinetics of ClRuH(CH₂)," *Organometallics*, 7, 675 (1988). doi: [10.1021/om00093a017](https://doi.org/10.1021/om00093a017)
10. E. A. Carter and W. A. Goddard III, "Correlation-Consistent Singlet-Triplet Gaps in Substituted Carbenes," *J. Chem. Phys.*, 88, 1752 (1988). doi: [10.1063/1.454099](https://doi.org/10.1063/1.454099)
9. E. A. Carter and W. A. Goddard III, "New Predictions for Singlet-Triplet Gaps of Substituted Carbenes," *J. Phys. Chem.*, 91, 4651 (1987). doi: [10.1021/j100302a003](https://doi.org/10.1021/j100302a003)
8. E. A. Carter and W. A. Goddard III, "Methylidene Migratory Insertion into an Ru-H Bond," *J. Am. Chem. Soc.*, 109, 579 (1987). doi: [10.1021/ja00236a044](https://doi.org/10.1021/ja00236a044)
7. E. A. Carter and W. A. Goddard III, "Electron Correlation, Basis Sets, and the Methylene Singlet-Triplet Gap," *J. Chem. Phys.*, 86, 862 (1987). doi: [10.1063/1.452287](https://doi.org/10.1063/1.452287)
6. E. A. Carter and W. A. Goddard III, "Bonding in Transition Metal Methylene Complexes. III. Comparison of Cr and Ru Carbenes; Prediction of Stable L_nM(CXY) Systems." *J. Am. Chem. Soc.*, 108, 4746 (1986). doi: [10.1021/ja00276a011](https://doi.org/10.1021/ja00276a011)
5. E. A. Carter and W. A. Goddard III, "Bonding in Transition Metal Methylene Complexes. II. (RuCH₂)⁺, A Complex Exhibiting Low-Lying Methylidene-Like and Carbene-Like States." *J. Am. Chem. Soc.*, 108, 2180 (1986). doi: [10.1021/ja00269a010](https://doi.org/10.1021/ja00269a010)
4. E. A. Carter and W. A. Goddard III, "Relation between Singlet-Triplet Gaps and Bond Energies." *J. Phys. Chem.*, 90, 998 (1986). doi: [10.1021/j100278a006](https://doi.org/10.1021/j100278a006)
3. M. A. Hanratty, E. A. Carter, J. L. Beauchamp, W. A. Goddard III, A. E. Illies, and M. T. Bowers, "Electronic States of Chromium Carbene Ions Characterized by High Resolution Translational Energy Loss Spectroscopy," *Chem. Phys. Lett.*, 123, 239 (1986). doi: [10.1016/0009-2614\(86\)80064-1](https://doi.org/10.1016/0009-2614(86)80064-1)
2. W. A. Goddard III, J. J. Low, B. D. Olafson, A. Redondo, Y. Zeiri, M. L. Steigerwald, E. A. Carter, J. N. Allison, and R. Chang, "The Role of Oxygen and Other Chemisorbed Species on Surface Processes for Metals and Semiconductors; Approaches to Dynamical Studies of Surface Processes," Proceedings of the Symposium on The Chemistry and Physics of Electrocatalysis, J.D.E. McIntyre, .J. Weaver, and E.B. Yeager, Eds. (The Electrochemical Society, Inc., Pennington, New Jersey, 1984) Vol. 84-12, pp. 63-95.
1. E. A. Carter and W. A. Goddard III, "The Cr Methylidene Cation: CrCH₂⁺," *J. Phys. Chem.*, 88, 1485 (1984). doi: [10.1021/j150652a009](https://doi.org/10.1021/j150652a009)

CONFERENCE PROCEEDINGS

6. D.F. Johnson, E.A. Carter, "Structure, Bonding and Adhesion of Materials Interfaces with Density Functional Theory: Cr/Fe, SiC/Fe, MoSi₂/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. Moscovitz 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, 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.
- 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 CO₂ 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 CO₂ 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 *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 CO₂ 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 CO₂ 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 CO₂ 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 CO₂ 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 Martinez)
- April 2, 2017 “The Holy Grail: Chemistry enabling an economically viable CO₂ 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 CO₂ 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 Martinez)
- 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 N₂ 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 CO₂ reduction over GaP, CdTe, and CuInS₂ photoelectrodes?” talk at the *251st ACS Spring National Meeting*, San Diego, CA. (presented by Thomas Sentfle)
- 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 N₂ 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 CO₂ 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 CO₂ 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 CO₂ 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 CO₂ with Pyridinium Catalysts,” invited talk at the *CECAM Workshop on Future Challenges in CO₂-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 CH₄ Dehydrogenation on Ru-functionalized Cu and N₂ Dissociation on Fe-functionalized Au,” poster at the *AFOSR MURI Program Review Meeting*, Houston, TX. (presented by Mark Martinez)
- 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 CO₂ 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 Martinez)
- May 19, 2016 “How do surface reconstructions affect Py-catalyzed CO₂ 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 CO₂ 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 CO₂ Reduction over Semiconductor Photoelectrodes?,” poster at the *AFOSR MURI Annual Review Meeting*, San Diego, CA. (presented by Tom Senftle)
- Jan. 25, 2016 “Pyridine-catalyzed CO₂ 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-affiliates Partnership*, Princeton, NJ. (presented by Mohan Chen)
- Nov. 20, 2015 “Pyridine-catalyzed CO₂ 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-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 CO₂ 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 CO₂ Reduction on GaP Electrodes: Can Surface Hydrogen Atoms Play a Role?,” poster at the *Third Biennial CO₂ 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 CO₂ 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 CO₂ 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 CO₂ 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 CO₂ 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 CO₂,” poster at the *3rd 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 CO₂ reduction on GaP electrodes,” poster at the *3rd 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 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 $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ vs. the new $\text{SrFe}_{1+x}\text{MoxO}_{(6-\delta)}$ mixed ion-electron conductor,” talk at the *247th 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_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-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 *2nd 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_2 ,” poster at the *2nd Annual Meeting of the Princeton E-affiliates 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-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 *2nd Annual Meeting of the Princeton E-affiliates 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 Li₂O 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_{1-x}Sr_xFeO₃ and La_{1-x}Sr_xCoO₃,” 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 CO₂ 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)

4/3/2017

- 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 $\text{Sr}_2\text{Fe}_{2-x}\text{Mo}_x\text{O}_{6-d}$ (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 $\{\text{La,Sr}\}\text{MnO}_3$ (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 O_2 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