

EMILY ANN CARTER

PROFESSIONAL ADDRESS

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EDUCATION

1987	California Institute of Technology	Pasadena, CA
•	Degree: Ph. D. in Physical Chemistry	Advisor: William A. Goddard III
1982	University of California, Berkeley	Berkeley, CA
•	Degree: B.S. (high honors) in Chemistry	

PROFESSIONAL POSITIONS

2023-present	Associate Laboratory Director for Applied Materials and Sustainability Sciences , Princeton Plasma Physics Laboratory (PPPL) <i>Leading diversification of PPPL's research portfolio into the fundamental science of electromanufacturing, solar geoengineering, microelectronics, and quantum information. Established the Princeton University Associated Faculty appointment program at PPPL.</i>
2022-present	Senior Strategic Advisor for Sustainability Science at Princeton Plasma Physics Laboratory; Gerhard R. Andlinger Professor in Energy and the Environment; Professor of Mechanical and Aerospace Engineering, the Andlinger Center for Energy and the Environment, and Applied and Computational Mathematics; Associated Faculty of the Princeton Institute for Computational Science & Engineering and the High Meadows Environmental Institute, Princeton University
2022-present	Executive Vice Chancellor and Provost Emerita and Distinguished Professor of Chemical and Biomolecular Engineering Emerita, University of California, Los Angeles

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

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

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

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

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

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

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

RESEARCH ACTIVITIES

Development of accurate and efficient quantum mechanics simulation techniques, including pioneering embedded correlated wavefunction and orbital-free density functional theories. Discovery and design of materials for producing chemicals, materials, and fuels from renewable energy, with a specific emphasis on carbon dioxide utilization. Delivered over 600 invited/plenary lectures at conferences, universities, companies, and government laboratories worldwide. Trained 58

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

Web of Science P-4075-2014
Researcher ID

ORCID: [0000-0001-7330-7554](https://orcid.org/0000-0001-7330-7554)

Google Scholar: <https://scholar.google.com/citations?user=vluc7z8AAAAJ&hl=en>

Github: Codes developed in the Carter group are available through GitHub repositories:
<https://github.com/EACcodes>

AWARDS AND HONORS

- 2025 Physical Chemistry Division of the American Chemical Society Created the Emily A. Carter Early Career Award in Theoretical Chemistry
- 2025 Willis H. Flygare Memorial Lecturer in Physical Chemistry, University of Illinois, Urbana-Champaign
- 2025 Satish Saxena Distinguished Lecturer in Chemical Engineering, University of Illinois, Chicago
- 2024 Annabelle Lee Lecturer in Chemistry, Virginia Tech
- 2024 [Marsha I. Lester Award](#) for Exemplary Impact in Physical Chemistry, American Chemical Society, Physical Chemistry Division
- 2024 [Foreign Member](#), The Royal Society, London, Great Britain
- 2024 [Covestro Lecturer](#), University of Pittsburgh, Department of Chemical and Petroleum Engineering
- 2024 [William H. Nichols Medal](#), New York Section of the American Chemical Society
- 2023 Gilbert Newton Lewis Memorial Lecturer, College of Chemistry, University of California, Berkeley
- 2023 Robert S. Mulliken Award, Department of Chemistry, University of Chicago
- 2023 27th John Stauffer Lecturer in Chemistry, Stanford University
- 2022 Fellow, Royal Society of Chemistry
- 2022 Paint Branch Distinguished Lecturer in Applied Physics, University of Maryland, Institute for Research in Electronics and Applied Physics
- 2022 Richard S. H. Mah Lecturer, Northwestern University, Department of Chemical and Biological Engineering
- 2022 Harrison Shull Distinguished Lecturer, Indiana University Bloomington, Department of Chemistry
- 2021 Materials Theory Award, Materials Research Society
- 2020 Brumley D. Pritchett Lecturer, Georgia Institute of Technology, School of Materials Science and Engineering
- 2020 Member, European Academy of Sciences
- 2020 Chemistry & Biochemistry Distinguished Lecturer, University of California, Los Angeles

- 2019 John Scott Award, Board of City Trusts, Philadelphia, PA
- 2019 Camille & Henry Dreyfus Lectureship, University of Basel, Switzerland
- 2019 Inaugural WiSE Presidential Distinguished Lecturer, University of Southern California
- 2019 18th NCCR MARVEL Distinguished Lecturer, L'École Polytechnique Fédérale de Lausanne (EPFL), Switzerland
- 2019 Graduate Mentoring Award, McGraw Center for Teaching and Learning, Princeton University
- 2019 [Distinguished Alumni Award](#), California Institute of Technology
- 2019 Eyring Lecturer in Molecular Sciences, Arizona State University
- 2019 Mildred Dresselhaus Memorial Lecturer, Ras Al Khaimah Centre for Advanced Materials, United Arab Emirates
- 2019 Dow Foundation Distinguished Lecturer, University of California, Santa Barbara
- 2018 C. R. Mueller Distinguished Lecturer, Purdue University
- 2018 CME Leadership Award for Interdisciplinary Innovation, New York Section of the American Chemical Society
- 2018 Donald L. Katz Lectureship in Chemical Engineering, University of Michigan
- 2018 ACS Award in Theoretical Chemistry, American Chemical Society
- 2017 College of Engineering Fall Distinguished Lecturer, University of California, Davis
- 2017 Emerson Center Lectureship Award, Emory University
- 2017 Fritz London Memorial Lecturer, Duke University
- 2017 Julian C. Smith Lecturer in Chemical and Biomolecular Engineering, Cornell University
- 2017 Albert J. Moscowitz Memorial Lecturer in Chemistry, University of Minnesota
- 2017 Distinguished Lecturer in Theoretical and Computational Chemistry, University of California, San Diego
- 2017 Outstanding Referee of the Physical Review journals
- 2017 Irving Langmuir Prize in Chemical Physics, American Physical Society
- 2016 Schiesser Lecturer, Lehigh University
- 2016 Pitzer Lecturer on Theoretical Chemistry, Ohio State University
- 2016 Almlöf–Gropen Lecturer, Centre for Theoretical and Computational Chemistry at the University of Oslo and the University of Tromsø, Norway
- 2016 R. H. Betts Memorial Award Lecturer, University of Manitoba, Winnipeg, Canada
- 2016 Fred Kavli Innovations in Chemistry Lecturer, American Chemical Society
- 2016 Member, National Academy of Engineering
- 2015 Joseph O. Hirschfelder Prize in Theoretical Chemistry, Theoretical Chemistry Institute at the University of Wisconsin, Madison
- 2014 Fellow, National Academy of Inventors
- 2014 Malcolm Dole Distinguished Summer Lecturer in Physical Chemistry, Northwestern University

- 2014 Ira Remsen Award, Maryland Section of the American Chemical Society, Johns Hopkins University
- 2014 Women in STEM Award for Outstanding Research Scholarship, Princeton University
- 2014 Linnett Visiting Professor of Chemistry, University of Cambridge
- 2013 Hoyt C. Hottel Lecturer in Chemical Engineering, Massachusetts Institute of Technology
- 2013 Kenneth S. Pitzer Lecturer, Department of Chemistry, University of California, Berkeley
- 2013 Mathematics of Planet Earth Simons Public Lecturer, Institute for Pure and Applied Mathematics, University of California, Los Angeles
- 2013 Lord Lecturer, Department of Chemistry, Allegheny College
- 2013 Sigillo D'Oro (Golden Sigillum) Medal, Italian Chemical Society, Scuola Normale Superiore, Pisa, Italy
- 2013 Article selected for *The Journal of Chemical Physics* 80th Anniversary Collection (Chen Huang and Emily A. Carter, "Potential-functional embedding theory for molecules and materials," *J. Chem. Phys.*, **135**, 194104 (2011).)
- 2013 Francis Clifford Phillips Lectureship, Xi Chapter of the Phi Lambda Upsilon National Honorary Chemical Society and the Department of Chemistry, University of Pittsburgh
- 2013 Tedori-Callinan Lectureship, Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania
- 2013 Naval Research Laboratory Distinguished Lectureship, Naval Research Laboratory, Washington, DC
- 2013 W. Allan Powell Lectureship, Virginia Section of the American Chemical Society and the University of Richmond
- 2012 Docteur Honoris Causa from L'École Polytechnique Fédérale de Lausanne, Switzerland (EPFL)
- 2012 Fellow, American Chemical Society
- 2012 Honorary Mathematical and Physical Sciences Distinguished Lecturer, National Science Foundation
- 2012 Dean's Distinguished Lecturer, College of Science and Technology, Temple University
- 2011 MIT Distinguished Speaker in Computational Science and Engineering, Massachusetts Institute of Technology
- 2011 August Wilhelm von Hofmann Lecture Award, German Chemical Society
- 2011 Jerome B. Cohen Lecturer in Materials Science and Engineering, Northwestern University
- 2011 Ernest Davidson Lecturer in Theoretical Chemistry, University of North Texas
- 2011 Gerhard R. Andlinger Professor in Energy and the Environment, Princeton University

- 2010 Molecular Foundry Distinguished Lecturer, Lawrence Berkeley National Laboratory
- 2010 Coover Lecturer in Chemistry, Iowa State University
- 2010 Material Simulation Distinguished Lecturer, Pennsylvania State University
- 2010 Pelz Memorial Lecturer in Mechanical and Aerospace Engineering, Rutgers University
- 2010 Noyes Lecturer in Physical Chemistry, University of Texas, Austin
- 2009 Member, International Academy of Quantum Molecular Science
- 2008 EaSTChem Visiting Fellow, Universities of Edinburgh and St. Andrews, Scotland
- 2008 Member, National Academy of Sciences
- 2008 Fellow, American Academy of Arts & Sciences
- 2008 Welch Distinguished Lecturer in Chemistry
- 2008 Coulson Lecturer in Theoretical Chemistry, University of Georgia
- 2008 Kivelson Lecturer in Physical Chemistry, University of California, Los Angeles
- 2007-08 Old Dominion Faculty Fellow, Council of the Humanities, Princeton University
- 2007 American Chemical Society Award for Computers in Chemical and Pharmaceutical Research
- 2006 Arthur W. Marks '19 Professor, Princeton University
- 2005 Merck-Frosst Lecturer in Chemistry, Concordia University
- 2004 Fellow, Institute of Physics
- 2002 Dean's Recognition Award for Research, University of California, Los Angeles
- 2002 McDowell Lecturer in Physical Chemistry, University of British Columbia, Canada
- 2000 Fellow, American Association for the Advancement of Science
- 1998 Fellow, American Physical Society
- 1998 Hanson-Dow Award for Excellence in Teaching, University of California, Los Angeles
- 1996-97 Defense Science Study Group Member
- 1996 Dr. Lee Visiting Research Fellowship in the Sciences, Christ Church, Oxford University, England
- 1995 Peter Mark Memorial Award, American Vacuum Society
- 1995 Fellow, American Vacuum Society
- 1993 Herbert Newby McCoy Research Award, University of California, Los Angeles
- 1993 Medal of the International Academy of Quantum Molecular Science
- 1993 Exxon Faculty Fellowship in Solid State Chemistry, American Chemical Society Inorganic Division Award
- 1993 Glenn T. Seaborg Research Award, University of California, Los Angeles
- 1993-95 Alfred P. Sloan Research Fellow
- 1992-97 Camille and Henry Dreyfus Teacher-Scholar Award
- 1990-91 Union Carbide Innovation Recognition Award

- 1989-90 Faculty Member of Distinction (Undergraduate Teaching Award), University of California, Los Angeles
- 1989-90 Union Carbide Innovation Recognition Award
- 1988-93 Camille and Henry Dreyfus Foundation Distinguished New Faculty Award
- 1988-93 National Science Foundation Presidential Young Investigator Award
- 1986-87 SOHIO Fellowship in Catalysis, California Institute of Technology (Caltech)
- 1985-86 International Precious Metals Institute and Gemini Industries Research Grant Award
- 1984 Sigma Xi, California Institute of Technology (Caltech)
- 1982-85 National Science Foundation Predoctoral Fellowship
- 1982 Phi Beta Kappa, University of California, Berkeley
- 1982 Mabel Kittredge Wilson Prize in Chemistry, University of California, Berkeley
- 1981-82 Bruce Howard Memorial Scholar, University of California, Berkeley
- 1981 Coblenz Society Award for Molecular Spectroscopy, University of California, Berkeley
- 1981 Mildred Jordan Sharp Torch and Shield Award, University of California, Berkeley
- 1979-80 Theodore and Edith Braun Scholar, University of California, Berkeley
- 1978-82 Alumni Scholar, University of California, Berkeley
- 1978-82 Regents Scholar, University of California, Berkeley

NEWS/MEDIA INTERVIEWS

- 2024 August 19, 2024 – Featured in Politico’s [E&E news](#) regarding US reusing captured CO₂ for concrete, aviation fuel
- August 7, 2024 – Featured in [National Academies news](#) regarding NASEM report about the role for carbon dioxide utilization in U.S. economy and identifying research gaps and opportunities
- 2023 November 25 – Interview on the “Girl Power Gurus” podcast as an [international leader in sustainability science](#)
- October 29 – Featured in [Forbes](#) regarding energy efficiency as a panacea for power
- June 28 – Interview with David Zierler at the [Caltech Heritage Project](#) regarding the paramount issue of climate change and sustainability
- May 5 – Featured in [C-Change Conversation](#) regarding the processes of transforming CO₂ emissions from burning coal, oil, and gas into useful products
- April 3 – Featured in [Vogue Business](#) regarding Why Gucci’s latest fragrance is made from recycled carbon
- April 1 – Featured in [PAW](#) regarding Princeton Plasma Physics Lab Takes on Sustainability Science
- 2022 December 8 – Featured in [OilPrice.com](#) regarding scientists inventing a new way to convert ammonia into hydrogen

- December 3 – Featured in [SciTechDaily](#) regarding a new catalyst turning a smelly gas byproduct into a cash cow
- December 2 – Featured in [E&E News](#) regarding NASEM report of capturing carbon dioxide and conversion into useful products is possible but requires extensive new infrastructure and large clean energy inputs
- December 1 – Featured in [Innovation Map](#) regarding Houston startup founders reporting on clean energy tech efficacy
- December 1 – Featured in [National Academies news](#) regarding NASEM report that industry and government should begin planning carbon dioxide utilization in circular economy
- November 28 – Featured in [SciTechDaily](#) regarding development of light-powered nanomaterial catalyst that could be key for hydrogen economy
- November 28 – Featured in [Green Car Congress](#) regarding development of earth-abundant photocatalyst for conversion of ammonia into hydrogen
- November 27 – Featured in [Earth.com](#) regarding unlocking hydrogen's potential as a green fuel
- November 25 – Featured in [Tech Xplore](#) regarding researchers creating green fuel with the flip of a light switch
- November 25 – Featured in [Science Daily](#) regarding a new inexpensive catalyst that could be key for hydrogen economy
- November 25 – Featured in [Techfragments](#) regarding a catalyst using light to turn ammonia into hydrogen fuel
- November 24 – Featured in [Phys.org](#) regarding a light-powered catalyst that could be key for hydrogen economy
- November 24 – Featured in [Mirage News](#) regarding Rice lab's key light-activated nanomaterial for hydrogen economy
- February 9 – Interview with Times Radio UK (in association with The Times and Sunday Times) regarding JET fusion energy breakthrough
- January 4 – Interview with Times Radio UK (in association with The Times and Sunday Times) regarding China's fusion research
- 2021 December 7 – Featured for the [2021 MRS Materials Theory Award](#) regarding quantum-derived materials solutions for a sustainable future
- 2020 January 17 – Featured in [ACS Chemical & Engineering News](#) regarding the development of an improved process for synthesis gas ("syngas") production
- January 16 – Quoted in *LA Times* on carbon conversion entitled "[Turning carbon into concrete could win UCLA team a climate victory — and \\$7.5 million](#)"
- 2019 November 15 – Featured in *The Philadelphia Inquirer* article entitled "[Philadelphia science prize goes to climate change and electronics researchers from Penn. UCLA](#)"
- October 21 – Interview with *Physics Magazine* entitled "[Waiting for the Quantum Simulation Revolution](#)"
- May 29 – Interview with 'She Roars' Podcast on [universities in the service of humanity at Princeton and beyond](#)

- January 25 – Quoted in *China Daily* on China's Vice-President Wang Qishan call on innovation, multilateralism, and shaping a shared future entitled "[Global vision presented in Davos speech](#)"
- January 24 – Interview with Yahoo! Finance entitled "[The focus on the 4th Industrial Revolution at Davos](#)"
- January 21 – Interview with Bloomberg TV on [Engineering's value to society](#)
- 2018 September 19 – Interview with *ACS Energy Letters* Editor-in-Chief, Prashant V. Kamat, "[A Conversation with Emily Carter](#)," *ACS Energy Lett.*, **3**, 2470 (2018)
- 2017 January 18 – Interview with Reuters Money on [climate change, innovation, and women in tech](#), aired via Facebook Live
- January 16 – Featured in a World Economic Forum article entitled "[Smashing the glass ceiling: 6 Davos leaders explain how they did it](#)"
- 2016 May 5 – Quoted in the New York Times on ExxonMobil's pursuit of carbon capture technology entitled "[Exxon Mobil Backs FuelCell Effort to Advance Carbon Capture Technology](#)"
- January 19 – Published an Op-Ed in the Houston Chronicle entitled "[In era of cheap oil, our choices are clear: consume more or spark change](#)"
- 2014 February – Co-wrote a Change.org petition to "[stop gender discrimination in science](#)"; this, as well as a follow-up interview with Nature entitled "[Chemists call for boycott over all-male speaker line up](#)"
- 2010 February 26 – Featured in [Popular Science](#) and [Science Daily News](#) regarding the discovery of an equation for materials innovation
- 2009 June 12 – Interview with NJNews television regarding [EFRC on Combustion Science](#), aired on Channel 13
- 2006 June 5 – Featured in the Princeton Weekly Bulletin entitled "[Carter shapes future breakthroughs, one atom at a time, one student at a time](#)"
- 2005 January 31 – Published an invited Op-Ed piece in the Daily Princetonian entitled "[Few Women in the Sciences? It's the Culture, Stupid](#);" this, as well as [a response by Paul R. Ehrlich](#)
- 1999 August – Interview with German TV (Bayrischer Rundfunk) about research

MEMBERSHIPS IN PROFESSIONAL SOCIETIES

The Royal Society; elected Foreign Member in 2024

Royal Society of Chemistry; elected Fellow in 2022

European Academy of Sciences; elected Member in 2020

National Academy of Engineering; elected Member in 2016

National Academy of Inventors; elected Fellow in 2014

International Academy of Quantum Molecular Science; elected Member in 2009

National Academy of Sciences; elected Member in 2008

American Academy of Arts and Sciences; elected Fellow in 2008

Institute of Physics; elected Fellow in 2004
American Association for the Advancement of Science (1999 -); elected Fellow in 2000
Materials Research Society (1998 -)
American Vacuum Society (1989 -); elected Fellow in 1995
American Physical Society (1984 -); elected Fellow in 1998
American Chemical Society (1981 -); elected Fellow in 2012

EDITORIAL SERVICES TO SCHOLARLY PUBLICATIONS

Co-Guest Editor, *The Journal of Physical Chemistry* (Virtual Special Issue), "Honoring Michael R. Berman," 2022-23
Member, Editorial Advisory Board, *Energy & Environmental Science*, 2021-
Member, Editorial Advisory Board, *Advanced Theory and Simulations*, 2017-
Member, Editorial Advisory Board, *Journal of the American Chemical Society*, 2017-
Member, Inaugural Editorial Advisory Board, *ACS Central Science*, 2015-18
Member, Editorial Advisory Board of *Journal of Physical Chemistry Letters*, 2014-15
Member, Editor-in-Chief Search Committee, *Science*, 2012-13
Member, Editorial Advisory Board of *Journal of Chemical Theory and Computation*, 2010-19
Member, Editor-in-Chief Search Committee, *Journal of Chemical Physics*, 2007-08
Member, Editorial Board of *Annual Review of Physical Chemistry*, 2006-10
Member, Editorial Advisory Board of *Accounts of Chemical Research*, 2005-07
Guest Editor, *Accounts of Chemical Research* special issue on *Computational and Theoretical Chemistry*, 2004-05
Member, Editor-in-Chief Search Committee, *Journal of Physical Chemistry*, 2003-04
Member, Editorial Board of *SIAM Journal on Multiscale Modeling, and Simulation*, 2001-07
Member, Editorial Board of *Modelling and Simulation in Materials Science and Engineering*, 2001-12
Member, Editorial Advisory Board of *ChemPhysChem*, 2000-14
Member, Editorial Board of *Journal of Chemical Physics*, 2000-02
Guest Editor, *Journal of Physical Chemistry* William A. Goddard issue, 1999-2000
Member, Advisory Editorial Board of *Chemical Physics Letters*, 1998-2009
Member, Advisory Editorial Board of *PhysChemComm*, 1998-2002
Member, Editorial Board of the *Encyclopedia of Chemical Physics and Physical Chemistry*, 1999-2001
Member, Editorial Advisory Board of *Journal of Physical Chemistry*, 1995-2000
Member, Editorial Advisory Board of *Surface Science*, 1994-99
Specialist Editor of *Computer Physics Communications*, 1993-94
Member, Editorial Advisory Board of *Molecular Simulation*, 1991-96

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

PROFESSIONAL/COMMUNITY SERVICE

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

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

Outreach activities June 5 - Invited Speaker, Ivy+ 2025 MOR Leadership Workshop, Princeton University
 May 15 - Invited Speaker at the 2025 Annual Meeting, MIT Alumni of Northern New Jersey, Newark, New Jersey
 April 16 - Invited Speaker, Science Salon, NY Academy of Sciences, New York, NY
 April 14 - Invited Speaker, BES Early Career Network (ECN) DOE Fireside Chat, Zoom Series
 March 21 - Invited Speaker, "Carbon Utilization Infrastructure, Markets, Research and Development," NAE Section 3 Zoom Webinar Series
 March 20 - Invited Panelist, "Celebrating Women Leading Innovation and Change," School of Engineering and Applied Science, Princeton University, Princeton, NJ

- February 5 – Invited Speaker, “A Conversation about Climate Intervention Strategies: The Work Ahead,” The Old Guard of Princeton, Princeton, NJ
- 2024 Chair, Scientific Advisory Board, Equatic, Inc., 2024-
Member, Sectional Committee 3 (Chemistry), The Royal Society, 2024-
Member, Stanford University Chemical Engineering External Advisory Committee, 2024
- Outreach activities:* September 18 – Presenter, “[Carbon Utilization, Infrastructure, Research and Development: A Final Report](#),” National Academies of Sciences, Engineering, and Medicine (NASEM) Division Committee on Engineering and Physical Sciences Meeting (held virtually), Washington, DC
- August 19 – Presenter, “[Carbon Utilization Infrastructure, Markets, and Research and Development: A Final Report](#),” National Academies of Sciences, Engineering, and Medicine (NASEM) Public Briefing (held virtually), Washington, DC
- August 7 – Presenter, “Carbon Utilization Infrastructure, Markets, and Research and Development: A Final Report,” National Academies of Sciences, Engineering, and Medicine (NASEM) Sponsor Briefing, Pittsburgh, PA
- March 25 – Invited Speaker, [Lab Showcase: Meet the Princeton Plasma Physics Laboratory: Powering Possibilities for a Clean Energy Future](#),” Federal Laboratory Consortium for Technology Transfer, Washington DC
- March 21 – Invited Distinguished Panelist, [Trends in Translational Research and Innovations in Material Science and Engineering](#),” NAI-NJIT Forum on Sustainable Societies: Advances in Material Science and Engineering, Newark, NJ
- 2023 Co-Lead, Simons Foundation International Collaboration on Solar Radiation Management Science, 2023-
Member, John Scott Award Advisory Committee, 2023-2025
Member, Planning Committee for the 2023 Annual NAE Meeting Forum
- Outreach activities:* October 27 – Panel Moderator, [Andlinger Center for Energy and the Environment Annual Meeting](#): Next-Generation Technologies for Carbon Capture, Utilization, and Storage, Princeton, NJ
- October 23-25 – Chair, [NASEM Webinar Series: Carbon Dioxide Utilization Markets, Infrastructure, Research and Development](#)
- September 18 – Invited Speaker, “Weighing Technology Choices for Climate Mitigation: Now, Later, or Never, and Where?” Princeton Human Values Forum (HVF), Princeton University
- August 30 – Invited Speaker, “Applied Materials and Sustainability Sciences: New Directions for PPPL,” Princeton Collaborative Research Facility (PCRF), Princeton Plasma Physics Lab
- May 26 – Invited Speaker, “Seizing the Climate Mitigation Window: New Initiatives at PPPL and Princeton,” Andlinger Center for Energy and the Environment, Princeton Reunions 2023
- April 5 – Invited Panelist, Princeton NuEnergy U.S. Dept. of Energy EERE Grant Launch, “Innovation in NJ – Growing NJ’s Clean Energy Economy”
- March 15 – Invited Speaker, PPPL Young Professionals Network Spotlight Event

- 2022 Chair, [Committee on Carbon Utilization Infrastructure, Markets, Research and Development](#), National Academies of Science, Engineering, and Medicine (NASEM) (2022-2024)
- [Member, Kavli Foundation Board of Directors](#), 2022-2026
- Member, Visiting Committee for the California Institute of Technology Division of Chemistry and Chemical Engineering
- Outreach activities:* March 1-3 – Chair & Moderator, NASEM Webinar Series: Technology, Infrastructure, and Policy for Carbon Utilization
- March 29 – Invited Presenter, NASEM Division on Engineering and Physical Sciences (DEPS) Committee Meeting
- April 4 – Invited Guest Speaker, Princeton NuEnergy (PNE) FY2022 Q1 Quarterly Conference
- April 27 – Invited Speaker, Collaborative Opportunities in Hydrogen RDD&D Workshop, Andlinger Center for Energy and the Environment, Princeton University
- May 20 – Invited Speaker, “Transforming Carbon Dioxide for a Sustainable Future,” Andlinger Center for Energy and the Environment, Princeton Reunions 2022
- June 30 – Contributed Presenter, “National Academies Congressionally Mandated Study on Carbon Utilization Infrastructure, Markets, and RD&D,” 19th International Conference on Carbon Dioxide Utilization (ICCDU), Princeton, NJ
- September 14 – Keynote Speaker, “Keys to Becoming a Successful Faculty Member,” Princeton Rising Stars in Physics Conference 2022, Princeton, NJ
- September 19-20 – Workshop Organizer, Simons Foundation Science of Solar Geoengineering Workshop, New York, NY
- November 30 – Presenter, “Carbon Dioxide Utilization Markets and Infrastructure: Status and Opportunities: A First Report,” National Academies of Sciences, Engineering, and Medicine (NASEM) Congressional Briefing (held virtually), Washington, DC
- December 1 – Presenter, “Carbon Dioxide Utilization Markets and Infrastructure: Status and Opportunities: A First Report,” National Academies of Sciences, Engineering, and Medicine (NASEM) Public Briefing (held virtually), Washington, DC
- December 5 – Invited Panelist, “A zero-emissions world is not a carbon-free world?” Deloitte-Andlinger Center Leadership Roundtable, Princeton, NJ
- 2021 Facilitator for the Research Corporation for Science Advancement (RSCA) 2021 Scialog Negative Emissions Science (NES) Conference
- Member, Decadal External Review Committee for the Kavli Foundation
- Outreach activities:* October 29 – Invited Speaker: Sustainability and Plasma Sciences, Virtual Visit by the Honorable Jennifer M. Granholm, U.S. Secretary of Energy, Princeton Plasma Physics Laboratory (PPPL), Princeton, NJ
- February 11 – [Interview](#), An Intergenerational Chat Between STEMInists, United Nations (UN) Women for YOUth Newsletter (International Day of Women and Girls in Science), University of California, Los Angeles, Los Angeles, CA

- February 22 – [Invited Speaker/Panelist](#): The Carbon Continuum – Transition to a Net-Zero World, Institute for Carbon Management (ICM), University of California, Los Angeles, Los Angeles, CA
- April 1 – [Interview](#), Carbon sequestration: a critical but less-understood piece of the climate puzzle, Institute of the Environment and Sustainability (IoES), University of California, Los Angeles, Los Angeles, CA
- April 1 – [Invited Speaker/Panelist](#): Overcoming leadership challenges in digital teaching, Times Higher Education (THE) Live USA 2021, London, United Kingdom
- 2020 Member, Search Committee for University of California, Riverside Provost and Executive Vice Chancellor
- Outreach activities:* October 1 – Invited Speaker, Los Angeles Cleantech Incubator (LACI) Power Day, Los Angeles, CA
- July 10 – Panelist, Higher Education Leadership, Virtual California Higher Education Sustainability Conference (CHESC), University of California, Santa Barbara, Santa Barbara, CA
- 2019 Member, NAE Dean’s Roundtable on Linking Academic Engineering Research and Defense Basic Science, 2019-20
- Member, External Advisory Committee of the University of Chicago Institute for Molecular Engineering
- Member, External Review Committee of the Columbia University Fu Foundation School of Engineering and Applied Science
- Outreach activities:* December 12 – Panelist, Way Forward and Actions – How is California Leading the Charge?, Environmental and Climate Change Literacy Project and Summit (ECCLPS), University of California, Los Angeles, Los Angeles, CA
- November 12 – Round Table Panelist, Female Perspective, Jung Female Investigators’ Program, University of Basel, Basel, Switzerland
- October 1 – [Featured Speaker](#), What is a University?, 10 Questions: Centennial Edition, University of California, Los Angeles, Los Angeles, CA
- May 9 – College of Science and Technology Spring Commencement Speaker, Temple University, Philadelphia, PA
- May 6 – Invited Speaker, Welcome Address, Building the Future: New Technological Frontiers in Cities, Princeton University, Princeton, NJ
- April 28 – Featured Speaker, Johns Hopkins University Presidential Brunch Gathering on Sustainability, Johns Hopkins University, Baltimore, MD
- February 25 – Session Chair on Computer Simulation, 11th Annual International Workshop on Advanced Materials (IWAM 2019), Ras Al Khaimah, United Arab Emirates
- January 24 – Panelist, CNBC presents: A Just Energy Transition for the World Panel Discussion, World Economic Forum Annual Meeting 2019, Davos, Switzerland
- January 24 – Panelist, The Promise and Progress of Bioengineering, World Economic Forum Annual Meeting 2019, Davos, Switzerland

- 2018 Member, 2019 Irving Langmuir Prize Selection Committee, 2018-19
 Member, National Academies of Sciences, Engineering, and Medicine (NASEM)
 External Review Committee of the Gulf Research Program, 2018-19
- Outreach activities:* October 4 – Invited Speaker, An Introduction to Engineering and Applied Science at Princeton, China Executive Summit 2018, Princeton University, Princeton, NJ
 May 15 – Invited Speaker, ACS Princeton Local Section May Sectional Meeting, Princeton University, Princeton, NJ
 April 7 – Keynote Speaker, AIChE Regional Conference, Princeton University, Princeton, NJ
 January 26 – Invited Speaker, Women in Leadership Breakfast, Garden Court Hotel, Palo Alto CA
- 2017 October 25 – Speaker, Welcome: Thoughts on the Intersection of Biomedical Research and Data Science, Ahead of the Curve: New Frontiers in Biomedical Data Science, Princeton University, Princeton, NJ
- Outreach activities:* October 18 – Organizing Committee Member and Panel Chair, New Directions in Carbon Dioxide Utilization, The Royal Society of London 2017 Sackler Forum on Dealing with Carbon Dioxide at Scale, Buckinghamshire, UK
 September 6 – Invited Speaker, Overcoming Grand Challenges of the Twenty-First Century: The View from Princeton Engineering, Canyon Partners Research Retreat, Beverly Hills, CA
 May 11 – Invited Speaker, Princeton Alumni Breakfast and Conversation, Henrietta’s Table at The Charles Hotel, Cambridge, MA
 April 26 – Invited Speaker, Annual Dinner of the Princeton Club of Chicago on The Future of Engineering at Princeton, University Club of Chicago, Chicago, IL
 April 4 – Panelist, Women in COMP Post-Doctoral Breakfast, 253rd ACS Spring National Meeting, San Francisco, CA
 February 8 – Invited Speaker, 55th Reunion Reception and Dinner with Princeton Class of 1962, New York Yacht Club, New York, NY
 January 19 – IdeasLab Panelist, Responding to Climate Change with Princeton University, World Economic Forum Annual Meeting 2017, Davos, Switzerland
 January 18 – Panelist, Princeton's Breakfast Panel: Income Inequality and Opportunities to Improve the Human Condition, World Economic Forum Annual Meeting 2017, Davos, Switzerland
- 2016 Member, Molecular Sciences Software Institute (MolSSI) Advisory Board, 2016-17
 Member, Lawrence Berkeley National Laboratory (LBNL) Advisory Board, 2016-25
 Member, Secretary of Energy Advisory Board Task Force on CO₂ Utilization and Negative Emissions, 2016-17 (<https://www.energy.gov/seab/downloads/final-report-task-force-co2-utilization>)
 Member, ExxonMobil Corporate Strategic Research (CSR) Capability Reassessment Committee, 2016
 Member, International Advisory Committee, World Association of Theoretical and Computational Chemists (WATOC) 2017 Conference

- Outreach activities:* December 2 – Invited Speaker, An Overview of Engineering Landscape and Princeton's School of Engineering and Applied Science, President's Retreat on Engineering, Princeton, NJ
- November 15 – Invited Speaker, Sustainable Engineering and Development Society Dinner, Princeton University, Princeton, NJ
- November 10 – Keynote Speaker, Celebrate Princeton Invention 2016, Princeton University, Princeton, NJ
- October 4 – Invited Speaker, Women in Science Colloquium Dinner, Princeton University, Princeton, NJ
- May 28 – Panel Moderator, Princeton Alumni-Faculty Forum, Out of the Box: What's New in Alternative Energy?, Princeton University, Princeton, NJ
- May 18-20 – Organizer and Session Chair, Andlinger Center Building Opening Celebration and Symposium, Princeton University, Princeton, NJ
- April 20 – Invited Speaker, Princeton Preview Faculty Panel, Princeton University, Princeton, NJ
- 2015 *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, 2014-17
- Member, 2015 National Academy of Sciences Award in Chemical Sciences Selection Committee
- Member, SLAC National Accelerator Laboratory Scientific Policy Committee, 2014-16
- Member, International Organizing Committee for the International Congress of Quantum Chemistry, 2014-17
- Outreach activities:* September 10 – Invited Speaker, Butler/PEI Energy Table Discussion & Dinner on The Future of Energy Technologies and Andlinger Center Resources, Butler College, Princeton University, Princeton, NJ
- March 29 – Keynote Speaker, A Tale of Two Evolving Trajectories: Perspectives on a Life in Science and the Future of Energy, Women in STEM Symposium, Princeton University, Princeton, NJ
- March 4 – Princeton Graduate Alumni Dinner Speaker, The Future of Energy (with Dean Vince Poor), Crowne Plaza Hotel, Palo Alto, CA
- January 4 – After-Dinner Speaker, Food, Water, Energy and the Environment, Princeton Food Salon, Princeton, NJ

- 2013 Member, National Academy of Sciences Class Membership Committee, 2013-14
Advisory Council Liaison, NSF Mathematical and Physical Sciences Subcommittee on Optics and Photonics, 2013-14
- Outreach activities:* November 15 – Invited Speaker, Class of 1951 Mini-Reunion, Princeton University, Princeton, NJ
- November 13 – Invited Speaker, Old Guard of Princeton, “Achieving a Sustainable Energy Future via Quantum Mechanics and the Andlinger Center,” Princeton University, Princeton, NJ
- June 26 – 2013 Princeton-CEFRC Summer School Career Panel Discussion, Princeton University, Princeton, NJ
- June 19 – Panelist, Senate/NAS Science and Technology Policy Forum on Energy, Capitol Hill, Washington, DC
- June 1 – Moderator, Princeton Alumni-Faculty Forum Panel, Can We Turn Things Around? Sustainability and Climate Change, Princeton, NJ
- May 9 – Last Lecture for the Class of 2013, “Energy Choices for the 21st Century & Beyond,” Princeton University, Princeton, NJ
- January 9 – Invited Speaker, The Role of Science in Moving the Planet to Green Energy and a Sustainable Future, Nassau Club, Princeton, NJ
- 2012 Member, NSF Mathematical and Physical Sciences Advisory Council, 2012-15
Member, National Academy of Sciences Class Membership and Chemistry in Service to Society Committees, 2012-13
Chair, DOE-BES Council on Chemical and Biochemical Sciences, 2012-13
- Outreach activities:* October 19 – Panelist, What’s Next in Energy, Aspire Colloquium, Princeton University, Princeton, NJ
- June 2 – Moderator, Princeton Alumni-Faculty Forum Panel, Managing Our Expectations: Long-Term Energy Solutions, Princeton, NJ
- May 31 – Panelist, Opportunities and Obstacles in Large-Scale Biomass Utilization – The Role of Chemical Sciences, Chemical Sciences Roundtable, Washington, DC
- April 14 – Moderator, Energy Policy Panel, Princeton Colloquium on Public and International Affairs “The State of the States,” Princeton, NJ
- 2011 Member, International Advisory Board of the Winton Programme for the Physics of Sustainability, Cambridge University, 2011-17
- Outreach activities:* July 14 – Moderator, A Conversation on Global Sustainability, Leading Through Change: A Princeton University Conference, Half Moon Bay, CA
- May 25 – Panelist, A View from Senior EFRC Representatives, Science for our Nation’s Energy Future, Energy Frontier Research Centers Summit & Forum, Washington, DC
- April 16 - Keynote Speaker, Our Future, Our Challenge: 2011 High School Student Eco-Conference, Princeton Day School, Princeton, NJ
- March 1 - Discussant, The Sunlight Derby – How to Win the Never-ending Race to Optimize Energy Risk in the 21st Century, JP Morgan Chase Global Markets Symposium, Key Biscayne, FL

- February 12 – Moderator, Clean Energy Panel, Global China Connection Princeton International Conference, Princeton, NJ
- 2010 Chair, Energy Subdivision of the PHYS Division of the ACS, 2010-11
- Member, Board on Chemical Sciences and Technology, National Research Council, National Academy of Sciences, 2010-12
- Vice-Chair, DOE-BES Council on Chemical and Biochemical Sciences, 2010-11
- July 26-27 – Invited Panelist and Speaker, OSTP/DOE Workshop on Computational Materials Science and Chemistry for Innovation
- Outreach activities:* October 15 – After dinner speaker at Princeton University’s Aspire Leadership Assembly Dinner
- February 19 – After dinner speaker at Princeton University’s Annual Giving Reception and Dinner
- 2009 Conference co-organizer, “Chemical Carbon Mitigation – A Physiochemical Approach, *American Chemical Society Symposium*, Spring 2011, Anaheim, California, 2009-11
- Co-organizer, DOE-BES workshop on Theories of Excited States in Molecules and Nanostructures, 2009-10
- Chair-Elect, Energy Subdivision of the PHYS Division of the ACS, 2009-10
- Outreach activities:* November 17 – Spoke at a Capitol Hill press conference about the impact of American Recovery and Reinvestment Act of 2009 investments in basic scientific research
- November 16 – Spoke at Princeton University Graduate School High Table about new projects in energy research
- March 25 – Invited Speaker on “Women in Research Computing,” Office of Information Technology, Princeton University
- 2008 Member, DOE-BES Council on Chemical and Biochemical Sciences, 2008-11
- Member, International Advisory Board, 4th Multiscale Materials Modeling Conference, October 2008, Florida State University
- 2007 Member, NSF Workshop on Predictive Modeling of Materials at the Nanoscale
- Member, International Scientific Advisory Board, Centre of Excellence in Theoretical and Computational Chemistry, Norway, 2007-10
- Conference co-organizer, “Bold Predictions in Theoretical Chemistry: A Symposium in Honor of One of the Boldest, Bill Goddard, on the Occasion of his 70th Birthday, *American Chemical Society National Meeting*, August 2007, Boston, Massachusetts
- Outreach activities:* Dec 14 - "Pizza with Professors in PRISM", Princeton University, Princeton, NJ
- Dec 13 - Panelist for workshop “Keys to Becoming a Successful Faculty Member,” PICASso Career Workshop, Princeton University, Princeton, NJ
- Dec. 13 – Speaker, “Keys to Becoming a Successful Faculty Member,” PICASso Career Workshop, Princeton University, Princeton, NJ
- April 19 – Speaker, “Mentoring in the Workplace,” Office of Information Technology, Princeton University

- 2006 Member, NSF Review Panel for Cyber-Enabled Chemistry
 Member, DOE-BES Council for Chemical Sciences
 Member, Steering Committee for the Thomas Young Centre for Theory and Simulation of Materials, London, 2006-12
- 2005 Chair, American Conference on Theoretical Chemistry
 Chair, Division of Chemical Physics, American Physical Society
 Member, National Science Foundation Mathematical and Physical Sciences Theory Steering Committee
- Outreach activities:* Sept 24 – Spoke about the need for women in engineering careers to 63 high school girls at the Mother-Daughter Luncheon hosted by Today's World Learning Center Foundation, Ryland Inn, Whitehouse, NJ
- Sept. 22 – Calculus Cameo on Combustion Dynamics to Princeton Freshmen.
- Sept. 12 - Member, Freshman Orientation Panel for the Princeton University Science and Technology Council
- February 4 – Spoke about Materials and Combustion Research to 110 high school girls on a SEAS outreach trip to New York City, organized by the National Coalition of Girls Schools
- January 26 – What's in a Flame? (Combustion Chemistry) presentation at Community Park Elementary School Career Day
- 2004 Chair, Division of Chemical Physics, American Physical Society
 International Advisory Committee, "Conference on Computational Physics," Genoa, Italy, 1-4 September, 2004
 International Advisory Committee, 3rd International Conference on "Computational Modeling and Simulation of Materials" Acireale, Sicily, Italy, May 29-June 5, 2004
 Symposium co-organizer, "Multiscale and Stochastic Modeling Methods," *SIAM Conference on Mathematical Aspects of Materials Science*, Los Angeles, CA, May 23-26, 2004
 Program Chair, Division of Chemical Physics, American Physical Society March Meeting, Montreal, Canada, 22-26 March, 2004
 Member, National Science Foundation Mathematical and Physical Sciences Theory Steering Committee
- 2003 Chair-Elect, Division of Chemical Physics, American Physical Society
 Co-organizer, American Chemical Society Symposium, "New electronic structure methods: from molecules to materials," April, 2003
 Member, Executive Committee for "Materials and Nanotechnology" Strategic Planning Workshop (Princeton University)
- 2002 Vice-Chair, Division of Chemical Physics, American Physical Society
 Organizing Committee Member, Institute for Pure and Applied Math Workshop on Modeling and Simulation for Materials, 18-22 November, 2002

- Conference co-organizer, "Molecular Modeling and Computation: Perspectives and Challenges," Center for Integrative Multiscale Modeling and Simulation, Caltech, Pasadena, CA, 15-16 November, 2002
- Chair, Institute for Pure and Applied Mathematics Workshop on Linear Scaling Electronic Structure Methods, UCLA, 1-4 April, 2002
- Host, Career-Day visitors, Marlborough School (Los Angeles), 25 March 2002.
- 2001 Two lectures, demonstrations, and video presentations etching and corrosion of materials at the UCLA University Elementary School (March 15, 2001)
- Interviewed by graduate student minoring in Women Studies (May 15, 2001)
- Panelist, Women in Science Faculty Roundtable (May 15, 2001)
- 2000 International Advisory Committee Member, 10th International Conference on Solid Films and Surfaces (ICSFS-10)
- Member, Los Alamos National Laboratory Theoretical Division Advisory and Review Committee, 2000-05
- Member, Physics and Astronomy Classification Scheme (PACS) Working Group, April 2000
- Lecture on phases, molecular motion, energy, atomic structure, and molecular dynamics to 4th grade science students at Willows Community School in Los Angeles, March 17, 2000
- 1999 Sole Faculty Representative of the University of California system at the Science Coalition Signature Event, the purpose of which was to explain to Congress, in one-on-one meetings with Congressional Representatives or their staff, the importance of funding basic scientific research at Universities (Sept. 22, 1999)
- Proposal Coordinator and Proposed Director of a UCLA Materials Research Science and Engineering Center (pre-proposal submitted Sept. 10, 1999)
- Member, NSF Division of Materials Research Committee of Visitors, February 24-26, 1999
- 1998 Member, NSF Materials Research Science and Engineering Center Reverse Site Visit Review Panel, May 4-7, 1998
- Reviewer for the National Research Council's Committee on Review and Evaluation of the Army Chemical Stockpile Disposal Program's Report on "Using Supercritical Water Oxidation to Treat Hydrolysate from VX Neutralization," February 3, 1998
- 1996 January 1996-December 1997: Executive Committee Member, Electronic Materials and Processing Division of the American Vacuum Society
- 1995 Panelist, Diversity Forum at the National Organization for the Professional Advancement of Black Chemists and Chemical Engineers, 20 April 1995
- Conference co-organizer, "Metal-Metal Bonding: From Clusters to Surfaces," American Chemical Society National Meeting, Anaheim, CA, 2-7 April, 1995
- American Chemical Society Awards Committee for the ACS Award for Encouraging Women into Careers in the Chemical Sciences (1995-1997)
- 1994-1997 Executive Committee Member, Division of Computational Physics of the American Physical Society

- 1994 Discussion Leader, Career Paths and Strategies for Success as a Woman in Science, at Caltech, 10 November 1994
Participant, Sigma Xi Planning Conference for the Sigma Xi 1995 Forum on Science Policy, 8-11 September 1994
1994 ACS Division of Physical Chemistry Procter & Gamble Award Committee
Panelist, Women in Science Roundtable Discussion: Personal Experiences, Strategies for Success, and a Look to the Future, University of Toronto, Canada, 19 May 1994
Discussion Leader, "On Issues Concerning Women in the Workplace," UCLA Chemistry and Biochemistry Department, 29 April 1994
University of California Regents Scholarship Interviewer, 16 April 1994
Panelist, 1994 Workshop on "Women in the Sciences: Rising to the Challenge," at UCLA, 27 January 1994
- 1993 Conference Chair, "14th Annual West Coast Theoretical Chemistry Conference," UCLA, CA, 17-19 June 1993
- 1992 Panelist, 1992 National Science Foundation Postdoctoral Fellowships in Chemistry
- 1992-1994 Executive Committee Member, Surface Science Division of the American Vacuum Society
- 1992-1995 Executive Committee Member, Division of Physical Chemistry of the American Chemical Society
- 1991 Conference co-organizer, "Richard B. Bernstein Memorial Symposium," Los Angeles, CA, 19-20 April 1991
Participant, "1991 Workshop on Chemical Education," University of Utah, Salt Lake City, Utah, 22-24 March 1991
- 1990 Conference co-organizer, "Physics, Chemistry, and Materials Science of Clusters", ONR Contractors Conference, Lake Arrowhead, CA, 21 - 23 January 1990
- 1989 Caltech/MIT High School Visitation Program (1989-1992)

LIST OF PUBLICATIONS

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479. Z. Wei, J.-N. Boyn, J.M. P. Martirez, and E. A. Carter, "Accelerating Embedding Potential Optimization by Reconstructing the Pseudo-Valence Electron Density," *J. Chem. Theory Comput.* **21**, 7782 (2025). doi.org/10.1021/acs.jctc.5c00488
478. Z. Wei and E. A. Carter, "Embedded Random Phase Approximation for Magnetic Systems: H₂ Dissociative Adsorption on Fe(110)," *J. Chem. Phys.* **163**, 034120 (2025). <https://doi.org/10.1063/5.0271416>
477. D. V. Potapenko, Z. Chen, S. Xu, X. Yang, I. Waluyo, A. Gilman, E. A. Carter, and B. E. Koel, "Methanol Adsorption and Dissociation on GaP(110) Studied by Ambient Pressure X-ray Photoelectron Spectroscopy," *Surface Science*, **758**, 122743 (2025). doi.org/10.1016/j.susc.2025.122743 Part of the special issue and chosen as the cover article in "60 years of Surface Science: Achievements and Perspectives".

476. J. M. P. Martirez, S. Kurdziel, and E. A. Carter, "First-Principles Insights into the Thermocatalytic Cracking of Ammonia-Hydrogen Blends on Fe(110). 2. Kinetics," *Journal of Physical Chemistry C*, **129**, 6697 (2025). doi.org/10.1021/acs.jpcc.4c07303
475. A. D. Lele, Z. Shi, S. Khetan, E. A. Carter, J. M. P. Martirez, and Y. Ju, "Machine-learned force field for molecular dynamics simulation of non-equilibrium ammonia synthesis on iron catalysts," *Journal of Physical Chemistry C*, **129**, 4937 (2025). doi.org/10.1021/acs.jpcc.4c07596
474. J.-N. Boyn and E. A. Carter, "Elucidating and contrasting the mechanisms for Mg and Ca sulfate ion-pair formation with multi-level embedded quantum mechanics/molecular dynamics simulations," *Journal of Chemical Physics*, **161**, 224501 (2024). doi.org/10.1063/5.0235460.
473. E. A. Carter, S. Atsumi, M. Byron, J. Chen, S. Comello, M. Fan, B. Freeman, M. Fry, S. Jordaan, H. Mahgerefteh, A.-H. Park, J. Powell, A. R. Ramirez, V. Sick, S. Stewart, J. Trembly, J. Yang, J. Yuan, C. Wise, and E. Zeitler, "Carbon Utilization Infrastructure, Markets, and Research and Development: A Final Report," National Academies of Sciences, Engineering, and Medicine (NASEM). Washington DC: The National Academies Press. ISBN: 978-0-309-71775-5 (2024). [doi: 10.17226/27732](https://doi.org/10.17226/27732)
472. E. A. Carter, "Our Role in Solving Global Challenges: An Opinion," *J. Am. Chem. Soc.*, **146**, 21193 (2024). [doi: 10.1021/jacs.4c07374](https://doi.org/10.1021/jacs.4c07374)
471. X. Wen, J.-N. Boyn, J. M. P. Martirez, Q. Zhao, and E. A. Carter, "Strategies to obtain reliable energy landscapes from embedded multireference correlated wavefunction methods for surface reactions," *Journal of Chemical Theory and Computation*, **20**, 6037 (2024). [doi: 10.1021/acs.jctc.4c00558](https://doi.org/10.1021/acs.jctc.4c00558)
470. B. Bobell, J.-N. Boyn, J. M. P. Martirez, and E. A. Carter, "Modeling Bicarbonate Formation in an Alkaline Solution with Multi-Level Quantum Mechanics/Molecular Dynamics Simulations," *Molecular Physics Special Issue in Honour of Giovanni Ciccotti*, **123** (7-8), e2375370 (2025); published online in 2024. [doi: 10.1080/00268976.2024.2375370](https://doi.org/10.1080/00268976.2024.2375370)
469. X. Wen, J. M. P. Martirez, and E. A. Carter, "Plasmon-driven ammonia decomposition on Pd(111): Hole transfers role in changing rate-limiting steps," *ACS Catalysis*, **14**, 9539 (2024). [doi: 10.1021/acscatal.4c01869](https://doi.org/10.1021/acscatal.4c01869)
468. Z. Wei, J. M. P. Martirez, and E. A. Carter, "First-Principles Insights into the Thermodynamics of Variable-Temperature Ammonia Synthesis on Transition-Metal-Doped Cu (100) and (111)," *ACS Energy Lett.*, **9**, 3012 (2024). [doi: 10.1021/acsenerylett.4c01100](https://doi.org/10.1021/acsenerylett.4c01100)
467. A. G. Rajan, J. M. P. Martirez, and E. A. Carter, "Strongly Facet-Dependent Activity of Iron-Doped β -Nickel Oxyhydroxide for the Oxygen Evolution Reaction," *Phys. Chem. Chem. Phys.* 25th Anniversary Special Issue, **26**, 14721 (2024). [doi: 10.1039/D4CP00315B](https://doi.org/10.1039/D4CP00315B)
466. J.-N. Boyn and E. A. Carter, "Characterizing the Mechanisms of Ca and Mg Carbonate Ion-Pair Formation with Multi-Level Molecular Dynamics/Quantum Mechanics Simulations," *J. Phys. Chem. B*, **127**, 10824 (2023). [doi: 10.1021/acs.jpcc.3c05369](https://doi.org/10.1021/acs.jpcc.3c05369)

465. A. Acosta, J. M. P. Martirez, N. Lim, J. P. Chang, and E. A. Carter, "Effect of thickness and surface composition on the stability of polarization in ferroelectric $\text{Hf}_{1-x}\text{Zr}_x\text{O}_2$ thin films," *Phys. Rev. Mater.*, **7**, 124401 (2023). [doi: 10.1103/PhysRevMaterials.7.124401](https://doi.org/10.1103/PhysRevMaterials.7.124401)
464. Z. Wei, J. M. P. Martirez, and E. A. Carter, "Introducing the Embedded Random Phase Approximation: H_2 Dissociative Adsorption on Cu(111) as an Exemplar," *J. Chem. Phys.*, **159**, 194108 (2023). [doi: 10.1063/5.0181229](https://doi.org/10.1063/5.0181229)
463. M. B. Bertagni, R. H. Socolow, J. M. P. Martirez, E. A. Carter, C. Greig, Y. Ju, T. Lieuwen, M.E. Mueller, S. Sundaresan, R. Wang, M. A. Zondlo, and A. Porporato, "Minimizing the Impacts of the Ammonia Economy on the Nitrogen Cycle and Climate," *Proc. Natl. Acad. Sci. U.S.A.*, **120**, e2311728120 (2023). [doi: 10.1073/pnas.2311728120](https://doi.org/10.1073/pnas.2311728120)
462. J.-N. Boyn and E. A. Carter, "Probing pH-Dependent Dehydration Dynamics of Mg and Ca Cations in Aqueous Solutions with Multi-Level Quantum Mechanics/Molecular Dynamics Simulations," *J. Am. Chem. Soc.*, **145**, 20462 (2023). [doi: 10.1021/jacs.3c06182](https://doi.org/10.1021/jacs.3c06182)
461. J. M. P. Martirez and E. A. Carter, "Solvent dynamics are critical to understanding carbon dioxide dissolution and hydration in water," *J. Am. Chem. Soc.*, **145**, 1256 (2023). [doi: 10.1021/jacs.3c01283](https://doi.org/10.1021/jacs.3c01283)
460. E. A. Carter, M. A. Johnson, and S. R. Leone, "A Tribute to Michael R. Berman," *J. Phys. Chem. C*, **127**, 11421 (2023). [doi: 10.1021/acs.jpcc.3c03070](https://doi.org/10.1021/acs.jpcc.3c03070)
459. R. B. Wexler, G. S. Gautam, R. Bell, S. Shulda, N. A. Strange, J. A. Trindell, J. D. Sugar, E. Nygren, S. Sainio, A. H. McDaniel, D. Ginley, E. A. Carter, and E. B. Stechel, "Multiple and nonlocal cation redox in Ca–Ce–Ti–Mn oxide perovskites for solar thermochemical applications," *Energy Environ. Sci.*, **16**, 2550 (2023). [doi: 10.1039/d3ee00234a](https://doi.org/10.1039/d3ee00234a)
458. R. B. Wexler, E. B. Stechel, and E. A. Carter, "Materials Design Directions for Solar Thermochemical Water Splitting," in *Solar Fuels*, Vol. 3, Nurdan Demirci Sankir & Mehmet Sankir, Eds. (Wiley-Scrivener, USA), 3-64 (2023). [doi: 10.1002/9781119752097.ch1](https://doi.org/10.1002/9781119752097.ch1)
457. L. Li, M. F. Calegari Andrade, R. Car, A. Selloni, and E. A. Carter, "Characterizing Structure-Dependent TiS_2 /Water Interfaces using Deep-Neural-Network-Assisted Molecular Dynamics," *J. Phys. Chem. C*, **127**, 9750 (2023). [doi: 10.1021/acs.jpcc.2c08581](https://doi.org/10.1021/acs.jpcc.2c08581)
456. J. Cai, Q. Zhao, W.-Y. Hsu, C. Choi, J. M. P. Martirez, C. Chen, J. Huang, E. A. Carter, and Y. Huang, "Highly Selective Electrochemical Reduction of CO_2 into Methane on Nanotwinned Cu," *J. Am. Chem. Soc.*, **145**, 9136 (2023). [doi: 10.1021/jacs.3c00847](https://doi.org/10.1021/jacs.3c00847)
455. P. Chen, D. Fan, Y. Zhang, A. Selloni, E. A. Carter, C. B. Arnold, Y. Zhang, A. S. Gross, J. R. Chelikowsky, and N. Yao, "Observation of Electron Orbital Signatures of Single Atoms within Metal-Phthalocyanines using Atomic Force Microscopy," *Nat. Commun.*, **14**, 1460 (2023). [doi: 10.1038/s41467-023-37023-9](https://doi.org/10.1038/s41467-023-37023-9)

454. E. A. Carter, S. Atsumi, M. Byron, A. Chunev, S. Comello, M. Fan, M. Fry, H. Mahgerefteh, E. Massetti, A.-H. Park, J. Powell, A. R. Ramírez, V. Sick, C. Wise, and E. Zeitler, "Carbon Dioxide Utilization Markets and Infrastructure: Status and Opportunities: A First Report," National Academies of Sciences, Engineering, and Medicine (NASEM), Washington, DC: The National Academies Press, ISBN 978-0-309-69327-1 (2023). [doi: 10.17226/26703](https://doi.org/10.17226/26703)
453. Y. Yuan, L. Zhou, J. L. Bao, J. Zhou, A. Bayles, L. Yuan, M. Lou, M. Lou, S. Khatiwada, H. Robatjazi, E. A. Carter, P. Nordlander, and N. J. Halas, "Earth-abundant photocatalyst for H₂ generation from NH₃ with light-emitting diode illumination," *Science*, **378**, 889 (2022). [doi: 10.1126/science.abn5636](https://doi.org/10.1126/science.abn5636)
452. L. Yuan, J. Zhou, M. Zhang, X. Wen, J. M. P. Martirez, H. Robatjazi, L. Zhou, E. A. Carter, P. Nordlander, and N. J. Halas, "Plasmonic Photocatalysis with Chemically and Spatially Specific Antenna-Dual Reactor Complexes," *ACS Nano*, **16**, 17365 (2022). [doi: 10.1021/acsnano.2c08191](https://doi.org/10.1021/acsnano.2c08191)
451. R. B. Wexler and E. A. Carter, "Oxygen-Chlorine Chemisorption Scaling for Seawater Electrolysis on Transition Metals: The Role of Redox," *Adv. Theory Simul.*, 2200592 (2022). [doi: 10.1002/adts.202200592](https://doi.org/10.1002/adts.202200592)
450. J. M. P. Martirez and E. A. Carter, "First-Principles Insights into the Thermocatalytic Cracking of Ammonia-Hydrogen Blends on Fe(110): 1. Thermodynamics," *J. Phys. Chem. C*, **126**, 19733 (2022). (Virtual Special Issue: Honoring Michael R. Berman) [doi: 10.1021/acs.jpcc.2c06003](https://doi.org/10.1021/acs.jpcc.2c06003)
449. Q. Zhao, J. M. P. Martirez, and E. A. Carter, "Charting C-C coupling pathways in electrochemical CO₂ reduction on Cu(111) using embedded correlated wavefunction theory," *Proc. Natl. Acad. Sci. U.S.A.*, **119**, e2202931119 (2022). [doi: 10.1073/pnas.2202931119](https://doi.org/10.1073/pnas.2202931119)
448. Q. Zhao, J. M. P. Martirez, and E. A. Carter, "Electrochemical Hydrogenation of CO on Cu(100): Insights from Accurate Multiconfigurational Wavefunction Methods," *J. Phys. Chem. Lett.*, **13**, 10282 (2022). [doi: 10.1021/acs.jpcllett.2c02444](https://doi.org/10.1021/acs.jpcllett.2c02444)
447. A. M. Teale, T. Helgaker, A. Savin, C. Adamo, B. Aradi, A. V. Arbuznikov, P. W. Ayers, E. J. Baerends, V. Barone, P. Calaminici, E. Cancès, E. A. Carter, P. K. Chattaraj, H. Chermette, I. Ciofini, T. D. Crawford, F. D. Proft, J. F. Dobson, C. Draxl, T. Frauenheim, E. Fromager, P. Fuentealba, L. Gagliardi, G. Galli, J. Gao, P. Geerlings, N. Gidopoulos, P. M. W. Gill, P. Gori-Giorgi, A. Görling, T. Gould, S. Grimme, O. Gritsenko, H. J. A. Jensen, E. R. Johnson, R. O. Jones, M. Kaupp, A. M. Köster, L. Kronik, A. I. Krylov, S. Kvall, A. Laestadius, M. Levy, M. Lewin, S. Liu, P. -F. Loos, N. T. Maitra, F. Neese, J. P. Perdew, K. Pernal, P. Pernot, P. Piecuch, E. Rebolini, L. Reining, P. Romaniello, A. Ruzsinszky, D. R. Salahub, M. Scheffler, P. Schwerdtfeger, V. N. Staroverov, J. Sun, E. Tellgren, D. J. Tozer, S. B. Trickey, C. A. Ullrich, A. Vela, G. Vignale, T. A. Wesolowski, X. Xu, and W. Yang, "DFT exchange: sharing perspectives on the workhorse of quantum chemistry and materials science," *Phys. Chem. Chem. Phys.*, **24**, 28700 (2022). (Hot Article) [doi: 10.1039/d2cp02827a](https://doi.org/10.1039/d2cp02827a)

446. M. Lou, J. L. Bao, L. Zhou, G. N. Naidu, H. Robatjazi, A. I. Bayles, H. O. Everitt, P. Nordlander, E. A. Carter, and N. J. Halas, "Direct H₂S Decomposition by Plasmonic Photocatalysis: Efficient Remediation plus Sustainable Hydrogen Production," *ACS Energy Lett.*, **7**, 3666 (2022). [doi: 10.1021/acsenergylett.2c01755](https://doi.org/10.1021/acsenergylett.2c01755)
445. H. Robatjazi, A. Schirato, A. Alabastri, P. Christopher, E. A. Carter, P. Nordlander, and N. J. Halas, "Reply to: Distinguishing thermal from non-thermal contributions to plasmonic hydrodefluorination," *Nat. Catal.*, **5**, 247 (2022). [doi: 10.1038/s41929-022-00768-5](https://doi.org/10.1038/s41929-022-00768-5)
444. S. Zhai, J. Nam, G. S. Gautam, K. Lim, J. Rojas, M. F. Toney, E. A. Carter, I.-H. Jung, W. C. Chueh, and A. Majumdar, "Thermodynamic guiding principles of high-capacity phase transformation materials for splitting H₂O and CO₂ by thermochemical looping," *J. Mater. Chem. A*, **10**, 3552 (2022). [doi: 10.1039/d1ta10391a](https://doi.org/10.1039/d1ta10391a)
443. A. Acosta, J. M. P. Martirez, N. Lim, J. P. Chang, and E. A. Carter, "Relationship between ferroelectric polarization and stoichiometry of HfO₂ surfaces," *Phys. Rev. Mater.*, **5**, 124417 (2021). [doi: 10.1103/PhysRevMaterials.5.124417](https://doi.org/10.1103/PhysRevMaterials.5.124417)
442. L. Li, J. M. P. Martirez, and E. A. Carter, "Identifying an Alternative Hydride Transfer Pathway for CO₂ Reduction on CdTe(111) and CuInS₂(112) Surfaces," *Adv. Theory Simul.*, **5**, 2100413 (2021). [doi: 10.1002/adts.202100413](https://doi.org/10.1002/adts.202100413)
441. O. Y. Long, G. S. Gautam, and E. A. Carter, "Assessing cathode property prediction *via* exchange-correlation functionals with and without long-range dispersion corrections," *Phys. Chem. Chem. Phys.*, **23**, 24726 (2021). [doi: 10.1039/d1cp03163e](https://doi.org/10.1039/d1cp03163e)
440. P. Chen, D. Fan, Y. Zhang, A. Selloni, E. A. Carter, C. B. Arnold, D. C. Dankworth, S. P. Rucker, J. R. Chelikowsky, and N. Yao, "Breaking a dative bond with mechanical forces," *Nat. Commun.*, **12**, 5635 (2021). (Editors' Highlight) [doi: 10.1038/s41467-021-25932-6](https://doi.org/10.1038/s41467-021-25932-6)
439. A. G. Rajan, J. M. P. Martirez, and E. A. Carter, "Coupled Effects of Temperature, Pressure, and pH on Water Oxidation Thermodynamics and Kinetics," *ACS Catal.*, **11**, 11305 (2021). [doi: 10.1021/acscatal.1c02428](https://doi.org/10.1021/acscatal.1c02428)
438. R. B. Wexler, G. S. Gautam, E. B. Stechel, and E. A. Carter, "Factors Governing Oxygen Vacancy Formation in Oxide Perovskites," *J. Am. Chem. Soc.*, **143**, 13212 (2021). (JACS Highly Cited Paper from 2020-21) [doi: 10.1021/jacs.1c05570](https://doi.org/10.1021/jacs.1c05570)
437. J. M. P. Martirez and E. A. Carter, "Metal-to-Ligand Charge-Transfer Spectrum of a Ru-Bipyridine-Sensitized TiO₂ Cluster from Embedded Multiconfigurational Excited-State Theory," *J. Phys. Chem. A*, **125**, 4998 (2021). (Virtual Special Issue on "125 Years of *The Journal of Physical Chemistry*") [doi: 10.1021/acs.jpca.1c02628](https://doi.org/10.1021/acs.jpca.1c02628)
436. J. M. P. Martirez and E. A. Carter, "Projector-Free Capped-Fragment Scheme within Density Functional Embedding Theory for Covalent and Ionic Compounds," *J. Chem. Theory Comput.*, **17**, 4105 (2021). [doi: 10.1021/acs.jctc.1c00285](https://doi.org/10.1021/acs.jctc.1c00285)

435. L. Zhou, M. Lou, J. L. Bao, C. Zhang, J. G. Liu, J. M. P. Martirez, S. Tian, L. Yuan, D. F. Swearer, H. Robotjazi, E. A. Carter, P. Nordlander, and N. J. Halas, "Hot carrier multiplication in plasmonic photocatalysis," *Proc. Natl. Acad. Sci. U.S.A.*, **118**, e2022109118 (2021). [doi: 10.1073/pnas.2022109118](https://doi.org/10.1073/pnas.2022109118)
434. Q. Zhao, J. M. P. Martirez, and E. A. Carter, "Revisiting Understanding of Electrochemical CO₂ Reduction on Cu(111): Competing Proton-Coupled Electron Transfer Reaction Mechanisms Revealed by Embedded Correlated Wavefunction Theory," *J. Am. Chem. Soc.*, **143**, 6152 (2021). [doi: 10.1021/jacs.1c00880](https://doi.org/10.1021/jacs.1c00880)
433. J. M. P. Martirez, J. L. Bao, and E. A. Carter, "First-Principles Insights into Plasmon-Induced Catalysis," *Annu. Rev. Phys. Chem.*, **72**, 99 (2021). [doi: 10.1146/annurev-physchem-061020-053501](https://doi.org/10.1146/annurev-physchem-061020-053501)
432. R. B. Wexler, G. S. Gautam, and E. A. Carter, "Optimizing kesterite solar cells from Cu₂ZnSnS₄ to Cu₂CdGe(S,Se)₄," *J. Mater. Chem. A*, **9**, 9882 (2021). [doi: 10.1039/d0ta11603c](https://doi.org/10.1039/d0ta11603c)
431. E. A. Carter, "Autobiography of Emily A. Carter," *J. Phys. Chem. A*, **125**, 1671 (2021). [doi: 10.1021/acs.jpca.0c10044](https://doi.org/10.1021/acs.jpca.0c10044); *J. Phys. Chem. C*, **125**, 4333 (2021). [doi: 10.1021/acs.jpcc.0c10436](https://doi.org/10.1021/acs.jpcc.0c10436)
430. A. J. Tkalych, H. Zhuang, and E. A. Carter, "An Integrated Methodology for Screening Hydrogen Evolution Reaction Catalysts: Pt/Mo₂C as an Example," in *Computational Materials, Chemistry, and Biochemistry: From Bold Initiatives to the Last Mile (In Honor of William A. Goddard's Contributions to Science and Engineering)*, Vol. 284, pp. 719-731, Richard Muller & Sadasivan Shankar, Eds. (Springer Series in Materials Science), ISBN 978-3-030-18777-4 (2021). [doi: 10.1007/978-3-030-18778-1_31](https://doi.org/10.1007/978-3-030-18778-1_31)
429. R. Sheil, J. M. P. Martirez, X. Sang, E. A. Carter, and J. P. Chang, "Precise Control of Nanoscale Cu Etching via Gas-Phase Oxidation and Chemical Complexation," *J. Phys. Chem. C*, **125**, 1819 (2021). [doi: 10.1021/acs.jpcc.0c08932](https://doi.org/10.1021/acs.jpcc.0c08932)
428. S. Xu and E. A. Carter, "CO₂ Photoelectrochemical Reduction Catalyzed by a GaP(001) Photoelectrode," *ACS Catal.*, **11**, 1233 (2021). [doi: 10.1021/acscatal.0c04240](https://doi.org/10.1021/acscatal.0c04240)
427. A. Gupta, A. G. Rajan, E. A. Carter, and H. A. Stone, "Ionic Layering and Overcharging in Electrical Double Layers in a Poisson-Boltzmann Model," *Phys. Rev. Lett.*, **125**, 188004 (2020). [doi: 10.1103/PhysRevLett.125.188004](https://doi.org/10.1103/PhysRevLett.125.188004)
426. L. Li, S. Xu, and E. A. Carter, "First-Principles Modeling of Sodium Ion and Water Intercalation into Titanium Disulfide Interlayers for Water Desalination," *Chem. Mater.*, **32**, 10678 (2020). [doi: 10.1021/acs.chemmater.0c03891](https://doi.org/10.1021/acs.chemmater.0c03891)
425. A. Gupta, A. G. Rajan, E. A. Carter, and H. A. Stone, "Thermodynamics of Electrical Double Layers with Electrostatic Correlations," *J. Phys. Chem. C*, **124**, 26830 (2020). [doi: 10.1021/acs.jpcc.0c08554](https://doi.org/10.1021/acs.jpcc.0c08554)
424. G. S. Gautam, E. B. Stechel, and E. A. Carter, "Exploring Ca-Ce-M-O (M = 3d Transition Metal) Oxide Perovskites for Solar Thermochemical Applications," *Chem. Mater.*, **32**, 9964 (2020). [doi: 10.1021/acs.chemmater.0c02912](https://doi.org/10.1021/acs.chemmater.0c02912)

423. A. G. Rajan and E. A. Carter, "Microkinetic model for pH- and potential-dependent oxygen evolution during water splitting on Fe-doped β -NiOOH," *Energy Environ. Sci.*, **13**, 4962 (2020). (Hot Article) [doi: 10.1039/d0ee02292f](https://doi.org/10.1039/d0ee02292f)
422. A. G. Rajan and E. A. Carter, "Discovering Competing Electrocatalytic Mechanisms and Their Overpotentials: Automated Enumeration of Oxygen Evolution Pathways," *J. Phys. Chem. C*, **124**, 24883 (2020). [doi: 10.1021/acs.jpcc.0c08120](https://doi.org/10.1021/acs.jpcc.0c08120)
421. Q. Zhao, X. Zhang, J. M. P. Martirez, and E. A. Carter, "Benchmarking an Embedded Adaptive Sampling Configuration Interaction Method for Surface Reactions: H₂ Desorption from and CH₄ Dissociation on Cu(111)," *J. Chem. Theory Comput.*, **16**, 7078 (2020). [doi: 10.1021/acs.jctc.0c00341](https://doi.org/10.1021/acs.jctc.0c00341)
420. L. Li, J. M. P. Martirez, and E. A. Carter, "Prediction of Highly Selective Electrocatalytic Nitrogen Reduction at Low Overpotential on a Mo-doped g-GaN Monolayer," *ACS Catal.*, **10**, 12841 (2020). [doi: 10.1021/acscatal.0c03140](https://doi.org/10.1021/acscatal.0c03140)
419. A. G. Rajan, J. M. P. Martirez, and E. A. Carter, "Why Do We Use the Materials and Operating Conditions We Use for Heterogeneous (Photo)Electrochemical Water Splitting?," *ACS Catal.*, **10**, 11177 (2020). [doi: 10.1021/acscatal.0c01862](https://doi.org/10.1021/acscatal.0c01862)
418. Q. Zhao and E. A. Carter, "Revisiting Competing Paths in Electrochemical CO₂ Reduction on Copper via Embedded Correlated Wavefunction Theory," *J. Chem. Theory Comput.*, **16**, 6528 (2020). [doi: 10.1021/acs.jctc.0c00583](https://doi.org/10.1021/acs.jctc.0c00583)
417. G. S. Gautam, E. B. Stechel, and E. A. Carter, "A First-Principles-Based Sub-Lattice Formalism for Predicting Off-Stoichiometry in Materials for Solar Thermochemical Applications: The Example of Ceria," *Adv. Theory Simul.*, **3**, 2000112 (2020). [doi: 10.1002/adts.202000112](https://doi.org/10.1002/adts.202000112)
416. R. B. Wexler, G. S. Gautam, and E. A. Carter, "Exchange-correlation functional challenges in modeling quaternary chalcogenides," *Phys. Rev. B*, **102**, 054101 (2020). [doi: 10.1103/PhysRevB.102.054101](https://doi.org/10.1103/PhysRevB.102.054101)
415. H. Robatjazi, J. L. Bao, L. Zhou, M. Zhang, P. Christopher, E. A. Carter, P. Nordlander, and N. J. Halas, "Plasmon-driven carbon-fluorine (C(*sp*³)-F) bond activation with mechanistic insights into hot-carrier-mediated pathways," *Nat. Catal.*, **3**, 564 (2020). [doi: 10.1038/s41929-020-0466-5](https://doi.org/10.1038/s41929-020-0466-5)
414. O. Y. Long, G. S. Gautam, and E. A. Carter, "Evaluating optimal *U* for 3d transition-metal oxides within the SCAN+*U* framework," *Phys. Rev. Mat.*, **4**, 045401 (2020). [doi: 10.1103/PhysRevMaterials.4.045401](https://doi.org/10.1103/PhysRevMaterials.4.045401)
413. H. Lischka, R. Shepard, T. Müller, P. G. Szalay, R. M. Pitzer, A. J. A. Aquino, M. M. Araújo do Nascimento, M. Barbatti, L. T. Belcher, J.-P. Blaudeau, I. Borges Jr., S. R. Brozell, E. A. Carter, A. Das, G. Gidofalvi, L. Gonzalez, W. L. Hase, G. Kedziora, M. Kertesz, F. Kossoski, F. B. C. Machado, S. Matsika, S. A. do Monte, D. Nachtigallova, R. Nieman, M. Oppel, C. A. Parish, F. Plasser, R. F. K. Spada, E. A. Stahlberg, E. Ventura, D. R. Yarkony, and Z. Zhang, "The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry," *J. Chem. Phys.*, **152**, 134110 (2020). [doi: 10.1063/1.5144267](https://doi.org/10.1063/1.5144267)

412. S. Xu and E. A. Carter, "Oxidation State of GaP Photoelectrode Surfaces under Electrochemical Conditions for Photocatalytic CO₂ Reduction," *J. Phys. Chem. B*, **124**, 2255 (2020). [doi: 10.1021/acs.jpcc.0c01236](https://doi.org/10.1021/acs.jpcc.0c01236)
411. J. M. P. Martirez and E. A. Carter, "Secondary Transition-Metal Dopants for Enhanced Electrochemical O₂ Formation and Desorption on Fe-Doped β -NiOOH," *ACS Energy Lett.*, **5**, 962 (2020). [doi: 10.1021/acsenergylett.9b02761](https://doi.org/10.1021/acsenergylett.9b02761)
410. J. M. P. Martirez and E. A. Carter, "Noninnocent Influence of Host β -NiOOH Redox Activity on Transition-Metal Dopants' Efficacy as Active Sites in Electrocatalytic Water Oxidation," *ACS Catal.*, **10**, 2720 (2020). [doi: 10.1021/acscatal.9b05092](https://doi.org/10.1021/acscatal.9b05092)
409. A. G. Rajan, J. M. P. Martirez, and E. A. Carter, "Facet-Independent Oxygen Evolution Activity of Pure β -NiOOH: Different Chemistries Leading to Similar Overpotentials," *J. Am. Chem. Soc.*, **142**, 3600 (2020). [doi: 10.1021/jacs.9b13708](https://doi.org/10.1021/jacs.9b13708)
408. L. Zhou, J. M. P. Martirez, J. Finzel, C. Zhang, D. F. Swearer, S. Tian, H. Robatjazi, M. Lou, L. Dong, L. Henderson, P. Christopher, E. A. Carter, P. Nordlander, and N. J. Halas, "Light-driven methane dry reforming with single atomic site antenna-reactor plasmonic photocatalysts," *Nat. Energy*, **5**, 61 (2020). (WOS Highly Cited and Hot Paper in 2021-22) [doi: 10.1038/s41560-019-0517-9](https://doi.org/10.1038/s41560-019-0517-9)
407. B. G. del Rio, G. S. Gautam, and E. A. Carter, "Deuterium addition to liquid Li-Sn alloys: implications for plasma-facing applications," *Nucl. Fusion*, **60**, 016025 (2019). [doi: 10.1088/1741-4326/ab523c](https://doi.org/10.1088/1741-4326/ab523c)
406. S. Xu and E. A. Carter, "Optimal functionalization of a molecular electrocatalyst for hydride transfer," *Proc. Natl. Acad. Sci. U.S.A.*, **116**, 22953 (2019). [doi: 10.1073/pnas.1911948116](https://doi.org/10.1073/pnas.1911948116)
405. S. Hadke, S. Levchenko, G. S. Gautam, C. J. Hages, J. A. Márquez, F. Oliva, V. Izquierdo-Roca, E. A. Carter, T. Unold, and L. H. Wong, "Suppressed Deep Traps and Bandgap Fluctuations in Cu₂CdSnS₄ Solar Cells with $\approx$ 8% Efficiency," *Adv. Energy Mater.*, **9**, 1902509 (2019). [doi: 10.1002/aenm.201902509](https://doi.org/10.1002/aenm.201902509)
404. C. Hepburn, E. Adlen, J. Beddington, E. A. Carter, S. Fuss, N. Mac Dowell, J. C. Minx, P. Smith, and C. Williams, "The technological and economic prospects for CO₂ utilization and removal," *Nature*, **575**, 87 (2019). (WOS Highly Cited and Hot Paper in 2021-22) [doi: 10.1038/s41586-019-1681-6](https://doi.org/10.1038/s41586-019-1681-6)
403. J. L. Bao and E. A. Carter, "Surface-Plasmon-Induced Ammonia Decomposition on Copper: Excited-State Reaction Pathways Revealed by Embedded Correlated Wavefunction Theory," *ACS Nano*, **13**, 9944 (2019). [doi: 10.1021/acsnano.9b05030](https://doi.org/10.1021/acsnano.9b05030)
402. W. C. Witt and E. A. Carter, "Kinetic energy density of nearly free electrons. II. Response functionals of the electron density," *Phys. Rev. B*, **100**, 125107 (2019). [doi: 10.1103/PhysRevB.100.125107](https://doi.org/10.1103/PhysRevB.100.125107)
401. W. C. Witt and E. A. Carter, "Kinetic energy density of nearly free electrons. I. Response functionals of the external potential," *Phys. Rev. B*, **100**, 125106 (2019). [doi: 10.1103/PhysRevB.100.125106](https://doi.org/10.1103/PhysRevB.100.125106)

400. J. L. Bao and E. A. Carter, "Rationalizing the Hot-Carrier-Mediated Reaction Mechanisms and Kinetics for Ammonia Decomposition on Ruthenium-Doped Copper Nanoparticles," *J. Am. Chem. Soc.*, **141**, 13320 (2019). [doi: 10.1021/jacs.9b06804](https://doi.org/10.1021/jacs.9b06804)
399. W. C. Witt, K. Jiang, and E. A. Carter, "Upper bound to the gradient-based kinetic energy density of noninteracting electrons in an external potential," *J. Chem. Phys.*, **151**, 064113 (2019). [doi: 10.1063/1.5108896](https://doi.org/10.1063/1.5108896)
398. D. F. Swearer, H. Robatjazi, J. M. P. Martirez, M. Zhang, L. Zhou, E. A. Carter, P. Nordlander, and N. J. Halas, "Plasmonic Photocatalysis of Nitrous Oxide into N₂ and O₂ Using Aluminum-Iridium Antenna-Reactor Nanoparticles," *ACS Nano*, **13**, 8076 (2019). [doi: 10.1021/acsnano.9b02924](https://doi.org/10.1021/acsnano.9b02924)
397. L. Li and E. A. Carter, "Defect-Mediated Charge-Carrier Trapping and Nonradiative Recombination in WSe₂ Monolayers," *J. Am. Chem. Soc.*, **141**, 10451 (2019). [doi: 10.1021/jacs.9b04663](https://doi.org/10.1021/jacs.9b04663)
396. S. Xu and E. A. Carter, "Balancing Competing Reactions in Hydride Transfer Catalysis via Catalyst Surface Doping: The Ionization Energy Descriptor," *J. Am. Chem. Soc.*, **141**, 9895 (2019). [doi: 10.1021/jacs.9b02897](https://doi.org/10.1021/jacs.9b02897)
395. S. Xu and E. A. Carter, "Theoretical Insights into Heterogeneous (Photo)electrochemical CO₂ Reduction," *Chem. Rev.*, **119**, 6631 (2019). [doi: 10.1021/acs.chemrev.8b00481](https://doi.org/10.1021/acs.chemrev.8b00481); Virtual Issue on "Carbon Capture & Conversion," *J. Am. Chem. Soc.*, **142**, 4955 (2020). (WOS Highly Cited Paper in 2021-22) [doi: 10.1021/jacs.0c02356](https://doi.org/10.1021/jacs.0c02356)
394. L. Zhou, D. F. Swearer, H. Robatjazi, A. Alabastri, P. Christopher, E. A. Carter, P. Nordlander, and N. J. Halas, "Response to Comment on "Quantifying hot carrier and thermal contributions in plasmonic photocatalysis"," *Science*, **364**, eaaw9545 (2019). [doi: 10.1126/science.aaw9545](https://doi.org/10.1126/science.aaw9545)
393. B. Foerster, V. A. Spata, E. A. Carter, C. Sönnichsen, and S. Link, "Plasmon damping depends on the chemical nature of the nanoparticle interface," *Sci. Adv.*, **5**, eaav074 (2019). [doi: 10.1126/sciadv.aav0704](https://doi.org/10.1126/sciadv.aav0704)
392. S. Berman, G. S. Gautam, and E. A. Carter, "Role of Na and Ca as Isovalent Dopants in Cu₂ZnSnS₄ Solar Cells," *ACS Sustain. Chem. Eng.*, **7**, 5792 (2019). [doi: 10.1021/acssuschemeng.8b05348](https://doi.org/10.1021/acssuschemeng.8b05348); "Virtual Special Issue on Theories, Mechanisms, Materials, and Devices for Solar Energy Conversion," *ACS Sustain. Chem. Eng.*, **7**, 10164 (2019). (Editorial) [doi: 10.1021/acssuschemeng.9b02925](https://doi.org/10.1021/acssuschemeng.9b02925)
391. X. Zhang and E. A. Carter, "Subspace Density Matrix Functional Embedding Theory: Theory, Implementation, and Applications to Molecular Systems," *J. Chem. Theor. Comp.*, **15**, 949 (2019). [doi: 10.1021/acs.jctc.8b00990](https://doi.org/10.1021/acs.jctc.8b00990)
390. B. G. del Rio, E. K. de Jong, and E. A. Carter, "Properties of fusion-relevant liquid Li-Sn alloys: An *ab initio* molecular-dynamics study," *Nucl. Mat. Energy*, **18**, 326 (2019). [doi: 10.1016/j.nme.2019.01.027](https://doi.org/10.1016/j.nme.2019.01.027)

389. J. M. P. Martirez and E. A. Carter, "Unraveling Oxygen Evolution on Iron-Doped β -Nickel Oxyhydroxide: The Key Role of Highly Active Molecular-like Sites," *J. Am. Chem. Soc.*, **141**, 693 (2019). (JACS Highly Cited Paper from 2018-19 and WOS Highly Cited Paper in 2021-22) [doi: 10.1021/jacs.8b12386](https://doi.org/10.1021/jacs.8b12386)
388. Z. Chen, J. M. P. Martirez, P. Zahl, E. A. Carter, and B. E. Koel, "Self-assembling of formic acid on the partially oxidized $p(2 \times 1)$ Cu(110) surface reconstruction at low coverages," *J. Chem. Phys.*, **150**, 041720 (2019). [doi: 10.1063/1.5046697](https://doi.org/10.1063/1.5046697)
387. S. Xu, L. Li, and E. A. Carter, "Why and How Carbon Dioxide Conversion to Methanol Happens on Functionalized Semiconductor Photoelectrodes," *J. Am. Chem. Soc.*, **140**, 16749 (2018). [doi: 10.1021/jacs.8b09946](https://doi.org/10.1021/jacs.8b09946)
386. G. S. Gautam, T. P. Senftle, N. Alidoust, and E. A. Carter, "Novel Solar Cell Materials: Insights from First-Principles," *J. Phys. Chem. C*, **122**, 27107 (2018). [doi: 10.1021/acs.jpcc.8b08185](https://doi.org/10.1021/acs.jpcc.8b08185)
385. Q. Ou and E. A. Carter, "Potential Functional Embedding Theory with an Improved Kohn–Sham Inversion Algorithm," *J. Chem. Theor. Comp.*, **14**, 5680 (2018). [doi: 10.1021/acs.jctc.8b00717](https://doi.org/10.1021/acs.jctc.8b00717)
384. L. Zhou, D. F. Swearer, C. Zhang, H. Robatjazi, H. Zhao, L. Henderson, L. Dong, P. Christopher, E. A. Carter, P. Nordlander, and N. J. Halas, "Quantifying hot carrier and thermal contributions in plasmonic photocatalysis," *Science*, **362**, 69 (2018). [doi: 10.1126/science.aat6967](https://doi.org/10.1126/science.aat6967)
383. G. S. Gautam and E. A. Carter, "Evaluating transition metal oxides within DFT-SCAN and SCAN+*U* frameworks for solar thermochemical applications," *Phys. Rev. Mater.*, **2**, 095401 (2018). [doi: 10.1103/PhysRevMaterials.2.095401](https://doi.org/10.1103/PhysRevMaterials.2.095401)
382. B. G. del Rio, M. Chen, L. E. González, and E. A. Carter, "Orbital-free density functional theory simulation of collective dynamics coupling in liquid Sn," *J. Chem. Phys.*, **149**, 094504 (2018). (Editor's Pick) [doi: 10.1063/1.5040697](https://doi.org/10.1063/1.5040697); Scilight: [doi: 10.1063/1.5054900](https://doi.org/10.1063/1.5054900)
381. A. J. Tkalych, J. M. P. Martirez, and E. A. Carter, "Thermodynamic Evaluation of Trace-Amount Transition-Metal-Ion Doping in NiOOH Films," *J. Electrochem. Soc.*, **165**, F907 (2018). [doi: 10.1149/2.0101811jes](https://doi.org/10.1149/2.0101811jes)
380. J. M. P. Martirez and E. A. Carter, "Effects of the Aqueous Environment on the Stability and Chemistry of β -NiOOH Surfaces," *Chem. Mater.*, **30**, 5205 (2018). [doi: 10.1021/acs.chemmater.8b01866](https://doi.org/10.1021/acs.chemmater.8b01866)
379. L. D. Chen, M. Bajdich, J. M. P. Martirez, C. M. Krauter, J. A. Gauthier, E. A. Carter, A. C. Luntz, K. Chan, and J. K. Nørskov, "Understanding the apparent fractional charge of protons in the aqueous electrochemical double layer," *Nat. Comm.*, **9**, 3202 (2018). [doi: 10.1038/s41467-018-05511-y](https://doi.org/10.1038/s41467-018-05511-y)
378. A. J. Tkalych, J. M. P. Martirez, and E. A. Carter, "Effect of transition-metal-ion dopants on the oxygen evolution reaction on NiOOH(0001)," *Phys. Chem. Chem. Phys.*, **20**, 19525 (2018). [doi: 10.1039/c8cp02849d](https://doi.org/10.1039/c8cp02849d)

377. G. S. Gautam, T. P. Senftle, and E. A. Carter, "Understanding the Effects of Cd and Ag Doping in Cu₂ZnSnS₄ Solar Cells," *Chem. Mater.*, **30**, 4543 (2018). doi: [10.1021/acs.chemmater.8b00677](https://doi.org/10.1021/acs.chemmater.8b00677)
376. S. Xu and E. A. Carter, "2-Pyridinide as an Active Catalytic Intermediate for CO₂ Reduction on p-GaP Photoelectrodes: Lifetime and Selectivity," *J. Am. Chem. Soc.*, **140**, 8732 (2018). doi: [10.1021/jacs.8b03774](https://doi.org/10.1021/jacs.8b03774)
375. H. L. Zhuang, M. Chen, and E. A. Carter, "Orbital-free density functional theory characterization of the β' -Mg₂Al₃ Samson phase," *Phys. Rev. Mater.*, **2**, 073603 (2018). doi: [10.1103/PhysRevMaterials.2.073603](https://doi.org/10.1103/PhysRevMaterials.2.073603)
374. R. Yin, Y. Zhang, F. Libisch, E. A. Carter, H. Guo, and B. Jiang, "Dissociative Chemisorption of O₂ on Al(111): Dynamics on a Correlated Wave-Function-Based Potential Energy Surface," *J. Phys. Chem. Lett.*, **9**, 3271 (2018). doi: [10.1021/acs.jpcclett.8b01470](https://doi.org/10.1021/acs.jpcclett.8b01470)
373. M. Lessio, T. P. Senftle, and E. A. Carter, "Hydride Shuttle Formation and Reaction with CO₂ on GaP(110)," *ChemSusChem*, **11**, 1558 (2018). doi: [10.1002/cssc.201800037](https://doi.org/10.1002/cssc.201800037)
372. V. A. Spata and E. A. Carter, "Mechanistic Insights into Photocatalyzed Hydrogen Desorption from Palladium Surfaces Assisted by Localized Surface Plasmon Resonances," *ACS Nano*, **12**, 3512 (2018). doi: [10.1021/acsnano.8b00352](https://doi.org/10.1021/acsnano.8b00352)
371. W. C. Witt, B. G. del Rio, J. M. Dieterich, and E. A. Carter, "Orbital-free density functional theory for materials research," *J. Mater. Res.*, **33**, 777 (2018). doi: [10.1557/jmr.2017.462](https://doi.org/10.1557/jmr.2017.462)
370. M. L. Clark, P. L. Cheung, M. Lessio, E. A. Carter, and C. P. Kubiak, "Kinetic and Mechanistic Effects of Bipyridine (bpy) Substituent, Labile Ligand, and Brønsted Acid on Electrocatalytic CO₂ Reduction by Re(bpy) Complexes," *ACS Catal.*, **8**, 2021 (2018). doi: [10.1021/acscatal.7b03971](https://doi.org/10.1021/acscatal.7b03971)
369. X. Zhang and E. A. Carter, "Kohn-Sham potentials from electron densities using a matrix representation within finite atomic orbital basis sets," *J. Chem. Phys.*, **148**, 034105 (2018). doi: [10.1063/1.5005839](https://doi.org/10.1063/1.5005839)
368. J. M. P. Martirez and E. A. Carter, "Prediction of a low-temperature N₂ dissociation catalyst exploiting near-IR-to-visible light nanoplasmonics," *Sci. Adv.*, **3**, eaao4710 (2017). doi: [10.1126/sciadv.aao4710](https://doi.org/10.1126/sciadv.aao4710)
367. K. Yu and E. A. Carter, "Extending density functional embedding theory for covalently bonded systems," *Proc. Natl. Acad. Sci. U.S.A.*, **114**, E10861 (2017). doi: [10.1073/pnas.1712611114](https://doi.org/10.1073/pnas.1712611114)
366. 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*, pp. 81-118, Mark Gordon, Ed. (John Wiley & Sons), ISBN: 978-1-119-12924-0 (2017). doi: [10.1002/9781119129271](https://doi.org/10.1002/9781119129271)
365. T. P. Senftle, M. Lessio, and E. A. Carter, "The Role of Surface-Bound Dihydropyridine Analogues in Pyridine-Catalyzed CO₂ Reduction over Semiconductor Photoelectrodes," *ACS Cent. Sci.*, **3**, 968 (2017). doi: [10.1021/acscentsci.7b00233](https://doi.org/10.1021/acscentsci.7b00233)

364. T. P. Senftle and E. A. Carter, "Theoretical Determination of Band Edge Alignments at the Water–CuInS₂(112) Semiconductor Interface," *Langmuir*, **33**, 9479 (2017). [doi: 10.1021/acs.langmuir.7b00668](https://doi.org/10.1021/acs.langmuir.7b00668)
363. M. Lessio, J. M. Dieterich, and E. A. Carter, "Hydride Transfer at the GaP(110)/Solution Interface: Mechanistic Implications for CO₂ Reduction Catalyzed by Pyridine," *J. Phys. Chem. C*, **121**, 17321 (2017). [doi: 10.1021/acs.jpcc.7b05052](https://doi.org/10.1021/acs.jpcc.7b05052)
362. B. G. del Rio, J. M. Dieterich, and E. A. Carter, "Globally-Optimized Local Pseudopotentials for (Orbital-Free) Density Functional Theory Simulations of Liquids and Solids," *J. Chem. Theory Comput.*, **13**, 3684 (2017). [doi: 10.1021/acs.jctc.7b00565](https://doi.org/10.1021/acs.jctc.7b00565)
361. H. Zhuang, M. Chen, and E. A. Carter, "Prediction and characterization of an Mg–Al intermetallic compound with potentially improved ductility via orbital-free and Kohn-Sham density functional theory," *Modelling Simul. Mater. Sci. Eng.*, **25**, 075002 (2017). [doi: 10.1088/1361-651X/aa7e0c](https://doi.org/10.1088/1361-651X/aa7e0c)
360. J. R. Vella, M. Chen, S. Fürstenberg, F. H. Stillinger, E. A. Carter, P. G. Debenedetti, and A. Z. Panagiotopoulos, "Characterization of the liquid Li-solid Mo (110) interface from classical molecular dynamics for plasma-facing applications," *Nucl. Fusion*, **57**, 116036 (2017). [doi: 10.1088/1741-4326/aa7e0d](https://doi.org/10.1088/1741-4326/aa7e0d)
359. A. J. Tkalych, H. Zhuang, and E. A. Carter, "A Density Functional + *U* Assessment of Oxygen Evolution Reaction Mechanisms on β -NiOOH," *ACS Catal.*, **7**, 5329 (2017). [doi: 10.1021/acscatal.7b00999](https://doi.org/10.1021/acscatal.7b00999); Correction: *ACS Catal.*, **8**, 6070 (2018). [doi: 10.1021/acscatal.8b01775](https://doi.org/10.1021/acscatal.8b01775)
358. R. Zhang, L. Bursi, J. D. Cox, Y. Cui, C. M. Krauter, A. Alabastri, A. Manjavacas, A. Calzolari, S. Corni, E. Molinari, E. A. Carter, F. J. García de Abajo, H. Zhang, and P. Nordlander, "How to Identify Plasmons from the Optical Response of Nanostructures," *ACS Nano*, **11**, 7321 (2017). [doi: 10.1021/acs.nano.7b03421](https://doi.org/10.1021/acs.nano.7b03421)
357. A. Das, T. Müller, F. Plasser, D. B. Krisiloff, E. A. Carter, and H. Lischka, "Local Electron Correlation Treatment in Extended Multireference Calculations: Effect of Acceptor–Donor Substituents on the Biradical Character of the Polycyclic Aromatic Hydrocarbon Heptazethrene," *J. Chem. Theor. Comp.*, **13**, 2612 (2017). [doi: 10.1021/acs.jctc.7b00156](https://doi.org/10.1021/acs.jctc.7b00156)
356. J. M. Dieterich, W. C. Witt, and E. A. Carter, "libKEDF: An Accelerated Library of Kinetic Energy Density Functionals," *J. Comput. Chem.*, **38**, 1552 (2017). [doi: 10.1002/jcc.24806](https://doi.org/10.1002/jcc.24806)
355. J. M. Dieterich and E. A. Carter, "Opinion: Quantum solutions for a sustainable energy future," *Nat. Rev. Chem.*, **1**, 0032 (2017). [doi: 10.1038/s41570-017-0032](https://doi.org/10.1038/s41570-017-0032)
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. P. 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); Virtual Issue on Carbon Capture and Conversion: *J. Am. Chem. Soc.*, **142**, 4955 (2020). [doi: 10.1021/jacs.0c02356](https://doi.org/10.1021/jacs.0c02356)
352. J. Cheng, K. Yu, F. Libisch, J. M. Dieterich, and E. A. Carter, "Potential Functional Embedding Theory at the Correlated Wave Function Level. 2. 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 Wave Function Level. 1. 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-Höinghaus, "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, "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 Sr_{1-x}K_xFeO₃," *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 CO₂ 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, and E. A. Carter, "Interaction of Pyridine and Water with the Reconstructed Surfaces of GaP(111) and CdTe(111) Photoelectrodes: Implications for CO₂ Reduction," *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. Robatjazi, J. M. P. Martirez, C. M. Krauter, S. Yazdi, M. J. McClain, E. Ringe, E. A. Carter, P. Nordlander, and N. J. Halas, "Heterometallic antenna-reactor complexes for photocatalysis," *Proc. Natl. Acad. Sci. U.S.A.*, **113**, 8916 (2016). (WOS Highly Cited Paper in 2021-22) [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 CO₂ 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. L. Windus, "Spin-Free [2]_{R12} Basis Set Incompleteness Correction to the Local Multireference Configuration Interaction and the Local Multireference 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. Scoullos, 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 Cu₂ZnSnS₄ 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.-W. Jiang, H. Zhuang, L.-W. 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 (La_{0.5}Sr_{0.5}Co_{0.25}Fe_{0.75}O_{3-δ})," *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 CH₃OC(=O) and ĊH₂OC(=O)H Radicals," *J. Phys. Chem. B*, **120**, 1590 (2016). [doi: 10.1021/acs.jpcc.5b07959](https://doi.org/10.1021/acs.jpcc.5b07959)
333. J. M. P. Martirez and E. A. Carter, "Thermodynamic Constraints in Using AuM (M = Fe, Co, Ni, and Mo) Alloys as N₂ Dissociation Catalysts: Functionalizing a Plasmon-Active Metal," *ACS Nano*, **10**, 2940 (2016). [doi: 10.1021/acs.nano.6b00085](https://doi.org/10.1021/acs.nano.6b00085)
332. L. Zhou, C. Zhang, M. McClain, A. Manjavacas, C. M. Krauter, S. Tian, F. Berg, H. Everitt, E. A. Carter, P. Nordlander, and N. Halas, "Aluminum Nanocrystals 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 Cu₂ZnSnS₄," *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. A. 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 GaP(110) Identifies 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. J. 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*, **119**, 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*, **61**, 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). doi: [10.1002/9781118853887.ch3](https://doi.org/10.1002/9781118853887.ch3)
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.jpcllett.5b00597](https://doi.org/10.1021/acs.jpcllett.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: A pointwise kinetic energy density analysis and numerical convergence investigation," *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. L. 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 NiO Band Gap Upon Formation of Li_xNi_{1-x}O alloys: 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 body-centered-cubic 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); Correction: F. Libisch, C. M. Krauter, and E. A. Carter, "Corrigendum to: Plasmon-Driven Dissociation of H₂ on Gold Nanoclusters," *Z. Phys. Chem.*, **230**, 131 (2016). [doi: 10.1515/zpch-2015-5001](https://doi.org/10.1515/zpch-2015-5001)

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 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-δ}, 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: 10.1039/c3sc22296a](https://doi.org/10.1039/c3sc22296a)
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). (WOS Highly Cited Paper in 2021-22) [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 Nonstoichiometric and Doped Wüstite," *J. Phys. Chem. C*, **116**, 17403 (2012). [doi: 10.1021/jp3047664](https://doi.org/10.1021/jp3047664)
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 Electrocatalysis," *J. Am. Chem. Soc.*, **134**, 13296 (2012). (WOS Highly Cited Paper in 2021-22) [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 Cu₂O," *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 CO₂," *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 Sr₂Fe_{1.5}Mo_{0.5}O_{6-δ}, 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). (WOS Highly Cited Paper in 2021-22) [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 aluminium 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: 10.1021/nl200356n](https://doi.org/10.1021/nl200356n)
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. Lignères, 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 density functional theory + 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 β -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. Lignères, 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: An LDA+U study," *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, "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 nonlocal 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 an 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 Line Shapes 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: 10.1080/00268970802204645](https://doi.org/10.1080/00268970802204645)
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 aluminium *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 Computational and 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 Quasi-continuum 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, "An 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. Lignères, 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 continuum 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, "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 Open-Shell Singlet Diradical Ground States," *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 along the Reaction Path of CH₃CH₂ + O₂ → H₂C=CH₂ + HOO: Evidence for Vibronic State Mixing and Neutral Hydrogen Transfer," *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. Millennium 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 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, "Multi-reference 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. Kluener, 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. [doi: 10.1142/9789812811882_0010](https://doi.org/10.1142/9789812811882_0010)
107. R. L. Hayes, E. Fattal, N. Govind, and E. A. Carter, "Long Live Vinylidene! A New View of the $\text{H}_2\text{C}=\text{C} \rightarrow \text{HC}\equiv\text{CH}$ 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 heteroceramic 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, 117-184 (2002). doi.org/10.1007/0-306-46949-9_5
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). <https://pubs.acs.org/doi/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 uncertaintylike 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. Tazartes, 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-ICC10>3.0.CO;2-P](https://doi.org/10.1002/(SICI)1096-987X(199808)19:11<1300::AID-ICC10>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)-2 x 1," *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)-2 x 1," *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, "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 Direct Inversion in the Iterative Subspace Method," *J. Comp. Chem.*, **17**, 1836 (1996). [doi: 10.1002/\(SICI\)1096-987X\(199612\)17:16<1836::AID-ICC4>3.0.CO;2-O](https://doi.org/10.1002/(SICI)1096-987X(199612)17:16<1836::AID-ICC4>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, "Direct inversion in the iterative subspace-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, "A 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 multireference 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 Bonds 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, "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, " $O(N^3)$ 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 SiH_{2(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. [doi: 10.1016/B978-0-444-89022-1.50021-3](https://doi.org/10.1016/B978-0-444-89022-1.50021-3)
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 wave functions: 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 behavior," *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, "Coverage and temperature dependence of the morphology of strained metal 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 Chromium Methylidene Cation: CrCH_2^+ ," *J. Phys. Chem.*, **88**, 1485 (1984). [doi: 10.1021/j150652a009](https://doi.org/10.1021/j150652a009)

PATENTS

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

Emily A. Carter, Ananth Govind Rajan, and John Mark P. Martirez, *A Method of Generating Oxygen by Electrochemical Water Splitting at Optimized Conditions of pH, Temperature, and Pressure*. International Patent Application No.: PCT/IB2022/057592. Filed August 13, 2022. *Operating Conditions for Optimal High-Temperature, High-Pressure Operation of Water Oxidation Electrolyzers Using Mixed Iron/Nickel Oxyhydroxide Catalysts*. U.S. Foreign Filing License No.: 620,196. Filed July 28, 2021. Indian Provisional Patent No.: 202141034520. Filed July 30, 2021. Indian Patent Issued April 28, 2023.

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

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

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

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

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

SEMINARS AND PAPER PRESENTATIONS (LAST FIVE YEARS ONLY)

A. *Invited Seminars*

- May 7, 2025 "The energy transition is no longer enough: Transformation, intervention, and adaptation," MITEI Presents: Advancing the Energy Transition Series, MIT Energy Initiative, Cambridge, MA
- May 2, 2025 "Carbon Dioxide Conversion for a Sustainable Future: Research and Policy," Willis H. Flygare Memorial Lecture in Physical Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL
- May 1, 2025 "Carbon Dioxide Conversion for a Sustainable Future: Research and Policy," Satish Saxena Distinguished Lecture in Chemical Engineering, University of Illinois at Chicago, Chicago, IL
- October 25, 2024 "Carbon Dioxide Conversion for a Sustainable Future: Research and Policy," 2024 Annabelle Lee Memorial Lecture in Chemistry, Virginia Tech, VA
- May 3, 2024 "How Quantum Mechanics Can Help Identify Mechanisms and Design Materials to Combat Climate Change," 2024 Covestro Lecture, Department of Chemical and Petroleum Engineering, University of Pittsburgh, PA
- May 2, 2024 "How a Scientist/Engineer Can Help the Transition to a Net-Negative Emissions Civilization," 2024 Covestro Lecture, Department of Chemical and Petroleum Engineering, University of Pittsburgh, PA
- March 20, 2024 "How Quantum Mechanics Can Help Identify Mechanisms and Materials to Combat Climate Change," HML Colloquia Series XX, KTH Royal Institute of Technology, Sweden (given virtually)
- September 26, 2023 "How Quantum Mechanics Can Help Identify Mechanisms and Materials to Combat Climate Change," 2023 G. N. Lewis Memorial Lecture, College of Chemistry, University of California, Berkeley, CA
- July 6, 2023 "How Quantum Mechanics Can Help Identify Mechanisms and Materials to Combat Climate Change," Zernike Institute of Advanced Materials Colloquium, University of Groningen, Groningen, The Netherlands
- May 15, 2023 "How Quantum Mechanics Can Help Identify Mechanisms and Materials to Combat Climate Change," 2023 Richard S. Mulliken Memorial Lecture, Department of Chemistry, University of Chicago, Chicago, IL
- May 2, 2023 "Carbon Utilization and Other Needed Technologies for the Transition to Net Zero," High Meadows Environmental Institute Spring 2023 Faculty Seminar, Princeton University, Princeton, NJ
- April 25, 2023 "How Quantum Mechanics Can Help Identify Mechanisms and Design Materials to Combat Climate Change," 27th John Stauffer Lectures in Chemistry, Stanford University, Palo Alto, CA

- April 24, 2023 “How a Scientist/Engineer Can Help the Transition to a Net-Negative Emissions Civilization,” 27th John Stauffer Lectures in Chemistry, Stanford University, Palo Alto, CA
- February 17, 2023 “How Low Temperature Plasma Science Can Contribute to Society,” PPPL Spring Graduate Student Seminar (AST 558), Plasma Physics Graduate Program, Princeton Plasma Physics Laboratory, Princeton, NJ
- January 11, 2023 “How Quantum Mechanics Helps Identify Mechanisms and Discover Materials to Combat Climate Change,” Department of Chemistry & Chemical Biology Seminar Series, McMaster University, Ontario, Canada (given virtually)
- October 25, 2022 “How Quantum Mechanics Helps Identify Mechanisms and Discover Materials to Combat Climate Change,” 2022 Paint Branch Distinguished Lecture in Applied Physics, University of Maryland, Institute for Research in Electronics and Applied Physics, College Park, MD.
- May 5, 2022 “How Quantum Mechanics Helps Identify Mechanisms and Discover Materials to Combat Climate Change,” 2022 Richard S. H. Mah Lecture on Modeling and Computation in Chemical Engineering, Northwestern University, Department of Chemical and Biological Engineering, Evanston, IL
- April 14, 2022 “From Physical Chemistry to Engineering and Beyond: How to Make a Difference,” Careers in Chemistry Inaugural Seminar Series, University of Washington, Seattle, WA (given virtually)
- February 18, 2022 “Quantum Design of Materials for a Sustainable Future,” Mechanical & Aerospace Engineering Spring 2022 Seminar Series, Princeton University, Princeton, NJ
- January 26, 2022 “How Quantum Mechanics Helps Identify Mechanisms and Discover Materials to Combat Climate Change,” 2022 Harrison Shull Distinguished Lecturer, Indiana University Bloomington, Department of Chemistry, Bloomington, IN (given virtually)
- November 9, 2020 “Designing Materials for Sustainable Energy from First Principles,” 2020 Brumley D. Pritchett Lecturer, Georgia Institute of Technology, School of Materials Science and Engineering, Atlanta, GA (given virtually)

B. Invited Lectures

- August 18, 2025 “Insights for Quantum-Based Simulations of Electrically Driven Catalysis for Sustainability,” at the *ACS Fall 2025 National Meeting*, in the *Recent Advances in Computational Heterogeneous and Electrocatalysis* session, Washington, DC
- July 22, 2025 “How Theoretical Chemistry Can Help Sustain Life on Earth,” Invited Speaker at the *Inaugural Meeting of the Marcus Center for Theoretical Chemistry*, California Institute of Technology, Pasadena, CA
- June 8, 2025 “Modeling Plasmonic Photocatalysis: Excited State Kinetics from First Principles,” Keynote Speaker at the *Plasmonically Powered Processes Gordon Research Conference*, Ventura, CA

- May 27, 2025 “Quantum-Derived Kinetics of Photo/electrocatalysis on Metals,” Invited Speaker at the *Lorentz Workshop on Predicting Barriers for Reactions on Metals*, Leiden, The Netherlands
- April 7, 2025 “Assessing Reaction Mechanisms of Electrocatalysis: Beyond Density Functional Theory,” Invited Speaker at the *2025 MRS Spring Meeting & Exhibit, in the Rational Design of Electrocatalysts: Insights into Structure-Function Relationships for Next-Generation Materials Symposium*, Seattle, WA
- March 24, 2025 “Carbon dioxide utilization landscape: A national academies assessment,” Invited Speaker and Panel Moderator at the *ACS Spring 2025 National Meeting*, in the *CO₂ Removal: Novel Materials for Scalable Direct Air Capture* session, San Diego, CA
- March 23, 2025 “Multiphysics simulations of atomic-scale mechanisms for initiating CO₂ mineralization,” Invited Speaker at the *ACS Spring 2025 National Meeting*, in the *Geochemical Pathways for Carbon Capture, Removal, Utilization, and Storage: Laboratory to Field* session, San Diego, CA
- August 20, 2024 “Marsha I. Lester Award for exemplary impact in physical chemistry,” Invited Speaker at the *ACS Fall 2024 National Meeting* in the *ACS PHYS Awards* session, Denver, CO
- August 18, 2024 “First principles insights into catalysis driven by clean electricity,” Invited Speaker at the *ACS Fall 2024 National Meeting* in the *Surfaces & Interfaces in Chemical & Biological Systems: Symposium in honor of Hai-Lung Dai* session, Denver, CO
- August 7, 2024 “Public Briefing: National Academies of Science Report, Carbon Utilization Infrastructure Markets Research and Development,” Invited Speaker at the *2024 FECM/NETL Carbon Management Research Project Review Meeting*, Pittsburgh, PA
- July 10, 2024 “Contributions to Climate Change Mitigation through Quantum Simulations,” *New Fellows Seminar*, The Royal Society, London, UK
- June 13, 2024 “Back to the Future with Blue Moon Dynamics for Climate Change Intervention,” Invited Speaker at the *2024 CECAM Workshop* on “From methods to applications: challenges and opportunities in contemporary simulations,” École Normale Supérieure, Paris, France
- April 30, 2024 “Initial Insights into Greener Ammonia Production from Quantum Simulations,” Invited Speaker at the *2024 Annual Carbon Mitigation Initiative Deep Dive* on “Hydrogen & Ammonia Economies: Novel Technical Solutions & Environmental Implications,” Princeton University, NJ
- April 12, 2024 “A Physical Chemist’s Journey to Combat Climate Change,” Nichols Medal Award Address, *William H. Nichols Distinguished Symposium* on “Physical Chemistry and Sustainability,” American Chemical Society (New York Chapter), White Plains, NY
- November 6, 2023 “Carbon Removal Strategies 2030,” invited webinar panelist, California Institute of Technology (Caltech), Pasadena, CA

- June 15, 2023 “Carbon Dioxide Utilization: Insights from Quantum Based Simulations,” Invited Speaker at the *Liquids, Glasses, and Other Adventures in Thermodynamics and Statistical Mechanics Symposium* in Celebration of Pablo Debenedetti’s 70th Birthday, Princeton University, Princeton, NJ
- May 29, 2023 “Carbon Dioxide Utilization Markets and Infrastructure: Status and Opportunities - A First Report from the U.S. National Academies of Sciences, Engineering, and Medicine,” Invited Speaker at the 2023 *Carbon Capture, Utilization and Storage Gordon Research Conference*, Les Diablerets, Switzerland
- May 24, 2023 “CO₂ Capture via Carbonate Mineralization from Seawater,” Invited Speaker at the *Princeton Catalysis Initiative Symposium*, Princeton University, Princeton, NJ
- May 4, 2023 “Exploring green strategies for ammonia/hydrogen production,” Invited Speaker at the 22nd *Annual Meeting of the Carbon Mitigation Initiative*, Princeton University, Princeton, NJ
- November 2, 2022 “Photo- and Electro-Catalysis via Embedded Correlated Wavefunction Theory: Examples and Outlook,” Invited Speaker at the *Simons Foundation Initiative on Catalysis and Related Topics Workshop*, New York, NY.
- August 29, 2022 “Catalyst Design and Discovery for Carbon Dioxide Utilization from First Principles,” Invited Plenary Speaker at the 19th *International Conference on Density-Functional Theory and its Applications (DFT2022)*, Brussels, Belgium (given virtually).
- August 22, 2022 “Replacing Fossil-Fuel-Driven Chemical Production by Photo- and Electro-catalysis Derived from Quantum Simulations,” Invited Lecture at the *ACS Fall 2022 National Meeting*, Chicago, IL (given virtually).
- May 23, 2022 “Sustaining the Planet Via (Photo)(Electro)Catalysis, from First Principles,” Invited Keynote at the 27th *North American Catalysis Meeting (NAM27)*, New York, NY.
- March 20, 2022 “Modeling of interfaces involved in sustainable energy technologies,” Invited Lecture at the *ACS Spring 2022 National Meeting*, San Diego, CA (given virtually).
- December 7, 2021 “Quantum-Derived Materials Solutions for a Sustainable Future,” Invited Lecture and Invited Panelist at the 2021 *MRS Fall Meeting & Exhibit*, Boston, MA (given virtually).
- August 24, 2021 “Quantum chemistry off the beaten path,” at the *ACS Fall 2021 National Meeting*, Atlanta, GA (held virtually).
- August 22, 2021 “Mechanisms of (photo)electrochemical conversion of CO₂ to fuels from first principles,” Invited Keynote at the *ACS Fall 2021 National Meeting*, Atlanta, GA (given virtually).
- June 15, 2021 “Excited-State and Electrochemical Reactions at Materials Interfaces: High Fidelity Modeling Now and in the Future,” Invited Keynote Lecture and Invited Panelist at the *Materials Research Society (MRS)/Kaoli Future of Materials Virtual Workshop: Computational Materials Science, Focus on Non-Equilibrium and Excited-State Dynamics in Materials* (held virtually).

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

C. Invited Talks Given by Research Group Members

- March 27, 2025 “Can embedded multiconfigurational wavefunction methods reveal fresh insights into the electrochemical CO₂ reduction pathways on copper?” at the *ACS Spring 2025 Meeting in the CO₂ Conversion & Utilization-II: Electrochemical CO₂ Conversion to Fuels and Valuable Chemicals: Mechanistic Understanding and Advanced Characterization Session*, San Diego, CA. (presented by Mark Martirez)
- January 30, 2025 “Embedded Correlated Wavefunction Theory for Plasmonic Photocatalysis: Past, Present, and Future,” at the *AFOSR MURI Kickoff Meeting; Combining Nonequilibrium Chemistries with Atomic Precision*, Rice University, Houston, TX. (presented by Mark Martirez)
- March 13, 2024 “Quantum mechanical insights into light-driven reactions on metallic nanoparticles,” at the *2024 Catalysis Society of New York Spring Symposium*, Agile Strategy Lab, New Jersey Institute of Technology, Newark, NJ. (presented by Mark Martirez)
- January 11, 2024 “Can embedded multiconfigurational wavefunction methods reveal fresh insights into the electrochemical CO₂ reduction pathways on copper?,” at the Lorentz-CECAM Workshop on “*Atomistic modelling of solid-liquid interfaces in electrocatalysis*,” Leiden University, Leiden, The Netherlands. (to be presented by Mark Martirez)
- August 13, 2023 Quantum-mechanical view of light-driven NH₃ activation on Pd- and Fe-decorated Al nanoparticles,” at the *ACS Fall 2023 National Meeting & Exposition in the Division of Catalysis Symposium on Molecular and Heterogeneous Photocatalysts: Advances in Experiments and Theory*, San Francisco, CA. (presented by Mark Martirez)
- June 23, 2023 “Understanding carbonate formation in aqueous solutions at the atomic level via multi-level quantum mechanics/molecular dynamics simulations,” invited talk (direct invitation to Jan-Niklas Boyn) at the *ACS Central Regional Meeting*, Dearborn, MI.
- March 21, 2023 “Capped density functional embedding theory for excited-state simulations of covalent compounds,” at the *Lorentz Center workshop on “Accelerating theoretical spectroscopy for complex multiscale materials*,” Leiden University, Leiden, The Netherlands. (presented by Mark Martirez)
- July 20, 2022 “Plasmonic heterogeneous catalysis: Excited-state surface chemistry understood via embedded correlated wavefunction theory,” at the *Centre Européen de Calcul Atomique et Moléculaire (CECAM) workshop on “Light-matter interaction and ultrafast nonequilibrium dynamics in plasmonic materials*,” University of Warwick, Coventry, England, United Kingdom. (presented by Mark Martirez)

D. Contributed Talks and Presentations

- May 19, 2025 “Electrolysis-driven CO₂ sequestration in mineralized carbonates and using the electrochemical CO₂ reduction reaction (CO₂RR) for global carbon neutralization,” poster at the *Princeton Catalysis Symposium*, Princeton, NJ. (presented by Hengfei Gu)
- April 10, 2025 “Carbon Utilization Infrastructure, Markets, and Research and Development,” poster at the *Carbon Capture, Utilization and Storage Gordon Research Conference, Co-Creating Sustainable Carbon Management Solutions for a Thriving Future Session*, Ventura, CA. (presented by Catherine Wise)
- March 19, 2025 “Embedded correlated wavefunction driven multi-level quantum mechanics/molecular dynamics simulations of aqueous reactions,” at the *APS Global Physics Summit in the Advances in Simulation and Modeling of Liquid Solutions and Solid-Liquid Interfaces Focus Session*, Anaheim, CA. (presented by Jan-Niklas Boyn)
- Sept. 24, 2024 “First-Principles Insights into the Thermodynamics of Variable-Temperature Ammonia Synthesis on Transition-Metal-Doped Cu(100) and (111),” at the *Andlinger Center for Energy and the Environment Peer-led Seminar Series*, Princeton, NJ. (presented by Ziyang Wei)
- Sept. 3, 2024 “Quantum mechanical insights into light-driven reactions on metallic nanoparticles,” at the *XIX International Conference on Theoretical Aspects of Catalysis (ICTAC 2024)*, Seville, Spain. (presented by Mark Martinez)
- August 21, 2024 “Toward understanding carbonate mineralization at the atomic level with multi-level quantum mechanics/molecular dynamics simulations,” talk at the *ACS Fall 2024 Meeting in the Advances in CO₂ Capture & Conversion: Mineralization, Direct Ocean Capture & Modeling session*, Denver, CO. (presented by Jan-Niklas Boyn)
- August 21, 2024 “Accelerated embedding potential optimization by reconstructing the pseudo-valence electron density,” talk at the *ACS Fall 2024 Meeting in the Addressing the Complexity of Correlated Quantum Many-Body Problems by Embedding & Downfolding session*, Denver, CO. (presented by Ziyang Wei)
- August 3, 2024 “Embedded random phase approximation,” talk at the *Emerging Frontiers in Computational Chemistry and Materials: A Symposium in Celebration of Emily Carter’s Achievements*, Asilomar, Pacific Grove, CA. (presented by Ziyang Wei)
- August 3, 2024 “Non-equilibrium alkane dehydrogenation via pulsed heating and quenching: A computational exploration,” talk at the *Emerging Frontiers in Computational Chemistry and Materials: A Symposium in Celebration of Emily Carter’s Achievements*, Asilomar, Pacific Grove, CA. (presented by Mark Martinez)
- August 3, 2024 “Understanding the dynamics of Mg and Ca carbonate formation in aqueous solution from multi-level electronic structure simulations” talk at the *Emerging Frontiers in Computational Chemistry and Materials: A Symposium in Celebration of Emily Carter’s Achievements*, Asilomar, Pacific Grove, CA. (presented by Jan-Niklas Boyn)

- August 2, 2024 “Quantum Mechanics Simulation of Ammonia Formation by Nitrate Reduction on Copper Surfaces,” poster at the *Emerging Frontiers in Computational Chemistry and Materials: A Symposium in Celebration of Emily Carter’s Achievements*, Asilomar, Pacific Grove, CA. (presented by Vyshnavi Vennelakanti)
- June 27, 2024 “Quantum Mechanics Simulation of Ammonia Formation by Nitrate Reduction on Copper Surfaces,” poster at the *2024 Deep Modeling for Molecular Simulation* workshop, Princeton, NJ. (presented by Vyshnavi Vennelakanti)
- June 17, 2024 “Toward understanding carbonate mineralization at the atomic level with multi-level quantum mechanics/molecular dynamics simulations,” poster at the *2024 American Conference on Theoretical Chemistry*, Chapel Hill, NC. (presented by Jan-Niklas Boyn)
- June 17, 2024 “Introducing the Embedded Random Phase Approximation: H₂ Dissociative Adsorption on Cu(111) as an Exemplar,” poster at the *2024 American Conference on Theoretical Chemistry*, Chapel Hill, NC. (presented by Ziyang Wei)
- March 20, 2024 “Introducing the embedded random phase approximation: H₂ dissociative adsorption on Cu(111) as an exemplar,” talk at the *ACS Spring 2024 Meeting & Exposition in the Division of Computers in Chemistry*, New Orleans, LA. (presented by Ziyang Wei)
- Sept. 15, 2023 “DFT-Based Machine Learning Reactive Force Fields for Water and Aqueous NaCl and CO₂ Solutions,” at the *High Meadows Environmental Institute’s Summer of Learning Symposium*, Princeton University, Princeton, NJ. (presented by Huseyin Yagiz Devre)
- August 14, 2023 “Toward understanding carbonate mineralization at the atomic level with multi-level electronic structure simulations,” talk at the *ACS Fall 2023 National Meeting & Exposition in the Division of Energy and Fuels Symposium on Advances in Carbon Capture, Utilization, and Storage for a Sustainable Energy Future*, San Francisco, CA. (presented by Jan-Niklas Boyn)
- June 23, 2023 “Understanding carbonate formation in aqueous solutions at the atomic level via multi-level quantum mechanics/molecular dynamics simulations,” talk at the *2023 ACS Central Regional Meeting in the Computational Chemistry from Electrons to Macromolecules* session, Dearborn, MI. (presented by Jan-Niklas Boyn)
- March 28, 2023 “Understanding the dynamics of Mg and Ca carbonate formation in aqueous solution from multi-level electronic structure simulations” talk at the *ACS Spring 2023 National Meeting & Exposition in the Division of Physical Chemistry Symposium on Carbon Separation and Capture at the Atomistic Level: Theory and Experiment*, Indianapolis, IN. (presented by Jan-Niklas Boyn)
- Nov. 15, 2022 “Crystal Features Controlling Oxygen Vacancy Formation in ABO₃ Perovskites,” talk at the *2022 AIChE Annual Meeting*, Phoenix, AZ. (presented by Robert Wexler)
- Nov. 14, 2022 “Modeling the Combined Effects of Temperature, Pressure, and pH on Oxygen Evolution Thermodynamics and Kinetics,” talk at the *2022 AIChE Annual Meeting*, Phoenix, AZ. (presented by Ananth Govind Rajan)
- Oct. 14, 2022 “Explaining plasmon-activated ammonia and hydrogen decomposition on Pd and Fe-decorated Al nanoparticles via first-principles atomic-scale simulations,” poster at the *Andlinger Center for Energy and the Environment 2022 Annual Meeting*, Princeton, NJ. (presented by Xuelan Wen)

- Oct. 14, 2022 “Plasmonic heterogeneous catalysis: Excited-state surface chemistry understood via embedded correlated wavefunction theory,” poster at the *Andlinger Center for Energy and the Environment 2022 Annual Meeting*, Princeton, NJ. (presented by Mark Martirez)
- July 26, 2022 “Explaining plasmon-activated ammonia and hydrogen decomposition on Pd and Fe-decorated Al nanoparticles via first-principles atomic-scale simulations,” poster at the *American Conference on Theoretical Chemistry (ACTC) 2022*, Palisades Tahoe, CA. (presented by Xuelan Wen)
- July 20, 2022 “Plasmonic heterogeneous catalysis: Excited-state surface chemistry understood via embedded correlated wavefunction theory,” poster at the *Centre Européen de Calcul Atomique et Moléculaire (CECAM) workshop on “Light-matter interaction and ultrafast nonequilibrium dynamics in plasmonic materials,”* University of Warwick, Coventry, England, United Kingdom. (presented by Mark Martirez)
- June 30, 2022 “Intuitive materials design for solar thermochemical carbon dioxide splitting,” talk at the *19th International Conference on Carbon Dioxide Utilization (ICCDU)*, Princeton, NJ. (presented by Robert Wexler)
- May 25, 2022 “Explaining plasmon-activated ammonia and hydrogen decomposition on Pd and Fe-decorated Al nanoparticles via first-principles atomic-scale simulations,” poster at the *2022 AFOSR Molecular Dynamics and Theoretical Chemistry Program Review*, Arlington, VA. (presented by Xuelan Wen)
- May 10, 2022 “Influence of Thickness and Surface Composition on the Stability of Ferroelectric Polarization in Ultrathin HfO₂,” talk at the *2022 MRS Spring Meeting & Exhibit*, Honolulu, HI. (presented by Adrian Acosta)
- March 16, 2022 “Crystal Features Controlling Oxygen Vacancy Formation in ABO₃ Perovskites,” talk at the *APS March Meeting 2022*, Chicago, IL. (presented by Robert Wexler)
- Feb. 9, 2022 “Perpendicular magnetic anisotropy in FeGa(110)/Pt(111) thin film interfaces,” talk at the *TANMS Annual Research Strategy Meeting (ARSM) 2022 Virtual Symposia*, held virtually. (presented by Adrian Acosta)
- Nov. 8, 2021 “Revisiting Electrochemical CO₂ Reduction on Copper: Reaction Mechanisms Revealed By Embedded Correlated Wavefunction Theory,” talk at the *2021 AIChE Annual Meeting*, Boston, MA. (presented by Qing Zhao)
- Oct. 25-28, 2021 “Characterization of Plasma-Thermal Cu ALE Processes and Etch Products,” talk at the *AVS 67th Virtual Symposium*, Charlotte, NC. (presented by Xia “Gary” Sang)
- Oct. 11, 2021 “Gas-Phase Directional Etching of Copper Via Surface Oxidation and Chemical Complexation,” invited talk at the *240th ECS Digital Meeting*, Orlando, FL, held virtually. (presented by Prof. Jane Chang)
- June 2, 2021 “Precise Control of Nanoscale Cu Etching via Gas-Phase Oxidation and Chemical Complexation,” invited talk at the *239th ECS Digital Meeting with the 18th International Meeting on Chemical Sensors (IMCS)*, Chicago, IL. (presented by Prof. Jane Chang)
- April 20, 2021 “First-Principles Screening of Ca-Ce-M-O (M = 3d transition metal) Oxide Perovskites for Solar Thermochemical Applications,” talk at the *2021 Virtual MRS Spring Meeting & Exhibit*, Seattle, WA. (presented by Sai Gautam Gopalakrishnan)

- April 20, 2021 "Designer Perovskites with Dual Reduction on A and B Sites; Lowering the Peak Temperature of Thermochemical Hydrogen Production Cycles," talk at the *2021 Virtual MRS Spring Meeting & Exhibit*, Seattle, WA. (presented by Robert Bell)
- April 14, 2021 "Atomic-level understanding of sodium ion and water intercalation into titanium disulfide interlayers for water desalination," talk at the *ACS Spring 2021 National Meeting & Exposition*, San Antonio, TX, held virtually. (presented by Lesheng Li)
- April 14, 2021 "Oxygen evolution at low-lattice-coordinated NiOOH sites for water oxidation: Mechanism and doping strategies," talk at the *ACS Spring 2021 National Meeting & Exposition*, San Antonio, TX, held virtually. (presented by Mark Martirez)
- April 14, 2021 "Facet-Independent Oxygen Evolution Activity of Pure β -NiOOH: Different Chemistries Leading to Similar Overpotentials," talk at the *ACS Spring 2021 National Meeting & Exposition*, San Antonio, TX, held virtually. (presented by Ananth Govind Rajan)
- April 13, 2021 "Marcus-Theory Based Microkinetic Model for pH- and Potential-Dependent Water Splitting," talk at the *ACS Spring 2021 National Meeting & Exposition*, San Antonio, TX, held virtually. (presented by Ananth Govind Rajan)
- April 12, 2021 "Identification of a single-atom catalyst for electrochemical ammonia synthesis based on transition metal doped graphene-like GaN," talk at the *ACS Spring 2021 National Meeting & Exposition*, San Antonio, TX, held virtually. (presented by Lesheng Li)
- April 6, 2021 "Discovering Competing Electrocatalytic Mechanisms and their Overpotentials: Automated Enumeration of Oxygen Evolution Pathways," talk at the *ACS Spring 2021 National Meeting & Exposition*, San Antonio, TX, held virtually. (presented by Ananth Govind Rajan)
- April 6, 2021 "Efficient Machine-Learned Model for Oxide Perovskite Performance in Solar Thermochemical Technologies," talk at the *ACS Spring 2021 National Meeting & Exposition*, San Antonio, TX, held virtually. (presented by Robert Wexler)
- March 16, 2021 "First-principles evaluation of Ca-Ce-M-O (M = 3d transition metal) oxide perovskites for solar thermochemical applications," talk at the *APS March Meeting 2021*, held virtually. (presented by Sai Gautam Gopalakrishnan)
- Nov. 19, 2020 "Codoping $\text{Cu}_2\text{ZnSnS}_4$ with Cd, Ge, and Se: a recipe for suppressing deep traps," talk at the *ACS 2020 Virtual Postdoc Symposium*, San Francisco, CA. (presented by Robert Wexler)
- Nov. 19, 2020 "Accurate simulation of photochemical processes: From plasmon-driven photocatalysis to dye-sensitized photovoltaics," talk at the *ACS 2020 Virtual Postdoc Symposium*, San Francisco, CA. (presented by Mark Martirez)
- Nov. 17, 2020 "Suppressing Deep-Trap Formation in $\text{Cu}_2\text{ZnSnS}_4$ -Based Solar Cells," talk at the *2020 American Institute of Chemical Engineers (AIChE) Virtual Annual Meeting*, San Francisco, CA. (presented by Robert Wexler)
- Nov. 16, 2020 "Entropic Driving Forces of Ferrites for Two-Step Thermochemical Water and Carbon Dioxide Splitting," talk at the *International Mechanical Engineering Congress & Exposition (IMECE) 2020 Virtual Meeting*, Portland, OR. (presented by Shang Zhai)

- Nov. 16, 2020 “Entropy Source Analysis for Ferrites in Two-Step Thermochemical Splitting of Water and Carbon Dioxide,” talk at the 2020 American Institute of Chemical Engineers (AIChE) Virtual Annual Meeting, San Francisco, CA. (presented by Shang Zhai)
- Nov. 16, 2020 “Scratching the Surface: Simulating and Engineering the Interfaces of Materials for Sustainable Energy and Environmental Remediation,” poster at the 2020 American Institute of Chemical Engineers (AIChE) Virtual Annual Meeting, San Francisco, CA. (presented by Robert Wexler)
- Nov. 16, 2020 “Revisiting Electrochemical CO₂ Reduction on Copper Via Embedded Correlated Wavefunction Theory,” talk at the 2020 American Institute of Chemical Engineers (AIChE) Virtual Annual Meeting, San Francisco, CA. (presented by Qing Zhao)
- Nov. 16, 2020 “First-Principles Approaches for Accurate Predictions of Nanostructured Materials,” poster at the 2020 American Institute of Chemical Engineers (AIChE) Virtual Annual Meeting, San Francisco, CA. (presented by Qing Zhao)
- Nov. 16, 2020 “Identification of a Single-Atom Catalyst for Electrochemical Ammonia Synthesis Based on Transition Metal Doped Graphene-like GaN,” talk at the 2020 American Institute of Chemical Engineers (AIChE) Virtual Annual Meeting, San Francisco, CA. (presented by Lesheng Li)

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

- 2026 Invited Speaker at the “sMaR&T Seminar Series,” Materials Research and Technology Department, Luxembourg Institute of Science and Technology (LIST), Luxembourg.
- June 21-26, 2026 Invited Speaker at the “Engineering Considerations” session at the Gordon Research Conference on Climate Engineering, Newry, ME.
- June 15-19, 2026 Invited Speaker at the “Innovative nano- and hetero-structured functional materials for renewable energy applications” session of the “Advances in Functional Materials for Energy Harvesting, Storage, and Solar Fuels” symposium within CIMTEC 2026 - 16th International Ceramics Congress, Perugia, Italy.
- Feb. 19-21, 2026 Invited Speaker at the “4th International Conference on Materials Genome,” Amaravati, Andhra Pradesh, India.
- 2025 Invited Colloquium Speaker at the Sibley School of Mechanical and Aerospace Engineering, Cornell University, Ithaca, NY.
- 2025 Invited Seminar Speaker at the Department of Chemical Engineering, University of Texas, Austin, TX.
- 2025 Invited Colloquium Speaker at the Department of Physics & Astronomy, University of Delaware, DE.
- 2025 Invited Speaker at the “DGIST (virtual) Lecture Series,” Energy Science and Engineering Department, Daegu Gyeongbuk Institute of Science & Technology (DGIST), Daegu, Korea.
- Dec. 15-20, 2025 Invited Speaker at the “Computational Photocatalysis: Photophysics & Photochemistry at Interfaces. Machine Learning Bridges Theory and Experiment” symposium at the PacifiChem Congress 2025, Honolulu, HI.

- Dec. 15-20, 2025 Invited Speaker at the “*Challenges for Artificial Photosynthesis: Regulating Organic-Inorganic Functional Interfaces for Disruptive Solar Fuels Research*” symposium at the PacificChem Congress 2025, Honolulu, HI.
- Dec. 15-17, 2025 Distinguished Invited Speaker at the “*AI and Materials for Sustainability (AIMS-2025)*” conference at IIT Delhi in Abu Dhabi, Abu Dhabi, UAE.
- Nov. 3, 2025 Invited Speaker at the AIChE Annual Meeting celebrating the beginnings and future of the Computational Molecular Science and Engineering Forum (CoMSEF), Boston, MA.
- Oct. 14-17, 2025 Invited Plenary Speaker at the Mexican Chemical Society (SQM) on the “*100th Anniversary of Quantum Mechanics and its profound influence on the field of Chemistry,*” Monterrey, MX
- Oct. 12-16, 2025 Invited Keynote Speaker at the 248th Meeting of The Electrochemical Society on “*Computational Electrochemistry,*” Chicago, IL.
- Sep. 1-5, 2025 Invited Speaker at the *Lennard-Jones Centre Meeting 2025* at the Ray Dolby Centre, Cavendish Laboratory, University of Cambridge, UK
- Aug. 25-28, 2025 Invited Speaker at the “First principles modelling of interfaces for energy storage and conversion” Symposium at the *Psi-k 2025 Conference*, Lausanne, Switzerland.
- Aug. 4-8, 2025 Invited Keynote Speaker at the 2025 *SUNCAT Summer Institute* at the SLAC National Accelerator Laboratory, Menlo Park, CA
- July 23, 2025 Invited Speaker at the 2025 *Dynamics at Surfaces Gordon Research Conference*, Plymouth, NH.
- July 22-25, 2025 Invited Speaker at the special session on “Advanced Theoretical Methods in Nanoplasmonics and Molecular Plasmonics,” at the 15th *International Conference on Metamaterials, Photonic Crystals and Plasmonics (META 2025)*, Malaga, Spain.
- July 8-10, 2025 Invited Speaker at the CSI Workshop, Princeton University, Princeton, NJ.
- June 30-July 4, 2025 Invited Plenary Speaker at the 12th *International Conference on Materials for Advanced Technologies (ICMAT)*, Materials Research Society (MRS), Singapore.
- June 24-25, 2025 Distinguished Invited Speaker at the *International Symposium on AI for Electrochemistry (iSAIEC 2025)*, Xiamen University, China.
- June 22-27, 2025 Invited Speaker at the 13th *Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2025)*, Oslo, Norway.
- June 16-17, 2025 Invited Plenary Speaker at the SLAC National Accelerator Laboratory “*Driving critical chemical transformations with photons, electrons, and catalysts*” workshop, Menlo Park, CA.
- June 8-13, 2025 Invited Plenary Speaker at the 13th *International Conference on Chemical Kinetics*, Tahoe City, CA.
- April 23-24, 2025 Invited Speaker at the *AI and Climate Symposium*, UC Berkeley, Berkeley, CA.
- March 29, 2025 Invited Keynote Speaker at the *Forum on Digitalization Promoting Innovation in Large Enterprises — AI Empowering Industrial Development*, Beijing, China.
- Feb. 10-14, 2025 Invited Speaker at *Energy Week@Penn*, University of Pennsylvania, Philadelphia, PA.

- Dec. 16-20, 2024 Invited Plenary Speaker at the *Conference on Advances in Chemistry for Energy and Environment (CACEE-2024)*, Tata Institute of Fundamental Research, Mumbai, India.
- Dec. 1-6, 2024 Invited Speaker at the 2024 Materials Research Society Meeting on “*Plasmas for Materials Science—Opportunities at the Interface*,” Boston, MA.
- Nov. 12-15, 2024 Invited Speaker at the “Exploring Chiral Nanostructured Materials and Plasmonics for Energy Applications” Symposium at the *nanoGE Materials for Sustainable Development (MATSUS Fall 24) Conference*, Lausanne, Switzerland.
- Nov. 7, 2024 Invited Panelist at “*The Impact of Environment on Human Health*” Symposium, Princeton, NJ.
- Oct. 27-Nov. 1, 2024 Invited Speaker at the *Women in Catalysis* symposium at the 2024 AIChE Meeting, San Diego, CA.
- Oct. 6-11, 2024 Invited Lecturer at the PRiME 2024 Symposium on “*Fundamentals of Carbon Dioxide Reduction*,” Honolulu, HI.
- Sep. 30, 2024 Invited Speaker at the 77th Gaseous Electronics Conference (2024) on “*The Road to a Sustainable Energy Future and the Role of Plasmas*,” San Diego, CA.
- Sep. 22-25, 2024 Invited Speaker at the *International Conference on Molecular Electronic Structure*, Pescara, Italy.
- Sep. 8, 2024 Invited Plenary Speaker at the *Banff International Research Station (BIRS), of the Institute for Advanced Study in Mathematics (IASM), Symposium*, Hangzhou, China.
- July 14-18, 2024 Invited Speaker at the 10th *International Congresses on Ceramics (ICC10)* on “*Green Ceramics for Clean Energy and Sustainability*,” Montreal, Quebec, Canada.
- July 9-11, 2024 Keynote Speaker at the *GLObal Conference for Women Leaders and Emerging Researchers in Material Sciences (GLOW 2024)*, Nanyang Technological University, Singapore.
- June 20-24, 2024 Invited Lecturer at the *CIMTEC 2024 - Global Conference on “Materials in an Explosively Growing Informatics World*,” Montecatini Terme, Italy.
- June 17-19, 2024 Invited Speaker at the 3rd *Edition of the NanoSeries Conference on Nanotechnology*, Centro De Congressos Do Instituto Superior Técnico, University of Lisbon, Portugal.
- June 6-9, 2024 Invited Speaker at the 10th *Irsee Symposium at Schwäbisches Bildungszentrum on “Complexity at catalytically relevant interfaces*,” Irsee, Germany.
- March 17-21, 2024 Invited Speaker at the *American Chemical Society (ACS) Spring 2024 National Meeting* on “*The Role of Fundamental Interfacial Processes in Electrocatalysis under Division of Catalysis Science & Technology (CATL)*,” New Orleans, LA.
- March 4-8, 2024 Invited Lecturer at the 2024 APS March Meeting Focus Session on “*Density Functional Theory in Chemical Physics*,” Minneapolis, MN.
- Feb. 21, 2024 Invited Lecturer at the 2024 Presidential Lecture Series in Physics on “*Atmosphere: Earth to Exoplanets*,” New York, NY.
- 2023-2024 Invited Speaker at the *Catalysis Society of Metropolitan New York*, NY.
- Dec. 11-12, 2023 Invited Lecturer at the *Royal Society Discussion on “Green carbon for the chemical industry of the future*,” at the Royal Society, London, England, UK.

- Nov. 8, 2023 Keynote Speaker at *New Jersey Institute of Technology Research Day*, New Jersey Institute of Technology, Newark, NJ.
- Oct. 25-27, 2023 Plenary Lecturer at the *Sustainable Energy Workshop* at Brown University, Providence, RI.
- Oct. 23-26, 2023 Invited Lecturer at the *Exploration Conference "Interfaces and Mixing in Fluids, Plasmas, Materials,"* Kavli Institute for Theoretical Physics, University of California, Santa Barbara, Santa Barbara, CA.
- Oct. 9-10, 2023 Invited Keynote Speaker at the "*4th International Conference on Condensed Matter & Applied Physics*," Bikaner, Rajasthan, India.
- Sep. 11-14, 2023 Invited Lecturer at the *59th Symposium on Theoretical Chemistry (STC 2023)*, Zürich, Switzerland.
- Sep. 10-14, 2023 Invited Speaker at the *Climate Sustainability Workshop* at Spelman College, Atlanta, GA.
- July 11-12, 2023 Invited Panelist & Speaker at the *Climate Crossroads Summit at the National Academies*, Washington, D.C.
- June 14-16, 2023 Plenary Speaker at the *Australasian Leadership Computing Symposium*, Canberra, Australia.
- June 8, 2023 Panelist and guest of honor at the *Fourth Research Frontiers Forum, Climate Change and National Security: Goals, Gaps, and Game Changer*, Applied Physics Laboratory, Johns Hopkins University, Laurel, MD.
- June 4-8, 2023 Invited Speaker at the *Canadian Chemistry Conference and Exhibition (CSC 2023)*, Vancouver, British Columbia.
- May 28-June 2, 2023 Invited Keynote Speaker at the *243rd Electrochemical Society (ECS) Meeting*, Boston, MA.
- March 26-30, 2023 Invited Lecturer at the *ACS Spring 2023 National Meeting*, Indianapolis, IN.
- Nov. 15, 2022 Invited Lecturer at the *2022 AIChE Annual Meeting in Honor of Professor Keith E. Gubbins' 85th Birthday*, Phoenix, AZ.
- Nov. 9-12, 2022 Invited Facilitator at the *2022 Scialog NES Meeting*, Tucson, AZ.
- Aug. 25-30, 2022 Invited Sectional Lecturer at the *26th International Congress of Theoretical and Applied Mechanics (ICTAM2024)*, Daegu, Korea.
- July 21, 2022 Invited Distinguished Lecturer at the *U.S. Naval Research Laboratory (NRL) Chemistry Division 2022 Colloquium Series*, Washington, DC.
- July 18, 2022 Invited Plenary Lecturer at the *DOE Closing the Carbon Cycle Workshop*, Richland, WA.
- July 10-13, 2022 Invited Plenary Lecturer at the *NWChem-30 Conference*, Vancouver, BC.
- July 10-13, 2022 Invited Keynote Speaker at the *ACS Colloid and Surface Science Symposium*, Golden, CO.
- June 16-19, 2022 Invited Speaker at the *Schwäbisches Bildungszentrum 9th Irsee Symposium*, Irsee, Germany.

CURRENT EXTRAMURAL FUNDING SOURCES

Department of Energy, Basic Energy Sciences

Department of Energy, Fusion Energy Sciences

BP

Department of Defense, Multidisciplinary University Research Initiative