PROF. BRYAN M. WONG, PH.D.

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EDUCATION

Massachusetts Institute of Technology (M.I.T.) — **Cambridge, MA**
Ph.D. in Physical Chemistry, 2007
Thesis Committee Members: *Prof. Robert W. Field (Advisor), Prof. Troy Van Voorhis, Prof. Jianshu Cao*

Rice University — **Houston, TX**
B.S. in Physics and Chemistry, 2001, *Summa cum laude*

EMPLOYMENT

University of California, Riverside — **Riverside, CA**
Department of Chemistry
Professor — *2021 – Present*
Associate Professor — *2018 – 2021*
Assistant Professor — *2014 – 2018*

Department of Physics & Astronomy
Cooperating Faculty Member — *2017 – Present*

Materials Science & Engineering Program
Cooperating Faculty Member — *2014 – Present*

Department of Electrical & Computer Engineering
Cooperating Faculty Member — *2018 – Present*

Drexel University — **Philadelphia, PA**
Department of Chemistry
Department of Materials Science & Engineering
Assistant Professor — *2013 – 2014*

Sandia National Laboratories — **Livermore, CA**
Nanoelectronics and Nanophotonics Group
Senior Member of the Technical Staff — *2007 – 2013*

RESEARCH INTERESTS

My research group develops and applies *quantum-mechanical theoretical and computational techniques* to predict, understand, and rationally design chemical/material systems (either previously synthesized or yet to be made). My motivation arises from a deep interest in *electron dynamics* – a surprisingly rich research area that centers on the *non-equilibrium* (i.e., time-dependent) electronic properties of systems. A deep understanding of electron dynamics is extremely important since ***nearly all chemical, material, and biological processes occur out of equilibrium***, and our understanding of non-equilibrium excited-state processes in these systems is far from complete. The detailed understanding of electron dynamics enables numerous technological advancements, including plasmon-mediated photocatalysis, optically-induced charge separation, and light-harvesting nanomaterials. My research group's expertise in

developing/applying new electronic structure and time-dependent dynamics techniques brings to the field a unique capability for exploring these rich and emerging areas in complex chemical/material systems.

HONORS & AWARDS

2024 Top Cited Paper Award for "one of the top 1% most-cited papers in IOP Publishing's portfolio of journals from 2021-2023"
2024 *Environmental Science & Technology Letters* (*ES&T Letters*) Best Paper Award
2023 Google Cloud Research Innovator
2022 HPCWire Editors' Choice Award for Best Use of HPC in Response to Societal Plights (Urgent Computing, COVID-19)
2017 Regents Faculty Fellowship, UC Riverside
2017 ACS COMP OpenEye Outstanding Junior Faculty Award, American Chemical Society
2016 Department of Energy (DOE) Early Career Research Award
2015 NVIDIA GPU Award Finalist, American Chemical Society
2015 Original Work of Authorship for *pairbop v1.0*, Sandia National Laboratories
2014 R&D 100 Award for time-dependent calculations on *"Triplet Harvesting Plastic Scintillators"*
2014 Interfolio Scholar Gallery Award, Interfolio Inc.
2013 Employee Recognition Award, Sandia National Laboratories
2011 Best Poster Award Nominee, Materials Research Society
2011 Employee Recognition Award, Sandia National Laboratories
2007 Sigma Xi Scientific Research Society, Full Membership, M.I.T.
2007 IDEAS Competition and Fellowships Development Grant, M.I.T.
2001 *Summa cum laude*, Rice University
2001 Sigma Pi Sigma Physics Honor Society, Rice University
2001 Phi Lambda Upsilon Chemistry Honor Society, Rice University
2001 Bonner Book Award for the Most Outstanding Senior in Physics, Rice University
2001 Hypercube Scholar, Hypercube, Inc.
2001 Zevi and Bertha Salsburg Memorial Award in Chemistry, Rice University
2000 Hanszen College Fellow, Rice University
2000 NSF-REU Award, Rice Quantum Institute, Rice University
2000 Bonner Book Award for the Most Outstanding Junior in Physics, Rice University
2000 Golden Key National Honor Society, Rice University
1999 Richter Fellowship Award, Rice University
1997-2001 President's Honor Roll, Rice University
1997 Intel International Science and Engineering Fair Finalist
1996 Intel International Science and Engineering Fair Finalist

EXTERNAL FUNDING & CONTRACTS (AMOUNT TO MY GROUP: $9,868,320)

2025-2029 Air Force Office of Scientific Research (AFOSR), *"Harnessing Electron Dynamics Calculations and Experiments to Probe Time-Resolved Phenomena in Complex Plasmonic Systems."* **Total Award Amount: $1,000,000** (P.I.); **Amount to My Group: $575,000**

2025-2029 Department of Energy (DOE): National Renewable Energy Laboratory (NREL), *"Enhancing Federal Contract Opportunities through Strategic Training and Collaboration at the University of California, Riverside."* **Total Award Amount: $150,000** (single P.I.); **Amount to My Group: $150,000**

2025-2028 Department of Energy (DOE): Office of Basic Energy Sciences (BES), *"Excitons in Flatlands: First-Principles Explorations."* **Total Award Amount: $800,000** (co-P.I.); **Amount to My Group: $200,000**

2024-2029 Army Research Office (ARO), *"Propellant Burning Rate Control through Crystalline Oxidizer Microstructure."* **Total Award Amount: $994,500** (co-P.I.); **Amount to My Group: $180,000**

2024-2027 Nuclear Regulatory Commission (NRC), *"Predictive Quantum Calculations and Experiments to Design Scintillator Materials for Enhanced Monitoring of Nuclear Materials."* **Total Award Amount: $500,000** (P.I.); **Amount to My Group: $300,000**

2024-2027 Department of Energy (DOE): Office of Fossil Energy and Carbon Management (FECM), *"A Humanities-Driven STEM Approach for Student Training in Carbon Capture and Conversion."* **Total Award Amount: $999,990** (co-P.I.); **Amount to My Group: $475,531**

2024-2025 Department of Energy (DOE): Office of Fossil Energy and Carbon Management (FECM), *"Extraction of Rare Earth Elements and Critical Materials from Coal Ash Using Low-Cost Chloroaluminate Ionic Liquids and Derivatives."* **Total Award Amount: $100,000** (P.I.); **Amount to My Group: $50,000**

2023-2027 National Science Foundation (NSF): DMR – Designing Materials to Revolutionize and Engineer our Future (DMREF), *"Collaborative Research: DMREF: Organic Materials Architectured for Researching Vibronic Excitations with Light in the Infrared (MARVEL-IR)."* **Total Award Amount: $2,000,000** (co-P.I.); **Amount to My Group: $400,000**

2023-2026 Department of Energy (DOE): Office of Basic Energy Sciences (BES), *"Rational Design of Concentrated Electrolytes for Beyond Li-ion Batteries with Machine Learning and Quantum Calculations."* **Total Award Amount: $750,000** (co-P.I.); **Amount to My Group: $187,500**

2023-2026 Department of Energy (DOE): Office of Energy Efficiency and Renewable Energy (EERE), *"Large-Scale Density Functional Tight Binding (DFTB) Calculations to Probe Structural Effects and Bridge Multiple Length Scales in Hydrogen-Metal Systems."* **Total Award Amount: $300,000** (single P.I.); **Amount to My Group: $300,000**

2023-2025 Department of Energy (DOE): Office of Energy Efficiency and Renewable Energy (EERE), *"Single-Walled Carbon Nanotubes with Confined Chalcogens as the Catalysts and Electrodes for Oxygen Reduction Reaction in Fuel Cells."* **Total Award Amount: $300,000** (co-P.I.); **Amount to My Group: $150,000**

2022-2025 Department of Energy (DOE): Office of Fossil Energy and Carbon Management (FECM), *"An Experimental and Computational Approach to Investigating CO_2 Uptake of Cellulose-producing Algae from Cellulosic Ethanol Production."* **Total Award Amount: $400,000** (P.I.); **Amount to My Group: $200,000**

2022-2023 Department of Energy (DOE): Office of Fossil Energy and Carbon Management (FECM), *"Carbon Management with Advanced Materials: An Assessment of Experimental and Computational Capabilities."* **Total Award Amount: $200,000** (co-P.I.); **Amount to My Group: $100,000**

2021-2029 Army Research Office (ARO), *"High-Level GW Methods for Predicting Electronic Properties of 2D Materials in Heterostructures/Interfaces."* **Total Award Amount: $20,000** (single P.I.); **Amount to My Group: $20,000**

2021-2026 Department of Energy (DOE): Offices of Advanced Scientific Computing Research (ASCR) and Basic Energy Sciences (BES), *"DECODE: Data-Driven Exascale Control of Optically Driven Excitations in Chemical and Material Systems."* **Total Award Amount: $4,000,000** (P.I.); **Amount to My Group: $940,000**

2021-2025 National Science Foundation (NSF): CBET – Environmental Engineering, *"CDS&E: Harnessing Graphical Processing Units (GPUs) to Accelerate the Computational Efficiency of Air Quality Modeling Systems for*

Four-Dimensional Air Pollution Prediction." **Total Award Amount: $494,430** (P.I.); **Amount to My Group: $227,953**

2021-2025 Naval Engineering Education Consortium (NEEC), *"Harnessing Quantum Control Algorithms that Utilize and Enable New Machine Learning Applications with Entangled Qubits."* **Total Award Amount: $445,332** (single P.I.); **Amount to My Group: $445,332**

2021-2024 Department of Energy (DOE): Office of Fossil Energy (FE), *"Harnessing Plasma Experiments with Quantum Calculations for Low-Cost Hydrogen Production."* **Total Award Amount: $400,000** (co-P.I.); **Amount to My Group: $200,000**

2020-2025 Defense Threat Reduction Agency (DTRA), *"A URA for Materials Science in Extreme Environments."* **Total Award Amount: $3,000,000** (co-P.I.); **Amount to My Group: $729,643**

2020-2025 Department of Energy (DOE): Office of Fossil Energy (FE), *"Harnessing Quantum Information Science for Enhancing Sensors in Harsh Fossil Energy Environments."* **Total Award Amount: $500,000** (single P.I.); **Amount to My Group: $500,000**

2020-2025 National Science Foundation (NSF): CHE – Chemical Theory, Models and Computational Methods, *"EAGER: CDS&E: Field Programmable Gate Arrays (FPGAs) for Enhancing the Speed and Energy Efficiency of Quantum Chemistry Simulations."* **Total Award Amount: $270,347** (single P.I.); **Amount to My Group: $270,347**

2019-2023 Department of Energy (DOE): Office of Fossil Energy (FE), *"Probing Particle Impingement in Boilers and Steam Turbines Using High-Performance Computing with Parallel Central Processing Units (CPUs) and Graphics Processing Units (GPUs)."* **Total Award Amount: $400,000** (P.I.); **Amount to My Group: $200,000**

2019-2022 National Science Foundation (NSF): CHE – Environmental Chemical Science, *"D3SC: Data-Driven Modeling and Experimental Investigation for Discovery of Aquatic Chemistry Reaction Kinetics: New Tools for Water Reuse Applications."* **Total Award Amount: $501,059** (P.I.); **Amount to My Group: $281,409**

2018-2023 Department of Defense (DoD): Strategic Environmental Research and Development Program (SERDP), *"ER18-C2-1289 Treatment of Legacy and Emerging Fluoroalkyl Contaminants in Groundwater with Integrated Approaches: Rapid and Regenerable Adsorption and UV-Induced Defluorination."* **Total Award Amount: $749,999** (co-P.I.); **Amount to My Group: $105,000**

2018-2021 Office of Naval Research (ONR), *"A Rational Approach for Designing Lightweight, Energy-Efficient Components for Advanced Naval Materials."* **Total Award Amount: $450,000** (single P.I.); **Amount to My Group: $450,000**

2018-2020 National Science Foundation (NSF): CBET – Catalysis, *"EAGER: CDS&E: An Open-Source Software Package for Assessing and Controlling Photocatalytic Reactions."* **Total Award Amount: $200,000** (single P.I.); **Amount to My Group: $200,000**

2018-2019 Department of Defense (DoD): Strategic Environmental Research and Development Program (SERDP), *"A Combined Photo/Electrochemical Reductive Pathway Towards Enhanced PFAS Degradation."* **Total Award Amount: $198,576** (co-P.I.); **Amount to My Group: $25,000**

2017-2022 National Science Foundation (NSF): CHE – Environmental Chemical Science, *"Collaborative Research: Applicability Limits of Aqueous pK_a Values for Bulk and Surface Nanoparticle Processes."* **Total Award Amount: $310,847** (co-P.I.); **Amount to My Group: $155,424**

2017-2021 Department of Energy (DOE): Office of Fossil Energy (FE), *"Large-Scale, GPU-Enhanced DFTB Approaches for Probing Multi-Component Alloys."* **Total Award Amount: $250,000** (single P.I.)

2017-2021 Army Research Office (ARO), *"Quantitative and Mechanistic Analyses of Bond Selective Chemistry via Non-Thermal Excitation of Metal Nanostructures."* **Total Award Amount: $1,975,000** (co-P.I.); **Amount to My Group: $658,333**

2016-2021 Department of Energy (DOE): Early Career Research Program, *"Non-Empirical and Self-Interaction Corrections for DFTB: Towards Accurate Quantum Simulations for Large Mesoscale Systems."* **Total Award Amount: $750,000** (single P.I.); **Amount to My Group: $750,000**

2016-2019 National Science Foundation (NSF): CBET – Process Systems, Reaction Engineering and Molecular Thermodynamics, *"Dynamics of Solvation Effects on Lithium-Sulfur Electrochemical Processes in Sub-Nano Confinement."* **Total Award Amount: $329,695** (co-P.I.); **Amount to My Group: $164,848**

INTERNAL FUNDING AWARDS

2025-2026 University of California, Riverside – UC Riverside Artificial Intelligence ReSearch and Education Institute (RAISE@UCR) Seed Grant, *"Bridging Machine Learning and Quantum Dynamics Calculations to Probe Radiation-Induced Damage in Biological Systems."* **Total Award Amount: $30,000** (P.I.)

2025-2026 University of California, Riverside – Omnibus Travel Grant, **Total Award Amount: $620** (P.I.)

2025-2026 University of California, Riverside – Committee on Research Grant, *"Advanced Simulations for Designing Light-Harvesting Materials."* **Total Award Amount: $3,000** (P.I.)

2024-2025 University of California, Riverside – Omnibus Travel Grant, **Total Award Amount: $600** (P.I.)

2024-2025 University of California, Riverside – Committee on Research Grant, *"Predictive Simulations of Radiation-Induced Damage in DNA."* **Total Award Amount: $3,050** (P.I.)

2023-2024 University of California, Riverside – Committee on Research Grant, *"Harnessing Predictive Simulations to Design Corrosion-Resistant Materials."* **Total Award Amount: $5,000** (P.I.)

2023-2024 University of California, Riverside – Opportunity to Advance Sustainability Innovation and Social Inclusion Internal Funding Award (OASIS-IFA), *"Predictive Simulations and Experiments for High-Throughput Screening of Promising Hydrogen-Storage Materials."* **Total Award Amount: $25,000** (P.I.)

2023-2024 University of California, Riverside – Opportunity to Advance Sustainability Innovation and Social Inclusion Internal Funding Award (OASIS-IFA), *"Ammonia as a Hydrogen Carrier: Processing and Feasibility."* **Total Award Amount: $200,000** (co-P.I.)

2022-2023 University of California, Riverside – Committee on Research Grant, *"Harnessing Predictive Simulations to Design Advanced Sensor Materials."* **Total Award Amount: $9,000** (P.I.)

2022-2023 University of California, Riverside – Extramural Funding Opportunity Preparation Award, *"Harnessing Machine Learning Approaches to Efficiently Control Quantum Computers."* **Total Award Amount: $25,000** (co-P.I.)

2021-2022 University of California, Riverside – Omnibus Travel Grant, **Total Award Amount: $900** (P.I.)

2021-2022 University of California, Riverside – Extramural Funding Opportunity Preparation Award, *"Controlling Near-Surface NV Centers with Machine-Learned Quantum Control Algorithms for Enhanced Quantum Sensing."* **Total Award Amount: $25,000** (P.I.)

2020-2021 University of California, Riverside – Committee on Research Grant, *"Large-Scale Simulations and Machine-Learning Approaches for Designing Corrosion-Resistant Materials."* **Total Award Amount: $3,000** (P.I.)

2020-2021 University of California, Riverside – Omnibus Travel Grant, **Total Award Amount: $900** (P.I.)

2020-2021 University of California, Riverside – UC National Laboratory Fees Research Program, *"Harnessing Large-Scale Predictive Calculations for a More Accurate Assessment of COVID-19 Inhibitors and Their Binding Dynamics."* **Total Award Amount: $10,000** (P.I.)

2018-2019 University of California, Riverside – Omnibus Travel Grant, **Total Award Amount: $900** (P.I.)

2018-2019 University of California, Riverside – Collaborative Seed Grant, *"Electron-Phonon Interactions in the Confinement Regime."* **Total Award Amount: $10,000** (co-P.I.)

2018-2019 University of California, Riverside – Omnibus Travel Grant, **Total Award Amount: $950** (P.I.)

2017-2018 University of California, Riverside – Affordable Course Materials Initiative Grant. **Total Award Amount: $3,000** (P.I.)

2017-2018 University of California, Riverside – Collaborative Seed Grant, *"Treatment of Legacy and Emerging Fluoroalkyl Contaminants in Groundwater with Integrated Approaches: Rapid and Regenerable Adsorption and UV-Induced Defluorination."* **Total Award Amount: $10,000** (co-P.I.)

2017-2018 University of California, Riverside – Omnibus Travel Grant, **Total Award Amount: $1,000** (P.I.)

2016-2017 University of California, Riverside – Collaborative Seed Grant, *"New Computational Methods for Addressing Complex, Mesoscale Polymer Systems."* **Total Award Amount: $70,000** (P.I.)

2016-2017 University of California, Riverside – Omnibus Travel Grant, **Total Award Amount: $1,100** (P.I.)

2015-2018 University of California Office of the President, *"UCR – HBCU ASPIRE: A Summer Program in Research Engineering – Summer Research and Graduate Admission Pathways for Students from Historical Black Colleges and Universities."* **Total Award Amount: $254,104** (co-P.I.)

2015-2016 University of California, Riverside – Collaborative Seed Grant, *"Advanced Manufacturing Technologies for Next-Generation Rechargeable Battery Materials."* **Total Award Amount: $70,000** (co-P.I.)

2015-2016 UC Riverside Center for Catalysis, *"Multiscale Modeling for Multistep Catalysis: Inhomogeneity, Molecular Transport, and the Kinetics of Spatially Coordinated Reactions."* **Total Award Amount: $10,000** (co-P.I.)

2015-2016 University of California, Riverside – Collaborative Seed Grant, *"Hybrid Structure Modeling / Quantum Mechanical Methods for Enzyme Engineering."* **Total Award Amount: $10,000** (co-P.I.)

2015-2016 University of California, Riverside – Omnibus Travel Grant, **Total Award Amount: $1,300** (P.I.)

2013-2016 Sandia Laboratory Directed Research and Development (LDRD), *"Predicting Growth of Graphene Nanostructures Using High-Fidelity Atomistic Simulations."* **Total Award Amount: $1,560,000** (P.I.)

2010-2011 Sandia Laboratory Directed Research and Development (LDRD), *"First-Principles Predictions of Electronic Properties in Functionalized Graphene Nanoribbons."* **Total Award Amount: $80,000** (single P.I.)

2008-2009 Sandia Laboratory Directed Research and Development (LDRD), *"High Efficiency Infrared Detector Coupling Carbon Nanotubes with Photonic Crystals."* **Total Award Amount: $50,000** (single P.I.)

EXTERNAL COMPUTATIONAL RESOURCES

2026 National Energy Research Scientific Computing Center (NERSC) repository m4271, *"DECODE: Data-Driven Exascale Control of Optically Driven Excitations in Chemical and Material Systems."* **50,000 CPU Node hours and 10,000 GPU Node hours** (single P.I.)

2025 Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support (ACCESS) compute allocation award No. CHE250222, *"Ab initio Molecular Dynamics and Excited-State Simulations for Carbon Capture and Conversion."* **750,000 CPU hours** (single P.I.)

2025 National Energy Research Scientific Computing Center (NERSC) High-Impact Science at Scale, *"Massively Parallellized Real-Time Quantum Dynamics Simulations."* **25,000 CPU Node hours** (single P.I.)

2025 National Energy Research Scientific Computing Center (NERSC) repository m4271, *"DECODE: Data-Driven Exascale Control of Optically Driven Excitations in Chemical and Material Systems."* **80,000 CPU Node hours and 18,000 GPU Node hours** (single P.I.)

2024 Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support (ACCESS) compute allocation award No. PHY240322, *"Harnessing Quantum Dynamics for Enhancing Sensors in Harsh Environments."* **750,000 CPU hours** (single P.I.)

2024 Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support (ACCESS) compute allocation award No. CHE240173, *"Large-scale Ab Initio Molecular Dynamics of CO_2 Conversion in Algae."* **750,000 CPU hours** (single P.I.)

2024 National Energy Research Scientific Computing Center (NERSC) repository m4271, *"DECODE: Data-Driven Exascale Control of Optically Driven Excitations in Chemical and Material Systems."* **75,500 CPU Node hours and 18,000 GPU Node hours** (single P.I.)

2023 National Energy Research Scientific Computing Center (NERSC) repository m4271, *"DECODE: Data-Driven Exascale Control of Optically Driven Excitations in Chemical and Material Systems."* **100,000 CPU Node hours and 4,000 GPU Node hours** (single P.I.)

2022 Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support (ACCESS) compute allocation award No. EES220049, *"Computational Exploration of Air Quality Atmospheric Models for Four-Dimensional Air Pollution Prediction."* **800,000 CPU hours** (single P.I.)

2022 Extreme Science and Engineering Discovery Environment (XSEDE) compute allocation award No. TG-ENG160024, *"Advanced Computational Approaches to Probe Chemical Contaminants for Environmental Groundwater Applications."* **794,880 CPU hours** (single P.I.)

2021 Extreme Science and Engineering Discovery Environment (XSEDE) compute allocation award No. TG-ENG160024, *"Real-Time Quantum Dynamics Simulations for Predicting Radiation Damage Mechanisms in DNA."* **276,480 CPU hours and 19,600 GPU hours** (single P.I.)

2020 COVID-19 High Performance Computing Consortium, *"Harnessing Large-Scale Quantum-Based DFTB Calculations for a More Accurate Assessment of COVID-19 Inhibitors and Their Binding Dynamics."* $**250,000 worth of computing time on the Microsoft Azure cloud computing service** (single P.I.)

2020 National Energy Research Scientific Computing Center (NERSC) repository m3156, *"Real-Time Electron Dynamics of Large Chemical Systems."* **750,000 CPU hours** (single P.I.)

2019 NVIDIA Accelerated Data Science GPU Grant Program, **Titan V** awarded to B. M. Wong (single P.I.)

2019 National Energy Research Scientific Computing Center (NERSC) repository m3156, *"Real-Time Electron Dynamics and Self-Interaction Corrections in Large Chemical Systems."* **1,000,000 CPU hours** (single P.I.)

2018 National Energy Research Scientific Computing Center (NERSC) repository m3156, *"Real-Time Electron Dynamics and Self-Interaction Corrections in Large Chemical Systems."* **450,000 CPU hours** (single P.I.)

2018 Extreme Science and Engineering Discovery Environment (XSEDE) compute allocation award No. TG-ENG160024, *"Large-Scale Ab Initio Molecular Dynamics Simulations for Predicting Acid/Base Processes in Atmospheric Nanoparticles."* **66,816 CPU hours and 49,141 GPU hours** (single P.I.)

2017 NVIDIA Academic Hardware Grant Program, *"GPU Enhancements to DFTB for High-Throughput Ab Initio Molecular Dynamics Calculations of Multi-Component Alloys."* **Quadro P5000** (single P.I.)

2016 Extreme Science and Engineering Discovery Environment (XSEDE) compute allocation award No. TG-ENG160024, *"Predictive Modeling of Electrolytes for Electrochemical Energy Storage Systems."* **622,275 CPU hours** (single P.I.)

2016 NVIDIA Academic Hardware Grant Program, *"GPU-Enhanced Simulations of Energy-Efficient Light-Harvesting Systems."* **Tesla K40 GPU** (single P.I.)

2015 Extreme Science and Engineering Discovery Environment (XSEDE) compute allocation award No. TG-CHE150040, *"Density Functional Theory Calculations of Flexible Organic Polymers."* **50,000 CPU hours** (single P.I.)

2015 NVIDIA Academic Hardware Grant Program, *"GPU-Enhanced Simulations of Real-Time Electron Dynamics in Complex Environments."* **Tesla K40 GPU** (single P.I.)

2014 Extreme Science and Engineering Discovery Environment (XSEDE) compute allocation award No. TG-DMR140054, *"Large Scale Simulations for Understanding Growth Dynamics of Carbon Nanostructures on Metallic Surfaces."* **257,027 CPU hours** (single P.I.)

2013 Extreme Science and Engineering Discovery Environment (XSEDE) compute allocation award No. TG-CHE130052, *"Excited States of Functionalized Graphene Flakes."* **200,000 CPU hours** (single P.I.)

2010 NSF TeraGrid – National Center for Supercomputing Applications (NCSA) compute allocation award No. TG-CHE100066, *"First-Principles Predictions of Electronic Properties in Functionalized Graphene Nanoribbons."* **30,000 CPU hours** (single P.I.)

2008 NSF TeraGrid – National Center for Supercomputing Applications (NCSA) compute allocation award No. TG-CHE080076N, *"Noncovalent Interactions in Supramolecular Complexes."* **30,000 CPU hours** (single P.I.)

2007 NSF TeraGrid – National Center for Supercomputing Applications (NCSA) compute allocation award No. TG-CHE070084N, *"Thermochemistry of Large Amplitude Motions."* **25,000 CPU hours** (single P.I.)

SYNERGISTIC ACTIVITIES

Proposal Reviewer

American Chemical Society (ACS) Petroleum Research Fund
American Chemical Society (ACS) Chemical Computing Group (CCG) Excellence Awards for Graduate Students
Austrian Science Fund (FWF)
Center for Integrated Nanotechnologies (CINT)
Center for Nanoscale Materials (CNM), Argonne National Laboratory
National Science Centre Poland
US Department of Energy (DOE)

US Department of Energy (DOE) Office of Science Graduate Student Research Program
Division for Chemical Sciences, Netherlands Organization for Scientific Research
Israel Science Foundation Individual Research Grants
South Carolina EPSCoR Program
US National Science Foundation (NSF)
US National Science Foundation (NSF) Graduate Research Fellowship Program Awards

Journal Reviewer

See full list of journal reviews at https://www.webofscience.com/wos/author/record/1647258

PROFESSIONAL SOCIETY MEMBERSHIPS

American Chemical Society
American Nano Society
American Physical Society
Golden Key International Honor Society
Materials Research Society
Phi Lambda Upsilon Chemistry Honor Society
Royal Society of Chemistry
Sigma Pi Sigma Physics Honor Society
Sigma Xi Research Society
Society for Science & the Public

SERVICE ACTIVITIES

2025-2028 Chair, *R'Courses Governing Board, UC Riverside*
2024 Member, *Search Committee – Contracts and Grants Analyst II, Bourns College of Engineering, UC Riverside*
2023-2026 Associate Editor, *Scientific Reports*
2023-2025 Faculty Mentor, *Graduate Student Mentorship Program (GSMP), UC Riverside*
2023-2025 Member, *R'Courses Governing Board, UC Riverside*
2023 Member, *Search Committee – Contracts and Grants Analyst I, Bourns College of Engineering, UC Riverside*
2022-2025 Member, *Committee on Research, UC Riverside*
2022 Symposium Organizer, *Southern California Theoretical Chemistry (SoCal TheoChem) Symposium*
2022 Faculty Mentor, *Career Mentoring of Underrepresented STEM Students for the Professoriate (CUSP), UC Riverside*
2022 Member, *Search Committee – Contracts and Grants Analyst II, Bourns College of Engineering, UC Riverside*
2022 Member, *Bachelor Degree Completion Selection Committee, UC Office of the President*
2022-2023 Domain Co-Chair, Platform for Advanced Scientific Computing (PASC) Conference, *Chemistry and Materials Domain*
2021-2026 Member, *Building Emergency Staff (BES) – Materials Science & Engineering Building, UC Riverside*
2021-2023 Member, *Assessment Advisory Committee, UC Riverside*
2021-2022 Divisional Representative, *University Committee on Educational Policy, UC Office of the President*
2021 Member, *Search Committee – Director of Information Technology, Bourns College of Engineering, UC Riverside*
2021 Member, *Search Committee – Contracts and Grants Analyst II, Bourns College of Engineering, UC Riverside*
2021 Member, *Search Committee – Contracts and Grants Analyst III, Bourns College of Engineering, UC Riverside*
2021 Session Chair, *Pittsburgh Quantum Institute (PQI) Workshop*
2021-2023 Member and Representative, *Bourns College of Engineering Information Technology Steering Committee, UC Riverside*

2019-2022 Symposium Organizer, *Algorithm Development in Materials Science and Engineering, The Minerals, Metals and Materials Society*
2019-2022 Member, *Committee on Educational Policy, UC Riverside*
2018-2025 Member, *Online Master of Science (MSOL) in Engineering Oversight Committee, UC Riverside*
2018-2023 Member, *Student Mini-Grant Committee, UC Riverside*
2017-2023 Member, *Student Conduct and Academic Integrity Programs (SCAIP) Executive Committee, UC Riverside*
2017 Member, *Chemical & Environmental Engineering Undergraduate Program Committee, UC Riverside*
2017 Session Chair, *International Conference on Chemical Bonding*
2016-2023 Member, *Materials Science & Engineering Graduate Program Committee, UC Riverside*
2016-2023 Graduate Advisor for Admissions, *Materials Science & Engineering Program, UC Riverside*
2016-2017 Member, *Search Committee – Graduate Student Affairs (GSA) Officer, Materials Science & Engineering Program, UC Riverside*
2016-2017 Associate Editor, *RSC Advances*
2016 Symposium Organizer, *Time-Dependent Dynamics and Electronic Excited States*, ACS National Meeting, *Computers in Chemistry, American Chemical Society*
2016 Session Chair, ACS National Meeting, *Division of Energy & Fuels, American Chemical Society*
2016 Faculty Advisor, *Graduate Student Mentorship Program, UC Riverside*
2015-2018 Member, *Chemical & Environmental Engineering Graduate Program Committee, UC Riverside*
2015-2017 Member and Representative, *Bourns College of Engineering Information Technology Steering Committee, UC Riverside*
2015 Member, *Search Committee – Lecturer with Security of Employment (LSOE), Department of Chemical & Environmental Engineering, UC Riverside*
2015 Member, *Search Committee – Computational Materials Cluster Hire, UC Riverside*
2015 Member, *Public Relations and Communication Committee, UC Riverside*
2014-2026 Faculty Advisor, *Materials Research Society, UC Riverside*
2014 Member, *Materials Science & Engineering Undergraduate Program Committee, UC Riverside*
2013 Charter Member and Representative, *Institute for Energy and the Environment (IExE), Drexel University*
2013 Member, *College of Arts and Sciences Research Day Committee, Drexel University*
2013 Member, *Department of Chemistry Graduate Program Committee, Drexel University*
2012 Session Chair, ACS National Meeting, *Division of Inorganic Chemistry, American Chemical Society*
2010-2012 Workshop Organizer, *Enabling Predictive Simulation Research Institute, Sandia National Laboratories*
2009 Research Sponsor, *Department of Energy's Faculty and Student Teams (FaST) program for recruiting under-represented researchers in science and engineering, Sandia National Laboratories*
2000-2001 Vice President of the Society of Physics Students, *Rice University*

ACADEMIC MENTORING

Postdoctoral Associates

Dr. Yifan Yao (2025-present)
Dr. Pramod Verma (2025-present)
Dr. Kamal Sharkas (2023-present)
Dr. Min Choi (2021-present)
Dr. Gabriel Phun (2024-2025)
Dr. Qiang Xu (2022-2025): assistant professor at Jilin University
Dr. Mahmut Okyay (2022-2025): educator in Reno, Nevada
Dr. Wafa Maftuhin (2023-2024): lecturer at Universitas Negeri Surabaya
Dr. José Rodríguez-Borbón (2020-2024): scientific software developer
Dr. Sohag Biswas (2020-2024): postdoctoral associate at Scuola Normale Superiore

Dr. Zulfikhar A. Ali (2022-2023): data scientist at FICO
Dr. Kota Hanasaki (2020-2022): postdoctoral associate at University of Zurich
Dr. Yuanqi Gao (2020-2021): senior machine learning engineer at Lucid Motors
Dr. Ravindra Shinde (2019-2020): research scientist at the University of Twente
Dr. Sharma S.R.K.C. Yamijala (2017-2020): assistant professor at IIT Madras
Dr. Chao Lian (2018-2019): professor at the Institute of Physics Chinese Academy of Sciences
Dr. Fredy W. Aquino (2016-2019): software engineer at QSimulate
Dr. Mustafa Kurban (2018-2019): associate professor at Kırşehir Ahi Evran University
Dr. M. Belén Oviedo (2014-2016, *ICAM Postdoctoral Fellowship Awardee*): assistant professor at the Universidad Nacional de Córdoba
Dr. Michael E. Foster (2012-2014): consultant for Sandia National Laboratories
Dr. Jie Deng (2012): battery system engineer at Ford Motor Company
Dr. Jonathan W. Lee (2010-2012): senior engineering manager and project coordinator at UC Berkeley

Ph.D. Graduate Students
Mr. Simon Sandhofer (2022-present)
Mr. Yuan Chen (2022-2024)
Mr. Xian Wang (2019-2024), postdoctoral associate at Los Alamos National Laboratory
Mr. Steve D. Yang (2020-2023), data analyst at ATI, Inc.
Ms. Hyuna Kwon (2018-2023), postdoctoral associate at Lawrence Livermore National Laboratory
Mr. Anshuman Kumar (2017-2023, *Dissertation Year Program Awardee*), postdoctoral associate at the University of California, Davis
Mr. Zulfikhar A. Ali (2017-2022, *Graduate Research Mentorship Program Awardee*), data scientist at FICO
Mr. Niranjan V. Ilawe (2014-2018, *Dissertation Year Program Awardee*, *Chemical and Biological Defense Science & Technology (CBD S&T) Student Travel Awardee*): data engineer at Meta

M.S. Graduate Students
Mr. Simon Sandhofer (2020-2022): attending Ph.D. program at UC Riverside
Mr. Cameron Chevalier (2020-2021): attending Ph.D. program at UC Riverside
Mr. Michael Lurenana (2018-2020): senior environmental engineer at Burns & McDonnell
Mr. Akber Raza (2018-2019): GPU software engineer at Qualcomm
Mr. Ricardo Jenkins (2017-2018): research technician at BP/Castrol
Ms. Sarah I. Allec (2015-2018, *NASA MIRO Fields Fellowship Awardee*, *ACS Women Chemists Committee Travel Awardee*, *NSF Graduate Research Fellowship Program Awardee*): research scientist at Citrine Informatics
Ms. Lindsey Anderson (2015-2017): test management specialist at the Department of the Navy
Ms. Sangavi Pari (2015-2017, *Society of Women Engineers (SWE) Scholarship Program Awardee*): software engineer at Chewy
Mr. Marc N. Cercy Groulx (2014-2015): instrumentation engineer at PM Group

Other Graduate Students/Visiting Students
Mr. Prithviraj Yuvaraj (2021-2022): attending Ph.D. program at UC Riverside
Mr. Jose Rodriguez Borbon (2018-2020): postdoctoral associate at UC Riverside
Ms. Sharmistha Bardhan (2018-2019): software development engineer at Amazon
Mr. Khanh Do (2018): postdoctoral associate at Northeastern University
Mr. Kuai (David) Yu (2018): senior data scientist at Esri
Ms. Yue (Sarah) Zhu (2018): data scientist at Hewlett Packard

Ms. Lihua Xu (2017-2018, *Global Food Initiative Student Fellowship Awardee*): attending graduate school at Georgia Institute of Technology

Mr. Yijing Sun (2017): software engineer at Walmart

Ms. Yunduan Han (2017): software engineer at Unity Technologies SF

Ms. Alexandra E. Raeber (2013-2014, *NDSEG Fellowship Awardee*): postdoctoral associate at M.I.T.

Ms. Xi Chen (2013-2014): attending graduate school at Drexel University

Mr. Andrew W. Long (2012): senior data scientist at 3M

Mr. Timothy H. Hsieh (2010, *NSF Graduate Research Fellowship Program Awardee*): junior faculty member at the Perimeter Institute of Theoretical Physics

Ms. Angela Cheng (2010): research associate at Moeda

Undergraduate Students

Mr. Chase Lewis (2022), *Mr. Victor Cuchilla* (2021), *Ms. Selena Najar* (2021), *Mr. Caleb McClure* (2021), *Ms. Anagha Belavadi S* (2021), *Mr. Olawale Olatunde* (2020-2021), *Mr. Muslim Rana* (2020), *Mr. Hasan Usmani* (2020), *Ms. Ayah Seirafi* (2019-2020), *Ms. Ena Mikic* (2016-2017), *Ms. Eric Shang* (2017), *Ms. Crystal Xiao* (2017), *Mr. James Kwon* (2016), *Ms. Inger A. Wang* (2016), *Ms. Rishika Betrabet* (2015-2016), *Mr. Earl Garcia* (2015-2016), *Mr. Benjamin Cornejo* (2015-2016), *Ms. Horrara Diógenes* (2015), *Mr. Cesar Schadeck* (2015), *Mr. Thomas T. Dong* (2014), *Mr. Yash Kamothi* (2014), *Mr. Timothy J. Legere* (2014), *Ms. Shraddha Patel* (2014), *Ms. Adaugo Ukaegbu* (2014), *Mr. Mengyi Xu* (2014), *Ms. Gabrielle Arnold* (2013-2014), *Mr. Feng Long Chen* (2013-2014), *Mr. Nicholas Ly* (2013-2014), *Ms. Mi Tran* (2013-2014), *Mr. Andy Kung* (2010-2012), *Mr. Simon H. Ye* (2010, *NSF Graduate Research Fellowship Program Awardee*)

Advancement to Candidacy Committee Member

Xuefen Liu (2025), *Edward Zhu* (2025), *Duncan Quevedo* (2024), *Chao Gao* (2024), *Brandon Wagner* (2023), *Minseok Kim* (2022), *Marjuka Ferdousi Lazin* (2022), *Hyeonkyeong Lee* (2022), *Huawei Li* (2022), *Runtong Pan* (2022), *Steve D. Yang* (2022), *Gaurav Ahuja* (2021), *Quazi Mishkatul Alam* (2021), *Jianjun Chen* (2021), *Min Chiang Gary Ong* (2021), *Christopher Rudnicki* (2021), *Varun Trivedi* (2021), *Chuanye Xiong* (2021), *Zhaoxi Yang* (2021), *Allejandro Gallegos* (2020), *Hyuna Kwon* (2020), *Amin Kalantar Chahouki* (2019), *Anshuman Kumar* (2019), *Nicole Onishi* (2019), *Akber Raza* (2019), *Jiayan Shi* (2019), *Jianan Sun* (2019), *Ning Yu* (2019), *Yifan Zhao* (2019), *Weiyi Zhang* (2019), *Musen Zhou* (2019), *Ravindra V. Bhardwaj* (2018), *Kevin Chalek* (2018), *Setareh Jahansouz,*(2018), *Pegah Mirabedini* (2018), *Christos Stamatis* (2018), *Song Wang* (2018), *Xiaoyu Wen* (2018), *Lihua Xu* (2018), *Hadi Zamani Sabzi* (2018), *Zachary Zimmerman* (2018), *Sarah I. Allec* (2017), *Luping Han* (2017), *Watit Sontising* (2017), *Tianyi Yu* (2017), *Yangzhi Zhu* (2017), *Caroline Kim* (2016), *Kun Liu* (2016), *Jessica McKinley* (2016), *Laura de Sousa Oliveira* (2016), *Jonathan Spalding* (2016), *Dejan Stekovic* (2016), *Emmanuel Fofie* (2015), *Niranjan V. Ilawe* (2015), *Sanggon Kim* (2015), *Justin Neal* (2015), *Chad Priest* (2015), *Parawee Pumwongpitak* (2015), *Shijie Sheng* (2015), *Ashley Vizenor* (2014)

Thesis Defense Committee Member

Gaurav J. Ahuja, M.S. (2025), *Minseok Kim, Ph.D.* (2024), *Yujie Wang, Ph.D.* (2024), *Anshuman Kumar, Ph.D.* (2023), *Hyuna Kwon, Ph.D.* (2023), *Steve D. Yang, Ph.D.* (2023), *Zulfikhar A. Ali, Ph.D.* (2022), *Ming Lei, Ph.D.* (2022), *Simon Sandhofer, M.S.* (2022), *Hao Tang, M.S.* (2022), *Ning Yu, Ph.D.* (2022), *Musen Zhou, Ph.D.* (2022), *Yifan Zhao, Ph.D.* (2021), *Alejandro Alvarez Barragan, Ph.D.* (2019), *Setareh Jahansouz, Ph.D.* (2019), *Kun Liu, Ph.D.* (2019), *John Orta, M.S.* (2019), *Yangzhi Zhu, Ph.D.* (2019), *Leonard Apontti, M.S.* (2018), *Luping Han, Ph.D.* (2018), *Niranjan V. Ilawe, Ph.D.* (2018), *Sanggon Kim, Ph.D.* (2018), *Guanghui Li, Ph.D.* (2018), *Lindsey Anderson, M.S.* (2017), *Laura de Sousa Oliveira, Ph.D.* (2017), *Sangavi Pari, M.S.* (2017), *Parawee Pumwongpitak, Ph.D.* (2017), *Shijie Sheng, Ph.D.* (2017), *Yun Tian, Ph.D.* (2017), *Talin Avanesian, Ph.D.* (2016), *Chun-Te Kuo, M.S.* (2015), *Jonathan B. Soffer, Ph.D.* (2013)

TEACHING EXPERIENCE

University of California, Riverside **Riverside, CA**

2025 Spring, 2025 Fall, **CHEM 001C**: *General Chemistry*

Professor: An introduction to the basic principles of chemistry.

2024 Spring, **CHE 102**: *Catalytic Reaction Engineering*

Professor: Principles of surface reactions and heterogeneous catalysis. Catalyzed reaction kinetics, heterogeneous reactions, diffusion and heterogeneous catalysis, analysis and design of heterogeneous reactors.

2020 Summer, 2021 Summer, 2022 Summer, 2023 Summer, **CHE 114**: *Applied Fluid Mechanics*

Professor: An introduction to fluid statics, fluid flow, and flow of compressible and incompressible fluids in conduits and open-channel flow. Also covers flow past immersed bodies, transportation and metering of fluids, and agitation and mixing of liquids.

2019 Winter, 2020 Winter, 2021 Winter, 2022 Spring, **CHE 202**: *Transport Phenomena*

Professor: Topics include transport phenomena, potential flow, and boundary layer theories with applications to simultaneous heat, momentum, and mass transfer. Introduces numerical techniques used to solve advanced transport phenomena problems.

2016 Summer, 2017 Winter, 2018 Winter, 2022 Winter, 2023 Winter, **CHE 100**: *Engineering Thermodynamics*

Professor: An introduction to engineering thermodynamics with emphasis on chemical and environmental engineering systems. Topics include concepts of equilibrium, temperature, and reversibility; the first law and concept of energy; and the second law and concept of entropy. Also examines equations of state, thermodynamic properties, and engineering applications used in the analysis and design of closed and open systems.

2016 Winter, **MSE 201**: *Thermodynamic Foundations of Materials*

Professor: Covers the laws of thermodynamics and fundamental equations for multi-component elastic solids, electromagnetic media, and equilibrium criteria. Describes applications to solution thermodynamics, point defects in solids, elastic effects, phase diagrams, transitions, and interfaces. Includes nucleation theory, kinetics (diffusion of heat, mass, and charge), and coupled flows.

2016 Winter, **CEE 206**: *Advanced Chemical Engineering Thermodynamics*

Professor: Application of the laws of thermodynamics to phase and chemical reaction equilibrium. Introduction to statistical thermodynamics, molecular simulations, and the evaluation of thermodynamic properties from molecular simulations.

2015 Winter, 2015 Fall, 2016 Fall, 2017 Fall, 2018 Fall, 2019 Fall, 2020 Fall, 2021 Fall, 2022 Fall, **CEE 200**: *Advanced Engineering Computation*

Professor: Problem-solving techniques for basic engineering systems including heat and mass transfer, coupled reactions, fluid flow potential, and control.

2014 Fall, **ENGR 118**: *Engineering Modeling and Analysis*

Professor: Covers the formulation of mathematical models for engineering systems. Includes applying mass, momentum, and energy balances to derive governing differential equations; solving equations with the use of spreadsheets and other software packages; and fitting linear and nonlinear models to experimental data.

Drexel University **Philadelphia, PA**

2013, **CHEM 253**: *Thermodynamics and Kinetics*

Professor: Covers gas properties, gas laws, state functions, first, second, and third laws of thermodynamics, phase transformations, phase diagrams, chemical equilibrium, spontaneous reactions, Gibbs free energy, molecular motion,

diffusion, rates of chemical reactions, rate laws, molecular reaction dynamics, transition states, electron transfer. I have completely re-vamped this course by adding new computationally-based examples (both in lecture and in homework) to emphasize intuitive physical meaning and to include additional topics in materials science.

Massachusetts Institute of Technology (M.I.T.) **Cambridge, MA**

2005 Fall, **5.60**: *Thermodynamics and Kinetics*

Teaching Assistant: Presented 26 lectures and tutorials and graded assignments for course material. Assisted students individually with homework problems four times a week.

2002 Spring, **5.60**: *Thermodynamics and Kinetics*

Teaching Assistant: Presented 26 lectures and tutorials and graded assignments for course material. Assisted students individually with homework problems four times a week.

2001 Fall, **5.61**: *Physical Chemistry (Quantum Chemistry)*

Head Teaching Assistant: Organized class structure, presented 26 lectures and tutorials, prepared teaching materials for 6 problem sets, solutions, and 3 exams, and graded assignments for course material. Assisted students individually with homework problems two times a week.

Rice University **Houston, TX**

2001 Spring, **PHYS 126**: *General Physics II*

Teaching Assistant: Organized tutorials and recitation sections for course material. Assisted students individually with homework problems once a week.

2001 Spring, **NSCI 230**: *Computation in Science and Engineering*

Teaching Assistant: Organized 13 tutorials, wrote solution manuals, and graded assignments for course material. Assisted students individually with writing computer programs twice a week.

2000 Fall, **PHYS 125**: *General Physics I*

Teaching Assistant: Organized tutorials and recitation sections for course material. Assisted students individually with homework problems once a week.

2000 Spring, **NSCI 230**: *Computation in Science and Engineering*

Teaching Assistant: Organized 13 tutorials, wrote solution manuals, and graded assignments for course material. Assisted students individually with writing computer programs twice a week.

1999 Fall, **BIOS 201**: *Introductory Biology*

Teaching Assistant: Organized tutorials and recitation sections for course material once a month.

INVITED TALKS

2025 **Telluride Science Research Center**, Invited Talk, Telluride, CO: *Quantum Dynamics of Materials in External Fields: Software and Hardware Developments*, August 19, 2025

2024 **MRS Fall Meeting & Exhibit, Quantum Dynamics in Nanoclusters**, Invited Talk, Boston, MA: *Real-Time Quantum Dynamics in Plasmonic Nanoparticle Arrays*, December 3, 2024

2024 **Southern California Theoretical Chemistry Symposium**, Invited Talk, University of California at San Diego, CA: *Probing Electron Dynamics of Complex Material Systems in Real Time*, October 5, 2024

2024 **Telluride Science Research Center**, Invited Talk, Telluride, CO: *Probing Electron Dynamics of Complex Material Systems in Real Time*, July 10, 2024

2024 **Office of the Under Secretary of Defense for Research & Engineering, Basic Research Forum**, Invited Talk, Arlington, VA: *Quantum Simulations for Predicting Ground and Excited-State Dynamics of Material Systems*, April 5, 2024

2023 **California Polytechnic State University, Pomona, Department of Physics**, Pomona, CA: *Exploring Time-Dependent Quantum Physics in Material Systems*, November 16, 2023

2023 **AIChE National Meeting, Fundamental Theory and Characterization of Optoelectronic Materials**, Invited Talk, Orlando, FL: *Real Time Electron Dynamics of Chemical and Material Systems*, November 7, 2023

2023 **Johns Hopkins University, DIMP/Simulant Workshop**, Invited Talk, Baltimore, MD: *DIMP Decomposition Mechanisms on Metal Oxide Surfaces from Ab Initio Molecular Dynamics*, October 5, 2023

2023 **University of California at Berkeley, Berkeley Excited States Conference**, Invited Talk, Oakland, CA: *Probing Electron Dynamics of Complex Material Systems in Real Time*, February 16, 2023

2023 **University of California at Irvine, Department of Materials Science & Engineering**, Irvine, CA: *Probing Electron Dynamics of Complex Material Systems in Real Time*, February 9, 2023

2022 **Lawrence Berkeley National Laboratory, SciDAC-5 FASTMath Institute**, Invited Talk, Berkeley, CA: *Probing Electron Dynamics of Complex Chemical and Material Systems in Real Time*, June 28, 2022

2022 **University of Wyoming, Materials Science and Engineering Symposium**, Keynote Speaker, Laramie, WY: *Probing Electron Dynamics of Complex Chemical and Material Systems in Real Time*, April 29, 2022

2021 **Brandeis University, Department of Chemistry**, Waltham, MA: *Applications of Real-Time Electron Dynamics to Chemical and Material Systems*, November 22, 2021

2020 **Kansas State University, Theory and Simulation of Electronic and Optical Processes in Molecules and Materials**, Invited Talk, Manhattan, KS: *Unconventional Applications of Real-Time Electron Dynamics*, October 28, 2020

2020 **University of Illinois at Chicago, Department of Chemical Engineering**, Chicago, IL: *Energy-Transfer Mechanisms in Chemical Engineering Systems: A Real-Time Dynamics Perspective*, September 17, 2020

2020 **Department of Navy, Opportunity Awareness Workshop**, Invited Talk, Alexandria, VA: *A Rational Approach for Designing Lightweight, Energy-Efficient Components for Advanced Naval Materials*, August 11, 2020

2019 **Washington University in St. Louis, Department of Energy, Environmental & Chemical Engineering**, St. Louis, MO: *Energy-Transfer Mechanisms in Complex Chemical Systems: A Real-Time Dynamics Perspective*, October 11, 2019

2019 **Rutgers University, Workshop on Time-Dependent Density Functional Theory**, Invited Talk, New Brunswick, NJ: *A Primer on Real-Time TDDFT for Periodic Systems*, August 14, 2019

2019 **TMS Annual Meeting and Exhibition, Algorithm Development in Materials Science and Engineering**, Invited Talk, San Antonio, TX: *GPU-Enabled Algorithms for Ground-State and Excited-State Density Functional Tight Binding Simulations*, March 11, 2019

2019 **University of California at Davis, Department of Materials Science and Engineering**, Davis, CA: *Energy-Transfer Mechanisms in Complex Materials: A Real-Time Dynamics Perspective*, February 26, 2019

2019 **New York University, Department of Chemical and Biomolecular Engineering**, New York, NY: *Energy-Transfer Mechanisms in Complex Chemical Systems: A Real-Time Dynamics Perspective*, February 22, 2019

2019 **Dartmouth University, Department of Chemistry**, Hanover, NH: *Energy-Transfer Mechanisms in Complex Chemical Systems: A Real-Time Dynamics Perspective*, January 17, 2019

2019 **University of Florida, Department of Chemical Engineering**, Gainesville, FL: *Energy-Transfer Mechanisms in Complex Chemical Systems: A Real-Time Dynamics Perspective*, January 7, 2019

2018 **AIChE National Meeting, Electrochemical Storage Materials and Devices**, Invited Talk, Pittsburgh, PA: *Exploring Electrochemical Reaction Dynamics of Li^+-Solvation Structures with Large-Scale Quantum Mechanical Simulations*, October 28, 2018

2018 **Department of Navy, Opportunity Awareness Workshop**, Invited Talk, Atlanta, GA: *A Computational Materials Approach for Designing Lightweight, Energy-Efficient Components for Advanced Naval Materials*, August 30, 2018

2018 **ACS National Meeting, Division of Computers in Chemistry**, Invited Talk, Boston, MA: *Real-Time Density Functional Tight Binding: A New Computational Approach for Probing Plasmonic Properties of Large Material Systems*, August 21, 2018

2018 **Colorado School of Mines, Department of Metallurgical and Materials Engineering**, Golden, CO: *Real-Time Density Functional Tight Binding: A New Computational Tool for Probing Electronic Properties of Large Chemical Systems*, May 10, 2018

2018 **ACS National Meeting, Division of Polymer Chemistry**, Invited Talk, New Orleans, LA: *Polarizabilities of π-Conjugated Polymers Revisited: Improved Results from Broken-Symmetry, Range-Separated DFT*, March 18, 2018

2018 **California State University Fullerton, Department of Chemistry**, Fullerton, CA: *Real-Time Density Functional Tight Binding: A New Computational Tool for Probing Electronic Properties of Large Chemical Systems*, February 15, 2018

2017 **Rice University, Department of Chemical and Biomolecular Engineering**, Houston, TX: *Real-Time Density Functional Tight Binding: A New Computational Tool for Probing Electronic Properties of Large Chemical Systems*, August 24, 2017

2017 **5th International Conference on Chemical Bonding (ICCB),** Invited Talk, Kauai, HI: *Anomalous Optoelectronic Properties of Nanostructures from DFT and TD-DFT Calculations*, June 22, 2017

2017 **University of California at San Diego, Department of Chemistry**, San Diego, CA: *Real-Time Electron Dynamics of Large Complex Systems from a Density Functional Tight Binding Approach*, May 23, 2017

2017 **Southern California Theoretical Chemistry Symposium**, Invited Talk, University of California at Irvine, CA: *Real-Time Electron Dynamics of Large Complex Systems from a Density Functional Tight Binding Approach*, May 20, 2017

2017 **Aberdeen Proving Ground**, Invited Talk, Aberdeen, MD: *Real-Time Dynamics from DFTB: A New Computational Approach for Large Complex Systems*, May 15, 2017

2016 **ACS National Meeting, Division of Energy and Fuels**, Invited Talk and Session Chair, Philadelphia, PA: *Electron Dynamics of Large Systems from Real-Time TDDFTB*, August 23, 2016

2016 **ACS National Meeting, Division of Energy and Fuels**, Invited Talk, San Diego, CA: *Electron Dynamics of Large Systems from Real-Time TDDFTB*, March 15, 2016

2015 **University of Texas at El Paso, Department of Physics**, El Paso, TX: *Light-Harvesting Systems: from the Frequency Domain to the Time Domain*, November 25, 2015

2015 **University of California at Riverside, Department of Chemistry**, Riverside, CA: *Light-Harvesting Systems: from the Frequency Domain to the Time Domain*, November 23, 2015

2015 **California State University Northridge, Department of Physics**, Northridge, CA: *New Computational Tools for Probing Quantum Effects in Large Complex Systems*, March 6, 2015

2015 **University of California at Los Angeles, Department of Civil & Environmental Engineering**, Los Angeles, CA: *Real-Time Dynamics from Density Functional Tight Binding: A New Computational Tool for Probing Complex Heterogeneous Systems*, February 24, 2015

2014 **California State University San Bernardino, Department of Chemistry**, San Bernardino, CA: *Computers in Chemistry: Using Simulations for Running Virtual Experiments*, October 23, 2014

2014 **Telluride Science Research Center**, Invited Talk, Telluride, CO: *Charge-Transfer Dynamics with Explicit Solvent: Insights from RT-TDDFTB*, July 14, 2014

2014 **Virginia Tech, Department of Chemical Engineering**, Blacksburg, VA: *Predictive and Fast: First-Principles Calculations on Energy Transfer in Molecular Photovoltaics, Carbon Nanotubes and Nanowires*, March 3, 2014

2013 **Drexel University, Dean's Seminar**, Philadelphia, PA: *Computational Design for Molecular Photovoltaics, Carbon Nanotubes, and Nanowires*, November 13, 2013

2013 **Argonne National Laboratories, Materials Science Division**, Argonne, IL: *Energy Transfer in Molecular Photovoltaics, Carbon Nanotubes, and Nanowires – a First-Principles Perspective*, June 2013

2013 **University of California at Los Angeles, Department of Materials Science & Engineering**, Los Angeles, CA: *Energy Transfer in Molecular Photovoltaics, Carbon Nanotubes, and Nanowires – a First-Principles Perspective*, May 16, 2013

2013 **Tulane University, Department of Physics and Engineering Physics**, New Orleans, LA: *Non-Empirically Tuned Range-Separated DFT for Predicting Fundamental and Excitation Gaps*, April 19, 2013

2013 **Rice University, Department of Mechanical Engineering and Materials Science Seminar**, Houston, TX: *Energy Transfer in Molecular Photovoltaics, Carbon Nanotubes, and Nanowires*, March 21, 2013

2013 **University of Illinois at Urbana-Champaign, Department of Materials Science & Engineering Colloquium**, Urbana, IL: *Energy Transfer in Molecular Photovoltaics, Carbon Nanotubes, and Nanowires – a First-Principles Perspective*, February 2013

2012 **Jackson State University, Department of Chemistry**, Jackson, MS: *Rational Design of Light-Harvesting Molecules and Nanomaterials*, November 2012

2012 **Lawrence Livermore National Laboratories, Quantum Simulations Group**, Livermore, CA: *First-Principles Calculations of Molecular Photovoltaics and Nanomaterials*, October 2012

2012 **IBM Almaden Research Center**, San Jose, CA: *Nanoscale Electronic Effects in Heterostructure Nanowires*, October 2012

2012 **ACS National Meeting, Division of Inorganic Chemistry**, Invited Talk and Session Chair, San Diego, CA: *Unusual Nanoscale Effects of Electrons in Heterojunction Core/Shell Nanowires*, March 2012

2011 **Bradley University, Department of Physics**, Peoria, IL: *Computational Design of Light-Harvesting Molecules and Nanomaterials*, April 2011

2011 **Sandia National Laboratories, Materials Science & Technology External Review**, Albuquerque, NM: *First-Principles Computational Design of Light-Harvesting Molecules and Nanomaterials*, January 2011

OPEN-SOURCE SOFTWARE

SQUIRREL (Streamlined Quantum Unified Interface for Researching Real-time Excitations with Light): propagates the time-dependent Schrödinger equation on complex geometries in the presence of time-dependent electric and/or magnetic fields. The SQUIRREL software suite uses a suite of efficient propagation methods for various quantum dynamics applications, including a new perturbation-based element-dropping algorithm that improves computational performance with minimal loss of accuracy [for further details, see: S. N. Sandhofer, M. S. Okyay, and B. M. Wong*, *Computer Physics Communications*, **317**, 109861 (2025)].

VAN-DAMME (Versatile Approaches to Numerically Design, Accelerate, and Manipulate Magnetic Excitations): carries out massively-parallelized quantum optimal control (QOC) calculations of multi-qubit systems. To enable large QOC calculations, this software package utilizes symmetry-based techniques with custom GPU-enhanced algorithms [for further details, see: J. M. Rodríguez-Borbón, X. Wang, A. P. Diéguez, K. Z. Ibrahim, and B. M. Wong*, *Computer Physics Communications*, **296**, 109403 (2025)].

MISTER-T (Manipulating an Interacting System of Total Electrons in Real-Time): enables quantum optimal control for multi-electron systems on nonuniform meshes with arbitrary two-dimensional cross-sectional geometries. The software is enabled by forward and backward propagator integration methods to evolve the Kohn-Sham equations with a pseudoskeleton decomposition algorithm for enhanced computational efficiency [for further details, see: Y. Chen, M. S. Okyay, and B. M. Wong*, *Computer Physics Communications*, **302**, 109248 (2024)].

SHORYUKEN (Streamlined High-level Operations in Real-space to Yield, Understand, and Keep Exchange in Nanowires): calculates nonlocal exchange interactions in nanowires with arbitrary geometries, sizes, doping densities, and compositions. In addition to enabling new calculations of nonlocal exchange, this software package is a significant enhancement of our previous HADOKEN code and includes new algorithmic improvements as well as an improved treatment of surface states for nanowires with intrinsic polarization [for further details, see: Y. Chen, S. N. Sandhofer, and B. M. Wong*, *Computer Physics Communications*, **300**, 109197 (2024)].

TRAVOLTA (Terrific Refinements to Accelerate, Validate, and Optimize Large Time-dependent Algorithms): carries out massively parallelized quantum optimal control calculations on GPUs. This software package is a significant overhaul of our previous NIC-CAGE algorithm and also includes algorithmic improvements to the gradient ascent procedure to enable faster convergence [for further details, see: J. M. Rodríguez-Borbón, X. Wang, A. P. Diéguez, K. Z. Ibrahim, and B. M. Wong*, *Computer Physics Communications*, **296**, 109017 (2024)].

Quantum Optimal Control of Multi-Qubit Systems: accelerates quantum optimal control calculations of large multi-qubit systems used in a variety of quantum computing applications. By leveraging the intrinsic symmetry of finite groups, this software package reduces the computational runtime of qubit optimal control calculations by orders of magnitude while maintaining the same accuracy as the conventional method [for further details, see: X. Wang, M. S. Okyay, A. Kumar, and B. M. Wong*, *AVS Quantum Science*, **5**, 043801 (2023)].

FLUID-GPT (Fast Learning to Understand and Investigate Dynamics with a Generative Pre-trained Transformer): utilizes a Generative Pre-Trained Transformer 2 (GPT-2) with a convolutional neural network (CNN) for accurately predicting particle trajectories and erosion on an industrial-scale steam header geometry [for further details, see: S. D. Yang, Z. A. Ali, and B. M. Wong*, *Industrial & Engineering Chemistry Research*, **62**, 15278-15289 (2023)].

Semi-Supervised Machine Learning to Automatically Predict Bioactivities of PFASs: unsupervised/semi-supervised machine learning models to automatically predict bioactivities of PFASs in various human biological targets, including enzymes, genes, proteins, and cell lines [for further details, see: H. Kwon, Z. A. Ali, and B. M. Wong*, *Environmental Science & Technology Letters*, **10**, 1017-1022 (2023)].

Computational Fluid Dynamics and Machine Learning: harnesses convolutional neural network (CNN) and long- and short-term memory (LSTM) machine learning approaches to predict complex surface erosion profiles in steam distribution headers [for further details, see: S. D. Yang, Z. A. Ali, H. Kwon, and B. M. Wong*, *Industrial & Engineering Chemistry Research*, **61**, 8520-8529 (2022)].

HADOKEN (High-level Algorithms to Design, Optimize, and Keep Electrons in Nanowires): predicts electron confinement/localization effects in nanowires with various geometries, arbitrary number of concentric shell layers, doping densities, and external boundary conditions. This software package contains several examples and outputs on a variety of different nanowire geometries, boundary conditions, and doping densities to demonstrate its capabilities [for further details, see: C. Chevalier, and B. M. Wong*, *Computer Physics Communications*, **274**, 108299 (2022)].

NIC-CAGE (Novel Implementation of Constrained Calculations for Automated Generation of Excitations): calculates quantum optimal control fields that can drive a system from a known initial vibrational eigenstate to a specified final quantum state. This software utilizes newly derived analytic gradients for maximizing the transition probability based on a norm-conserving Crank–Nicolson propagation scheme [for further details, see: A. Raza, C. Hong, X. Wang, A. Kumar, C. R. Shelton, and B. M. Wong*, *Computer Physics Communications*, **258**, 107541 (2021)].

PFAS Carbon-Fluorine Bond Descriptors: a modified Java code [based on the approach in *J. Cheminformatics* **5**, 34 (2013)] for calculating molecular descriptors in various per- and polyfluroalkyl substances (PFAS). These molecular descriptors can be subsequently used in other machine learning algorithms to predict carbon-fluorine bond dissociation energies in other PFAS structures [for further details, see: A. Raza, S. Bardhan, L. Xu, S. S. R. K. C. Yamijala, C. Lian, H. Kwon, and B. M. Wong*, *Environmental Science & Technology Letters*, **2**, 624-629 (2019)].

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