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Affiliations

Department of Materials Science and Engineering, The Pennsylvania State University
Materials Research Institute, The Pennsylvania State University
Penn State Institutes of Energy and the Environment, The Pennsylvania State University

Education

Feb 2008	Ph.D. (Materials Science and Engineering), **MIT**
Mar 2004	M.S. (Mechanical Engineering), **École Polytechnique** (France)
Sep 2002	Eng. Diploma (Mechanical Engineering), **École Polytechnique** (France)

Awards and Fellowships

2021	Wilson Teaching Excellence Award, College of Earth and Mineral Sciences, **The Pennsylvania State University**
2021	Faculty of the Year Award, Materials Science and Engineering, **The Pennsylvania State University**
2019	**Corning** Faculty Fellowship in Materials Science and Engineering
2019	Montgomery-Mitchell Innovative Teaching Award, College of Earth and Mineral Sciences, **The Pennsylvania State University**
2017	**NSF** Faculty Early Career Development (CAREER) Award
2014	Ralph E. Powe Junior Faculty Award, **Oak Ridge National Laboratory**
2007 – 2009	French Institute for Computer Science (INRIA) Postdoctoral Fellowship, **Université Paris-Est**
2005 – 2006	Martin Family Society for Sustainability Fellowship, Laboratory for Energy and the Environment, **MIT**
2002 – 2003	Materials Science and Engineering Graduate Fellowship, **MIT**

Research

Energy conversion and storage
Materials for electrocatalysis
Materials for photocatalysis
Computational materials science
Modeling of electrified interfaces
Electronic-structure methods

Education

Feb 2008	**Ph.D., Materials Science and Engineering, MIT** (GPA: 5/5) Doctoral Thesis: *Towards first-principles electrochemistry* Academic Minor: *Energy sustainability* Elective courses: in Physics, Chemistry, and Applied Mathematics Supervisor: Prof. Nicola Marzari
Mar 2004	**M.S., Mechanical Engineering, École Polytechnique** (GPA: 5/5)
Sep 2002	**Eng. Diploma, Mechanical Engineering, École Polytechnique** (GPA: 4.81/5)

Professional Appointments

Jul 2019 – Present	Associate Professor Department of Materials Science and Engineering **The Pennsylvania State University**
Jul 2013 – Jul 2019	Assistant Professor Department of Materials Science and Engineering **The Pennsylvania State University**
Jan 2010 – Jun 2013	Permanent Researcher Department of Scientific Computing **École des Ponts, Université Paris-Est**
Nov 2007 – Sep 2009	Postdoctoral Researcher Department of Scientific Computing **École des Ponts, Université Paris-Est**

Publications

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At Penn State

S. Gelin, N. E. Kirchner-Hall, R. R. Katzbaer, M. J. Theibault, Y. Xiong, W. Zhao, M. M. Khan, E. Andrewlavage, P. Orbe, S. M. Baksa, M. Cococcioni, I. Timrov, Q. Campbell, H. Abruña, R. E. Schaak, **I. Dabo**, Ternary oxides of *s*- and *p*-block metals for photocatalytic solar-to-hydrogen conversion, under review, *PRX Energy* (2023).

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A. Dana, L. Mu, S. Gelin, S. B. Sinnott, **I. Dabo**, Cluster expansion by transfer learning from empirical potentials, under review, *Computational Materials Science* (2023)

E. Linscott, N. Colonna, R. De Gennaro, N. L. Nguyen, G. Borghi, A. Ferretti, **I. Dabo**, N. Marzari, koopmans: An open-source package for accurately and efficiently predicting spectral properties with Koopmans functionals (selected as *Editors' Choice*), *Journal of Chemical Theory and Computation* 19, 7097–7111(2023). DOI: 10.1021/acs.jctc.3c00652

H. Wang, Y. Xiong, H. Padmanabhan, Y. Wang, Z. Wang, R. Claes, G. Brunin, L. Min, R. Zu, M. T. Wetherington, Y. Wang, Z. Mao, G. Hautier, L.-Q. Chen, **I. Dabo**, V. Gopalan, Strong electron-phonon coupling driven pseudogap modulation and density-wave fluctuations in a correlated polar metal, *Nature Communications* 14, 5769 (2023). DOI: 10.1038/s41467-023-41460-x

Z. Li, T. Pei, W. Ying, W. V. Srubar III, R. Zhang, J. Yoon, H. Ye, **I. Dabo**, A. Radlinska, Can domain knowledge benefit machine learning for concrete property prediction? (selected as *Feature Article*), *Journal of American Ceramic Society* (2023). DOI: 10.1111/jace.19549

G. Kotsonis, S. Almishal, F. Vieira, V. Crespi, **I. Dabo**, C. Rost, J. P. Maria, High-entropy oxides: Harnessing crystalline disorder for emergent functionality, *Journal of the American Ceramic Society* 106, 5587-5611 (2023). DOI: 10.1111/jace.19252

C. McCormick, S. Baksa, J. Veglak, **I. Dabo**, R. Schaak, Chemical insights into the formation of metastable zinc cobalt sulfide solid-solution nanoparticles through simultaneous multi-

cation exchange, *Chemistry of Materials* 35, 5433-5446 (2023). DOI: 10.1021/acs.chemmater.3c00763

S. Calderon V, J. Hayden, S. M. Baksa, W. Tzou, S. Trolier-McKinstry, **I. Dabo**, J.-P. Maria, E. C. Dickey, Atomic-scale polarization switching in wurtzite ferroelectrics, *Science* 380, 1034 (2023). DOI: 10.1126/science.adh7670

A. Suceava, J. Hayden, K. P. Kelley, Y. Xiong, B. Fazlioglu-Yalcin, **I. Dabo**, S. Trolier-McKinstry, J.-P. Maria, V. Gopalan, Enhancement of second-order optical nonlinearities and nanoscale periodic domain patterning in ferroelectric boron-substituted aluminum nitride thin films, *Optical Materials Express* 13, 1522 (2023). DOI: 10.1364/OME.488459

S. McGee, A. Fest, C. Chandler, N. Nova, Y. Lei, J. Goff, S. B. Sinnott, **I. Dabo**, M. Terrones, L. Zarzar, Direct laser writing of multimetal bifunctional catalysts for overall water splitting, *American Chemical Society (ACS) Applied Energy Materials* 6, 3756-3768 (2023). DOI: 10.1021/acsaem.2c03973

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R. Slapikas, **I. Dabo**, S. B. Sinnott, Surface reconstruction of oxidized platinum nanoparticles using classical molecular dynamics simulations, *Computational Materials Science* 209, 111364 (2022). DOI: 10.1016/j.commatsci.2022.111364

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Prior to Penn State

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Dabo I., Wieckowski A., Marzari N., Vibrational recognition of adsorption sites for CO on platinum and platinum-ruthenium surfaces, *Journal of the American Chemical Society* 129, 11045 (2007), DOI: 10.1021/ja067944u

Book Chapters

Weitzner S. E. and **Dabo I.**, First-principles simulations of electrified interfaces in electrochemistry, in Heterogeneous catalysts: emerging techniques for design, characterization and applications edited by W. Y. Teoh, A. Urakawa, Y. H. Ng, P. H.-L. Sit, Wiley (2020)

Dabo I., Bonnet N., Li Y. L., Marzari N., Ab-initio electrochemical properties of electrode surfaces, in Fuel cell science: theory, fundamentals, and biocatalysis edited by A. Wieckowski and J. Nørskov, Wiley (2010)

Presentations

Invited oral presentations

Computational modeling of (photo)electrocatalytic materials and interfaces, Center for Enhanced Nanofluidic Transport, Energy Frontier Research Center, Massachusetts Institute of Technology, Virtual Seminar, March 2024

Extensive benchmarking of DFT + *ab initio U* calculations for predicting band gaps and optical properties, American Physical Society Meeting, Minneapolis, March 2024

Computational modeling of (photo)electrocatalytic materials and interfaces, Inaugural Workshop of the Initiative for Computational Catalysis (ICC), Flatiron Institute, New York, February 2024

Optical response of semiconductor materials beyond density-functional theory (seminar), Pennsylvania State University, *scheduled January 2024*

Data-Intensive discovery of earth-abundant semiconductors for solar-to-hydrogen conversion (seminar), CMU-Africa, October 2023

Koopmans functionals: basic concepts, Advanced Quantum-ESPRESSO School, University of Pavia (Italy), August 2023

Data-Intensive discovery of earth-abundant semiconductors for solar-to-hydrogen conversion (seminar), Cornell University, September 2023

Data-Intensive discovery of earth-abundant semiconductors for solar-to-hydrogen conversion (seminar), Stanford University, July 2023

Data-Intensive discovery of earth-abundant semiconductors for solar-to-hydrogen conversion, Wilson Science & Technology Forum, Virtual Seminar, April 2023

Transition-metal-free photocatalysts for solar-to-hydrogen conversion, American Physical Society Meeting, Las Vegas, March 2023

First-principles optimization and discovery of materials for energy conversion and storage (plenary), African Materials Society Meeting, Dakar (Senegal), December 2022

Computational discovery of water-splitting photocatalysts, Materials Day, Pennsylvania State University, October 2022

Data-intensive discovery of photocatalytic semiconductors for solar-to-hydrogen conversion, Materials Day, Boston University, October 2022

Extensive benchmarking of DFT+*U* for band-gap predictions and materials discovery, Workshop on Recent Developments in Electronic Structure, Columbia University, June 2022

First-principles optimization and discovery of materials for energy conversion and storage, Chemistry Seminar, University of Texas at Austin, April 2022

First-principles optimization and discovery of materials for energy conversion and storage, American Physical Society Meeting, Chicago, March 2022

First-principles optimization and discovery of materials for energy conversion and storage, Chemistry Seminar, University of Pennsylvania, February 2022

First-principles optimization and discovery of materials for energy conversion and storage, Chemical Engineering Seminar, University of Pittsburgh, January 2022

First-principles optimization and discovery of materials for energy conversion and storage, Theoretical, Computational and Data-Driven Chemistry Seminar, Imperial College London, Virtual Seminar, December 2021

First-principles optimization and discovery of materials for energy conversion and storage, Physics and Astronomy Colloquium, Stony Brook University, Virtual Seminar, October 2021

First-principles optimization and discovery of materials for energy conversion and storage, Department of Materials Science and Engineering, University of Maryland, Virtual Seminar, September 2021

First-principles discovery and optimization of materials and interfaces for electrochemical energy conversion, American Chemical Society Meeting, Atlanta, Virtual Seminar, August 2021

First-principles optimization and discovery of materials for energy conversion and storage, Center for Autonomous Materials Design, Duke University, Virtual Seminar, July 2021

What are materials? How to simulate them?, Science-U Make-It-Matter Camp, Pennsylvania State University, Virtual Seminar, July 2021

First-principles discovery and optimization of catalytic materials and disordered surfaces, Corning Glass Summit, Virtual Seminar, June 2021

First-principles optimization and discovery of materials for energy conversion and storage, Materials Science and Engineering Colloquium, Stanford University, Virtual Seminar, April 2021

Materials simulation and optimization from first principles, Chemical Engineering in the 21st Century: Challenges and Opportunities Meeting, National Academy of Sciences, Virtual Seminar, February 2021

Raising the success rate of data-driven materials discovery for the solar production of hydrogen fuels, African Physical Society Conference, The Abdus Salam International Centre for Theoretical Physics, Virtual Seminar, November 2020

First-principles discovery of materials for energy conversion and storage, Penn State/ American Ceramic Society/University of Kiel (PACK) Seminar Series, Virtual Seminar, November 2020

First-principles optimization and discovery of materials for energy conversion and storage, University of Delaware, Virtual Seminar, October 2020

First-principles discovery of materials for energy conversion and storage, National Science Foundation MRSEC Summer Seminar Series, Virtual Seminar, July 2020

Computational screening of photocatalytic electrodes for water splitting, TMS Conference, San Diego, February 2020

Computational screening of photocatalytic materials for solar-to-hydrogen conversion, African Materials Research Society Conference, Arusha, December 2019

Simulating materials for energy conversion and storage, Chemical Sciences Roundtable, National Academy of Sciences, Washington D.C., November 2019

High-throughput discovery of semiconductor photocatalysts for water splitting, Rutgers University, Newark, October 2019

Computational modeling and screening of semiconductor electrodes for solar-to-fuel conversion, Electrochemical Society Meeting, Atlanta, *October 2019*

First-principles modeling of layered electrodes for water splitting and charge storage, American Chemical Society Meeting, San Diego, August 2019

Computational modeling and screening of semiconductor electrodes for solar-to-fuel conversion, Nanoscience and Technology Colloquium, Argonne National Laboratory, Argonne, May 2019

Materials simulation and optimization from first principles, N. W. Taylor Lecture in Materials 2019: Materials from First Principles, University Park, April 2019

Charge separation and band alignment at photo-electrochemical interfaces, American Physical Society Meeting, Boston, March 2019

Large-scale simulations of solid-liquid interfaces under realistic electrochemical conditions for energy conversion and storage, American Chemical Society Meeting, New Orleans, March 2018

Large-scale simulations of solid-liquid interfaces under realistic electrochemical conditions for energy conversion and storage, American Research and Leadership Network, Pittsburgh, March 2018

Quantum-continuum simulations of solid-liquid interfaces under electrochemical conditions, TMS Conference, Phoenix, March 2018

Large-scale simulations of solid-liquid interfaces under realistic electrochemical conditions for energy conversion and storage, African Materials Research Society Conference, Gaborone (Botswana), December 2017

Large-scale simulations of solid-liquid interfaces under realistic electrochemical conditions for energy conversion and storage (seminar), Rensselaer Polytechnic Institute, Troy, November 2017

Large-scale simulations of solid-liquid interfaces under realistic electrochemical conditions for energy conversion and storage (seminar), Cornell, Ithaca, October 2017

Large-scale simulations of solid-liquid interfaces under realistic electrochemical conditions for energy conversion and storage, Penn Institute for Computational Science Conference, University of Pennsylvania, Philadelphia, October 2017

Large-scale simulations of solid-liquid interfaces under realistic electrochemical conditions for energy conversion and storage (seminar), Binghamton University, Binghamton, October 2017

Large-scale simulations of solid-liquid interfaces under realistic electrochemical conditions for energy conversion and storage (seminar), Carnegie Mellon, Pittsburgh, September 2017

Quantum–continuum simulations of solid–liquid interfaces under applied voltage, American Chemical Society Meeting, Washington, August 2017

Progress and challenges in density-functional theory, CECAM Workshop, Lausanne (Switzerland), July 2017

Towards first-principles shape control of electrocatalytic metal nanoparticles, Lorentz Workshop: Fundamentals of Electrocatalysis, Leiden (Netherlands), June 2017

Understanding the electrical response of semiconductor–electrolyte interfaces for efficient artificial photosynthesis (seminar), California State University, Los Angeles, April 2017

First-principles prediction of electrified interfaces under realistic electrochemical conditions, (seminar), École Polytechnique Fédérale de Lausanne, Lausanne, December 2016

First-principles prediction of the electrochemical stability of bimetallic catalysts for use as fuel cell electrodes, American Chemical Society Northeast Regional Meeting, Binghamton, October 2016

First-principles prediction of the electrochemical stability of bimetallic catalysts for use as fuel cell electrodes (seminar), Princeton University, Princeton, April 2016

First-principles prediction of the electrochemical stability of bimetallic catalysts for use as fuel cell electrodes (seminar), Wake Forest University, Winston-Salem, February 2016

First-principles prediction of solvation energies and redox potentials in aqueous environments, Pacifichem, Honolulu, December 2015

Thermodynamic stability of electrocatalytic surfaces in aqueous environments, American Institute of Chemical Engineers Meeting, Salt Lake City, November 2015

First-principles modeling of electrochemical and organic photovoltaic materials (seminar), Air Force, Valparaiso, April 2015

Computational materials discovery: Challenges and opportunities (seminar), Kyushu University, Fukuoka, February 2015

Computational spectroscopy of energy conversion and storage materials (seminar), Sandia National Laboratories, Albuquerque, October 2014

Modeling electrochemical interfaces under applied voltage, Materials Science Engineering Conference, Darmstadt, September 2014

First-principles electron spectroscopies of solar and battery materials (seminar), Rutgers University, New Brunswick, August 2014

Genomics of solar and battery materials from electron spectroscopies (seminar), Center of Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, July 2014

First-principles spectroscopy of materials for electrochemistry, photovoltaics, and optoelectronics (seminar), University of Paris-Sud, Orsay, March 2013

Challenges in computational materials spectroscopy for energy conversion and storage (seminar), Arizona State University, Tempe, January 2013

Electronic-structure predictions from Koopmans-compliant functionals, Correlation Meeting, Ecole Polytechnique, Palaiseau (France), December 2012

Bridging self-interaction corrections with Hubbard corrections, Workshop on Corrective Approaches to Density-Functional Theory for Strongly Correlated Systems, CECAM Workshop, Lausanne (Switzerland), June 2012

Quantum simulations of organic photovoltaic compounds, Young Engineers and Scientists Symposium, University of California, Berkeley, March 2012

Computational electronic-structure description of periodic molecular structures: reconciling Gaussians with plane waves (seminar), French Alternative Energies and Atomic Energy Commission (CEA), Saclay (France), September 2011

Koopmans' theorem and orbital-dependent density functionals (seminar), French Alternative Energies and Atomic Energy Commission (CEA), Grenoble (France), September 2011

Charge-carrier levels in materials from first principles (seminar), Ecole Polytechnique, Palaiseau (France), April 2011

First-principles simulation of electrochemical systems at fixed applied voltage, Pacifichem, Honolulu, December 2010

First-principles simulation of electrochemical reactions at catalytic electrodes, CECAM Workshop, Lausanne (Switzerland), July 2010

Self-interaction in density-functional approximations and Koopmans-based correction, CECAM Workshop, Lausanne (Switzerland), June 2010

Real-space correction scheme for computing the electrostatic potential of electronic systems (seminar), University of Minnesota, Minneapolis, October 2009

Non-Koopmans self-interaction correction in density-functional theory (seminar), French Alternative Energies and Atomic Energy Commission (CEA), Bruyères-le-Châtel (France), June 2009

How to cancel periodic-image errors in supercell ab-initio calculations (seminar), Pierre and Marie Curie University, Paris (France), April 2009

First-principles electrochemistry, Total Energy Workshop, International Center of Theoretical Physics, Trieste (Italy), January 2009

First-principles simulations at electrified-metal solution interfaces (seminar), International School for Advanced Studies, Trieste (Italy), December 2007

Challenges in first-principles surface electrochemistry, American Chemical Society Fall Meeting, Boston, August 2007

Contributed oral presentations

Predicting the stability of bimetallic transition metal alloy surfaces under realistic electrochemical conditions, Midwest Theoretical Chemistry Conference, University of Pittsburgh, Pittsburgh, June 2016

Electronic-structure calculations from Koopmans-compliant functionals, Electronic-Structure 2015 Workshop, University of Washington, Seattle, June 2015

Optical spectroscopies of materials from orbital-dependent approximations, American Physical Society Meeting, Baltimore, March 2013

Role of electronic localization in the phosphorescence of iridium sensitizing dyes, American Physical Society Meeting, Baltimore, March 2013

Restoring piecewise linearity in density-functional theory, Deutsche Physikalische Gesellschaft (DPG) Conference, Regensburg (Germany), March 2013

Accurate optical properties of organic photovoltaics from Koopmans functionals, Energy from the Sun, CECAM Conference, Cagliari (Italy), September 2012

Accurate beyond-DFT approach to the electronic structure of novel materials, PRACE Workshop, French Alternative Energies and Atomic Energy Commission (CEA), Saclay (France), June 2012

Electronic structure of organic photovoltaic compounds from first principles, 2nd Thomas Young Center (TYC) Energy Materials Workshop, King's College, London (United Kingdom), June 2012

Electronic and dielectric properties of photovoltaic compounds from first principles, American Physical Society Meeting, Boston, March 2012

First-principles surface chemistry under applied voltage, Electrochemical Society Meeting, Montreal (Canada), May 2011

Koopmans' condition for density-functional theory, American Physical Society Meeting, Dallas, March 2011

Non-Koopmans self-interaction correction to density-functional approximations, Psi-k Conference, Berlin (Germany), September 2010

First-principles simulation of electrochemical systems at fixed applied voltage, Density Functional Theory Meets Experiment Workshop, Institut für Festkörper- und Werkstoffforschung (IFW) of Dresden (Germany), August 2008

Real-space correction scheme for computing the electrostatic potential of electronic systems in vacuum and in polarizable media, Numerical Methods in Density-functional Theory Workshop, Technical University (TU) of Berlin (Germany), July 2008

Electrostatics in periodic boundary conditions and real-space corrections, American Physical Society Meeting, Denver, March 2007

Energetic, structural and vibrational properties of carbon monoxide on transition-metal surfaces: a linear-response approach to the energy puzzle, American Physical Society Meeting, Baltimore, March 2006

Vibrational recognition of adsorption sites from density-functional perturbation theory : CO/Pt(111), Electrochemical Society Meeting, Québec City (Canada), May 2005

Vibrational recognition of adsorption sites for CO adsorbed on transition-metal surfaces, American Physical Society Meeting, Los Angeles, March 2005

External Funding

As principal investigator

Title: " Predicting the formation of oxide layers on noble metals in aqueous media: Structural and dynamical properties of solid–liquid interfaces under voltage"
Sponsor: Department of Energy
Period of Performance: 09/01/2022-08/31/2025
Total Budget: $800,000
Role: Principal Investigator

Title: "CAREER: Large-scale quantum-continuum simulation of layered metal oxide semiconductor photoelectrodes under finite-temperature electrochemical conditions"
Sponsor: National Science Foundation
Period of Performance: 01/01/2017-12/31/2021
Total Budget: $565,000
Role: Principal Investigator

Title: "DMREF: INFEWS: Collaborative Research: Photocatalyst by design: Computational screening of reconstructed perovskite semiconductor electrodes for efficient solar-to-fuel conversion"
Sponsor: National Science Foundation
Period of Performance: 08/01/2017-07/31/2020
Total Budget: $1,270,000
Role: Principal Investigator

Title: "Predicting the formation of oxide layers on noble metals in aqueous media: Structural and dynamical properties of solid-liquid interfaces under voltage"
Sponsor: Department of Energy
Period of Performance: 09/01/2018-08/31/2021
Total Budget: $710,000
Role: Principal Investigator

Title: "Beyond-density-functional-theory prediction of novel pseudocapacitive electrodes"
Sponsor: Murata Manufacturing Co., Ltd. (Japan)
Period of Performance: 03/01/2016-08/31/2018
Total Budget: $121,000
Role: Principal Investigator

Title: "Cation intercalation and interface electrification in titanium carbide multilayer particles: Predicting the pseudocapacitance of shallow and deep cation-adsorption sites"
Sponsor: Murata Manufacturing Co., Ltd. (Japan)

Period of Performance: 11/01/2017-04/30/2020
Total Budget: $180,000
Role: Principal Investigator

As co-principal investigator

Title: "EFRC: Center for Electrochemical Dynamics and Reactions on Surfaces (CEDARS)"
Sponsor: Department of Energy
Period of Performance: 08/01/2022-07/31/2026
Total Budget: $10,350,000
Role: Co-Principal Investigator

Title: "Understanding and Designing Phosphide Solar Absorbers with High Carrier Lifetime"
Sponsor: Department of Energy
Period of Performance: 09/01/2022-08/31/2025
Total Budget: $4,500,000
Role: Co-Principal Investigator

Title: "MRSEC: Center for Nanoscale Science"
Sponsor: National Science Foundation
Period of Performance: 09/01/2020-08/31/2026
Total Budget: $18,787,000
Role: Co-Principal Investigator

Title: "A symmetry-based approach to minimum energy pathways"
Sponsor: National Science Foundation
Period of Performance: 07/01/2018-06/30/2021
Total Budget: $420,000
Role: Co-principal Investigator

Title: "COMMS: Center for Computational Mesoscale Materials Science"
Sponsor: Department of Energy
Period of Performance: 09/01/2023-08/31/2026
Total Budget: $2,773,131
Role: Co-principal Investigator

Title: "Computational mesoscale science and open software for quantum materials"
Sponsor: Department of Energy
Period of Performance: 08/01/2019-07/31/2023
Total Budget: $2,865,000
Role: Co-principal Investigator

Title: "Ferroelectricity in boron-substituted aluminum nitride"

Sponsor: Defense Advanced Research Project Agency
Period of Performance: 09/01/2020-08/31/2022
Total Budget: $386,000
Role: Co-principal Investigator

Title: "EFRC: Center for 3D Ferroelectric Microelectronics"
Sponsor: Department of Energy
Period of Performance: 08/01/2020-07/31/2024
Total Budget: $8,200,000
Role: Co-principal Investigator

Title: "Materials for electrochemical energy conversion"
Sponsor: Panasonic
Period of Performance: 01/01/2023-04/30/2024
Total Budget: $748,085
Role: Co-principal Investigator

As faculty participant

Title: "MRSEC: Center for Nanoscale Science"
Sponsor: National Science Foundation
Start Date: 09/01/2014-08/31/2020
Total Budget: $15,000,000
Portion of Support: 1 Graduate Student

Title: "Collaborative Research: I/UCRC Center for Atomically Thin Multifunctional Coatings"
Sponsor: National Science Foundation
Period of Performance: 07/15/2015-06/30/2020
Total Budget: $235,000
Portion of Support: Summer Salary

Title: "REU Site: Nanoscale physics and materials REU and RET at Penn State"
Sponsor: National Science Foundation
Start Date: 06/01/2019-04/30/2023
Total Budget: $350,000
Portion of Support: Summer Salary

Teaching

Fall 2019 – Present	Instructor **The Pennsylvania State University** MATSE 597/519 Computational materials science (graduate) (Teaching rating: 6.6/7)
Fall 2022 – Present Fall 2014 – Fall 2018	Instructor **The Pennsylvania State University** MATSE 501 Thermodynamics of materials (graduate) (Teaching rating: 6.6/7)
Spring 2022	Instructor **The Pennsylvania State University** MATSE 403 Solid state materials (undergraduate) (Teaching rating: 6.35/7)
Spring 2014 – Present	Instructor **The Pennsylvania State University** MATSE 419 Computational materials science (undergraduate) (Teaching rating: 6.4/7)
Spring 2012 – 2013	Instructor **École des Ponts, Université Paris-Est** Molecular simulation in materials science (graduate) (No teaching rating)
Fall 2007 – 2012	Instructor **École des Ponts, Université Paris-Est** Scientific computing (graduate) (No teaching rating)
Fall 2006	Teaching Assistant (Instructors: Prof. Y. Fink, Prof. N. Marzari) **MIT** 3.23 Electronic, optical, and magnetic properties (graduate) (No teaching rating)
Fall 2005, Fall 2004	Teaching Assistant (Instructors: Prof. D. Irvine, Prof. N. Marzari) **MIT** 3.012 Fundamentals of materials science (undergraduate) (No teaching rating)

Activities

Societies	Materials Research Society, American Physical Society (Member)
Editorial Boards	Science (AAAS) (Reviewing Editor) Computational Materials Science (Associate Editor) Nature Partner Journal (NPJ) Computational Materials (Member)
Software	Co-developer of modular computational capabilities for the simulation of quantum systems under electrochemical conditions with O. Andreussi and N. Marzari (www.quantum-environment.org) in Quantum-ESPRESSO (www.quantum-espresso.org)
Events	Co-organizer of Symposiym "Computational Discovery and Design of Material " (TMS Meeting, San Diego, 2023), Symposium "Atomic-Level Understanding of Materials in Fuel Cells and Electrolyzers" (MRS Meeting, Phoenix, 2019), Quantum-Espresso Workshop (Penn State, 2014 and 2018), Symposium "Frontiers of Electronic Structure Theory for Materials and Molecules" (APS Meeting, San Antonio, 2015), Seminar of Scientific Computing (University Paris-Est, Paris, 2009–2013).
Mentoring	Research Experiences for Undergraduates (REU), Upward Bound Math and Science (PREM), Summer Research Experiences for Teachers (RET), and Penn State Millennium Scholars Programs. 15 undergraduates, 2 teachers, and 3 high-school students mentored since 2014.

Advising

Postdoctoral Scholars (4)	Yanli Li (Xiamen University, China), Simon Gelin (Penn State; now Assistant Research Professor), Yasuaki Okada (Murata Manufacturing, Japan), Nicolas Poilvert (Bay Labs, CA)
Ph.D. Students (19)	Mohamed Ali (Penn State), Steven Baksa (Penn State), Aaron Bossen (Penn State), Maximiliano Burgess (Penn State), Quinn Campbell (Sandia), Cierra Chandler (Penn State), Weinan Chen (Mathworks), Amirezza Dana (Penn State), Julian Fanghanel (Penn State), James Goff (Penn State), Tara Karimzadeh Sabet (Penn State), Nathan Keilbart (LLNL), Nicole Kirchner-Hall (Penn State), Jason Munro (UC Berkeley), Seda Oturak (Penn State), Astoria Song (Penn State), Francisco Marques dos Santos Vieira (Penn State), Ziqi Wang (Penn State), Stephen Weitzner (LLNL), Vincent Xiong (Dartmouth)