Ismaila Dabo

Associate Professor · Materials Science and Engineering
The Pennsylvania State University

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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

2019	**Corning** Faculty Fellowship in Materials Science and Engineering
2019	G. Montgomery and Marion H. 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

At Penn State

Grieco C., Doucette G. S., Munson K. M., Swartzfager J. R., Munro J. M., Anthony J. E., **Dabo I.**, Asbury J. B., Vibrational probe of the origin of singlet exciton fission in TIPS-pentacene solutions, *Journal of Chemical Physics*, accepted (2019)

Keilbart N. D., Okada Y., **Dabo I.**, Probing the pseudocapacitance and energy-storage performance of RuO_2 facets from first principles, *Physical Review Materials* 3, 085405 (2019) (2019), DOI: 10.1103/PhysRevMaterials.3.085405

Akbarian D., Yilmaz D. E., Cao Y., Ganesh P., **Dabo I.**, Munro J., Van Ginhoven R., van Duin A. C. T., Understanding the influence of defects and surface chemistry on ferroelectric switching: A ReaxFF investigation of $BaTiO_3$, *Physical Chemistry and Chemical Physics* 21, 18240-18249 (2019), DOI: 10.1039/c9cp02955a

Campbell Q. and **Dabo I.**, Electrochemical stability and light-harvesting ability of silicon photoelectrodes in aqueous environments, *Journal of Chemical Physics* 151, 044109 (2019), DOI: 10.1063/1.5093810

Wilkinson C. J., Doss K., Hahn S. H., Keilbart N. D., Potter A. R., Smith N. J., **Dabo I.**, van Duin A. C. T., Kim S. H., Mauro J. C., Topological control of water reactivity on glass surfaces: Evidence of a chemically stable intermediate phase, *Journal of Physical Chemistry Letters* 10, 3955-3960 (2019), DOI: 10.1021/acs.jpclett.9b01275

Ong M., Guzman D., Campbell Q., **Dabo I.**, Jishi R. A.**,** $BaZrSe_3$: Ab-initio study of anion substitution for bandgap tuning in a chalcogenide material (selected as *Editor's Pick*), *Journal of Applied Physics* 125, 235702 (2019), DOI: 10.1063/1.5097940

Xiong Y. and **Dabo I.,** Influence of surface restructuring on the activity of $SrTiO_3$ photoelectrodes for photocatalytic hydrogen reduction, *Physical Review Materials* 3, 065801 (2019), DOI: 10.1103/PhysRevMaterials.3.065801

Campbell Q., Fisher D., **Dabo I.,** Voltage-dependent reconstruction of layered Bi_2WO_6 and Bi_2MoO_6 photocatalysts and its influence on charge separation for water splitting, *Physical Review Materials* 3, 015404 (2019), DOI: 10.1103/PhysRevMaterials.3.015404

Munro J. M., Liu V. S., Gopalan V., **Dabo I.**, DiSPy: Implementation of distortion symmetry for the nudged elastic band method, *Nature Partner Journal (NPJ) Computational Materials* 5, 52 (2019), DOI: 10.1038/s41524-019-0188-x

Ong M., Campbell Q., **Dabo I.**, Jishi R. A., First-principles investigation of $BiVO_3$ for thermochemical water splitting, *International Journal of Hydrogen Energy* 44, 1425 (2019), DOI: 10.1016/j.ijhydene.2018.11.125

de Pablo J., Jackson N. E., Webb M. A., Chen L. Q., Moore J., Morgan D., Pollock T., Schlom D., Toberer E., Analytis J., **Dabo I.**, DeLongchamp D., Fiete G., Grason G., Hautier G., Mo Y., Rajan K., Reed E., Rodriguez E., Stevanovic V., Suntivich J., Thornton K., Zhao J. C., Advancing and accelerating materials innovation: New frontiers for the Materials Genome Initiative, *Nature Partner Journal (NPJ) Computational Materials Science* 5, 41 (2019), DOI: 10.1038/s41524-019-0173-4

Weitzner S. E. and **Dabo I.**, Voltage effects on the stability of Pd ensembles in PdAu/Au(111) surface alloys, *Journal of Chemical Physics* 150, 041715 (2019), DOI: 10.1063/1.5054124

Aplan M. P., Grieco C., Lee Y., Munro J. M., Gray J. L., Wang Q., Seibers Z. D., Kuei B., Litofsky J. H., Kilbey S. M., **Dabo I.**, Asbury J. B., Gomez E. d., Conjugated block copolymers as model systems to examine mechanisms of charge generation in donor-acceptor materials, *Advanced Functional Materials* 29, 1804858 (2018), DOI: 10.1002/adfm.201804858

Aplan M. P., Munro J. M., Lee Y., Brigeman A. N., Grieco C., Wang Q., Giebink N. C., **Dabo I.**, Asbury J. B., Gomez E. D., Revealing the importance of energetic and entropic contributions to the driving force for charge photogeneration, *American Chemical Society (ACS) Applied Materials and Interfaces* 10, 39933-39941 (2018), DOI: 10.1021/acsami.8b12077

Munro J. M., Akamatsu H., Padmanabhan H., Liu V. S., Shi Y., Chen L.-Q., VanLeeuwen B. K., **Dabo I.**, Gopalan V., Discovering minimum energy pathways via distortion symmetry groups, *Physical Review B* 98, 085107 (2018), DOI: 10.1103/PhysRevB.98.085107

Liu V. S., VanLeeuwen B. K., Munro J. M., Padmanabhan H., **Dabo I.**, Gopalan V., Litvin D. B., Spatio-temporal symmetry: Crystallographic point groups with time translations and time inversion, *Acta Crystallographica* A74, 399-402 (2018), DOI: 10.1107/S2053273318004667

Weitzner S. E. and **Dabo I.**, Voltage-dependent cluster expansion for electrified solid–liquid interfaces: Application to the electrochemical deposition of transition metals, *Physical Review B* 96, 205134 (2017), DOI: 10.1103/PhysRevB.96.205134

Grieco C., Doucette G. S., Munro J. M., Kennehan E. R., Lee Y., Rimshaw A., Payne M. M., Wonderling N., Anthony J. E., **Dabo I.**, Gomez E. D., Asbury J. B., Triplet transfer mediates triplet pair separation during singlet fission in 6,13-bis(triisopropylsilylethynyl)-pentacene, *Advanced Functional Materials* 27, 1703929 (2017), DOI: 10.1002/adfm.201703929

Campbell Q. and **Dabo I.**, Quantum–continuum calculation of the surface states and electrical response of silicon in solution, *Physical Review B* 95, 205308 (2017), DOI: 10.1103/PhysRevB.95.205308

Keilbart N. D., Okada Y., Feehan A., Higai S., **Dabo I.**, Quantum–continuum simulation of the electrochemical response of pseudocapacitor electrodes under realistic conditions, *Physical Review B* 95, 115423 (2017), DOI: 10.1103/PhysRevB.95.115423

Ji X., Poilvert N., Liu W., Xiong Y., Cheng H. Y., Badding J. V., **Dabo I.**, Gopalan V., A silicon microwire under a three-dimensional anisotropic tensile stress, *Applied Physics Letters* 110, 091911 (2017), DOI: 10.1063/1.4977852

Sun D., Xiong Y., Sun Y., **Dabo I.**, Schaak R. E., Solution-synthesized In_4SnSe_4 semiconductor microwires with a direct band gap, *Chemistry of Materials* 29, 1095-1098 (2017), DOI: 10.1021/acs.chemmater.6b04216

Weitzner S. E. and **Dabo I.**, Quantum–continuum simulation of underpotential deposition at electrified metal–solution interfaces, *Nature Partner Journal (NPJ) Computational Materials* 3, 1-7 (2017), DOI: 10.1038/s41524-016-0004-9

Ji X., Lei S., Yu S.-Y., Cheng H. Y., Liu W., Poilvert N., Xiong Y., **Dabo I.**, Mohney S. E., Badding J. V., Gopalan V., Single-crystal silicon optical fiber by direct laser crystallization, *American Chemical Society (ACS) Photonics* 4, 85-92 (2017), DOI: 10.1021/acsphotonics.6b00584

Sasaki K., Toshiyuki K., Ideta K., Miki H., Hirajima T., Miyawaki J., Murayama M., **Dabo I.**, Removal mechanism of high concentration borate by co-precipitation with hydroxyapatite, *Journal of Environmental Chemical Engineering* 4, 1092-1101 (2016), DOI: 10.1016/j.jece.2016.01.012

Poilvert N., Borghi G., Nguyen N. L., Keilbart N. D., Wang K., **Dabo I.**, Koopmans-compliant self-interaction corrections, *Advances In Atomic, Molecular, and Optical Physics* 64, 105 (2015), DOI: 10.1016/bs.aamop.2015.06.008

Nguyen N. L., Borghi G., Ferretti A., **Dabo I.**, Marzari N., First-principles photoemission spectroscopy and orbital tomography in molecules from Koopmans-compliant functionals, *Physical Review Letters* 114, 166405 (2015), DOI: 10.1103/PhysRevLett.114.166405

Borghi G., Ferretti A., Nguyen N. L., **Dabo I.**, Marzari N., Koopmans-compliant functionals and their performance against reference molecular data, *Physical Review B* 90, 075135 (2014), DOI: 10.1103/PhysRevB.90.075135

Ferretti A., **Dabo I.**, Cococcioni M., Marzari N., Bridging density-functional and many-body perturbation theory: orbital-density dependence in electronic-structure functionals, *Physical Review B* 89, 195184 (2014), DOI: 10.1103/PhysRevB.89.195134

Bonnet N., **Dabo I.**, Marzari N., Electrostatic origin of the frequency shifts for chemisorbed molecules under potential bias, *Electrochimica Acta* 121, 210 (2014), DOI: 10.1016/j.electacta.2013.12.115

Dabo I., Ferretti A., Marzari N., Piecewise linearity and spectroscopic properties from Koopmans-compliant functionals, *Topics in Current Chemistry* 347, 193 (2014), DOI: 10.1007/128_2013_504

Prior to Penn State

Dabo I., Ferretti A., Park C.-H., Poilvert N., Cococcioni M., Marzari N., Donor and acceptor levels of organic photovoltaic compounds from first principles, *Physical Chemistry Chemical Physics* 15, 685 (2013), DOI: 10.1039/C2CP43491A

Himmetoglu B., Marchenko A., **Dabo I.**, Cococcioni M., Role of electronic localization in the phosphorescence of iridium sensitizing dyes, *Journal of Chemical Physics* 137, 154309 (2012), DOI: 10.1063/1.4757286

Dabo I., Resilience of gas-phase anharmonicity in the vibrational response of adsorbed carbon monoxide and breakdown under electrical conditions, *Physical Review B* 86, 035139 (2012), DOI: 10.1103/PhysRevB.86.035139

Blanchard M., Morin G., Lazzeri M., Balan E., **Dabo I.**, First-principles simulation of arsenate adsorption on the surface of hematite, *Geochimica et Cosmochimica Acta* 86, 182 (2012), DOI: 10.1016/j.gca.2012.03.013

Andreussi O., **Dabo I.**, Marzari N., Revised self-consistent continuum solvation in electronic-structure calculations, *Journal of Chemical Physics* 136, 064102 (2012), DOI: 10.1063/1.3676407

Li Y. L. and **Dabo I.**, Electronic levels and electrical response of periodic molecular structures from plane-wave orbital-dependent calculations, *Physical Review B* 84, 155127 (2011), DOI: 10.1103/PhysRevB.84.155127

Dabo I., Ferretti A., Poilvert N., Li Y. L., Marzari N., Cococcioni M., Koopmans' condition for density-functional theory (selected as *Editors' Suggestion*), *Physical Review B* 82, 115121 (2010), DOI: 10.1103/PhysRevB.82.115121

Giannozzi P., Baroni, S., Bonini N., Calandra M., Car R., Cavazzoni C., Ceresoli D., Chiarotti G. L., Cococcioni M., **Dabo I.**, Dal Corso A., Fabris S., Fratesi G., de Gironcoli S., Gebauer R., Gerstmann U., Gougoussis C., Kokalj A., Lazzeri M., Martin-Samos L., Marzari N., Mauri F., Mazzarello R., Paolini S., Pasquarello A., Paulatto L., Sbraccia C., Scandolo S., Sclauzero G., Seitsonen A. P., Smogunov A., Umari, P., Wentzcovitch, R. M., Quantum-ESPRESSO: a

modular and open-source software project for quantum simulations of materials, *Journal of Physics: Condensed Matter* 21, 395502 (2009), DOI: 10.1088/0953-8984/21/39/395502

Dabo I., Kozinsky B., Singh-Miller N. E., Marzari N., Electrostatics in periodic boundary conditions and real-space corrections, *Physical Review B* 77, 115139 (2008), DOI: 10.1103/PhysRevB.77.115139

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 (2019)

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

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

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

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

First-principles modeling of layered electrodes for water splitting and charge storage, American Chemical Society Meeting, San Diego, *scheduled 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: "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: "A symmetry-based approach to minimum energy pathways"

Sponsor: National Science Foundation
Period of Performance: 07/01/2018-06/30/2021
Total Budget: $419,915
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

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: $235,210
Portion of Support: Summer Salary

Teaching

Fall 2014 – Present	Instructor **The Pennsylvania State University** MATSE 501 Thermodynamics of materials (graduate) (Teaching rating: 6.6/7)
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	American Institute of Physics (AIP) Advances (Associate Editor) Nature Partner Journal (NPJ) Computational Materials (Member)
Journals	Reviewer for Computational Materials Science, Electrochimica Acta, Energy and Environmental Science, Journal of Chemical Physics, Journal of the Electrochemical Society, Nature Communications, Physical Chemistry Chemical Physics, Physical Review B, Physical Review Letters, Scientific Reports, Surface Science
Federal Agencies	Reviewer for the Department of Energy and the National Science Foundation
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 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, Upward Bound Math and Science, and Millennium Scholars Programs. 13 undergraduates and 3 high-school students mentored since 2014.

Advising

Postdoctoral Scholars (3)	Yanli Li (Xiamen University, China), Yasuaki Okada (Penn State), Nicolas Poilvert (Bay Labs, CA)
Ph.D. Students (13)	Steven Baksa (Penn State), Maximiliano Burgess (Penn State), Quinn Campbell (Sandia), Cierra Chandler (Penn State), Weinan Chen (Penn State), Julian Fanghanel (Penn State), James Goff (Penn State), Nathan Keilbart (LLNL), Nicole Kirchner-Hall (Penn State), Jason Munro (UC Berkeley), Francisco Marques dos Santos Vieira (Penn State), Stephen Weitzner (LLNL), Vincent Xiong (Penn State)