Jorge O. Sofo

Professor of Physics

Professor of Materials Science and Engineering

The Pennsylvania State University

104 Davey Laboratory PMB# 172

University Park PA 16802

Tel: +1-814-777-3450

Fax: +1-814-865-3604

e-mail: sofo@psu.edu

Degrees

* Ph.D. in Physics, Instituto Balseiro, Universidad Nacional de Cuyo, Bariloche, Argentina. December 1991. “Superconductivity in Systems with Local Interactions: from BCS to Bose Condensation.” Advisor: Prof. Carlos A. Balseiro.
* M.Sc. in Physics (Licenciatura) Instituto Balseiro, Universidad Nacional de Cuyo. Bariloche, Argentina. November 1988. “Magnetism and Transport in Semiconductor Heterostructures: a DFT approach.” Advisor: Prof. Carlos A. Balseiro.

Appointments

* Professor of Physics. The Pennsylvania State University. July 2011 to present.
* Professor of Materials Science and Engineering, The Pennsylvania State University. July 2011 to present.
* Director of the Materials Simulation Center, a facility of the Materials Research Institute, The Pennsylvania State University. November 2001 – July 2012.
* Associate Professor of Physics. The Pennsylvania State University. February 2002 – July 2011.
* Associate Professor of Materials Science and Engineering, The Pennsylvania State University. March 2003 - to July 2011.
* Fellow of the Fritz-Haber Institute of the Max Planck Society, Berlin, Germany. May 1st to June 15th, 2015.
* Visiting Scientist, Humboldt-Universität zu Berlin, Berlin, Germany. March 15th to April 30th, 2015.
* Visiting Professor, Università di Roma “La Sapienza”, Italy. December 15th to March 15th, 2015.
* Visiting Professor, Universidad de Chile, Santiago de Chile, Chile. November 2 to 30, 2014.
* Visiting Scientist, Humboldt-Universität zu Berlin, Berlin, Germany. July 25 to August 21, 2014.
* Visiting Scientist, Instituto Balseiro and Centro Atómico Bariloche, San Carlos de Bariloche, Argentina. June 22 to July 23, 2014.
* Visiting Researcher, Humboldt University of Berlin, Germany. July 12 to July 22, 2013.
* Visiting Professor, Pontificia Universidad Católica de Chile, Santiago de Chile, Chile. December 5 to December 12, 2009.
* Visiting Professor, Pontificia Universidad Católica de Chile, Santiago de Chile, Chile. 21st November 2008 to 1st December 2008.
* Visiting Professor, Université de la Mediterranée (CINaM), Marseille, France. July 13 to August 17, 2008.
* Visiting Professor, Pontificia Universidad Católica de Chile, August 1st to August 15th, 2007.
* Visiting Professor, University of Leoben, Austria. July 1st to July 31st, 2007.
* Distinguished Visiting Faculty, Oak Ridge National Laboratory. June 12 to July 7, 2006.
* Guest Professor, Institute of Theoretical Physics, Karl-Franzens Universität. Graz, Austria. June - July, 2001.
* Guest Professor, Institute of Theoretical Physics, Karl-Franzens Universität. Graz, Austria. May - June, 2000.
* Assistant Professor, Instituto Balseiro, Bariloche, University of Cuyo. February 1996 ‑ October 2001.
* Research Fellow of CONICET (National Research Council for Science and Technology of Argentina). July 1995 - December 2003.
* Research Associate at Oak Ridge National Laboratory, in a Cooperative Research and Development Agreement (CRADA) between Martin Marietta Energy Systems, Inc. and Marlow Industries, Inc. (Dallas, Texas). February 1993 - June 1995.
* Research Associate, The University of Tennessee. January 1992 - January 1993.

Honors

* Humboldt University Talent Travel Award, 2016.
* Cesar Milstein Award, 2011, 2014.
* Fellow of the American Physical Society since 2013.
* Fellow of the American Association for the Advancement of Science since 2016.

Grants

* Study of the metal-hydrogen interaction. ANPCyT-SECyT 03-00000-00680, Argentina. 1999-2000. Argentine Government Federal Agency of Promotion of Science and Technology, $50.000.
* Introduction of Parallel Programming Techniques at Instituto Balseiro, FOMEC, Argentina. 1999-2001. Argentine Department of Education $150,000. The project includes the assembly of a Beowulf cluster, currently working with 30 processors.
* Computational Simulation of Metal-Hydrogen Systems, CONICET Project 8014/96. 1999-2000. Argentine National Research Council $5,000.
* Study of the morphology and electronic structure of metallic and semiconducting surfaces. SCyT-ECOS A97E04. 1997 - 2001. Argentine Secretary of Science and Technology $30.000.
* Molecular Dynamics Simulation of Diffusion, Trapping and Recombination of Tritium in Beryllium. International Atomic Energy Agency 302-F4-ARG-8998. 1996-1997. $5,000.
* WIEN2002: Hands on Workshop on the WIEN2k Package. The Petroleum Research Fund. 2002. $3,600.
* WIEN2004: Hands on Workshop on the WIEN2k Package. The Petroleum Research Fund. 2004. $3,600.
* CAMLET: A Combined Ab-initio Manifold Learning Toolbox for Nanostructure Simulations. NSF Award CCF-0430349. 10/2004-9/2007. $231,000. Hongyuan Zha(PI) and Jorge O. Sofo.
* Graphene derived structures for two dimensional electronics. Seed grant. Center for Nanoscale Science. (MRSEC-NSF/PSU). 6/1/2008-5/31/2009. $50,000. Jorge O. Sofo (PI), G. D. Barber, P. C. Eklund, H. R. Gutierrez, T. E. Mallouk, P. S. Weiss, J. Zhu.
* Nanoscale Complexity at the Oxide/Water Interface. DOE. 2003-2010. $520,311. Serguei Lvov, James Kubicki, and Jorge Sofo.
* Center for Computational Materials Design (CCMD). NSF Award IIP-0541674. 09/01/05 - 08/31/10. $400,000. Zi-Kui Liu (PI), Long-Qing Chen, James D. Kubicki, Padma Raghavan, and Jorge O. Sofo.
* Search and Discovery of a New Crystalline Hydrocarbon: Graphane and Derived Compounds. ACS-PRF Award PRF# 46715-AC10. 9/1/2007-8/31/2009. $90,000. Jorge O. Sofo (PI). Under no-cost extension.
* Penn State Research Experiences for Undergraduates and Teachers Program in Condensed Matter Physics and Interdisciplinary Materials Research. NSF Award DMR- 0648837. 5/1/07 ‑ 4/30/11. $806,244. Moses Chan (PI), Jun Zhu, Jorge O. Sofo, and Ronald Redwing.
* Nanoscale Complexity at the Oxide-Water Interface – . DOE. 04/01/2010-06/30/2013. $153,000/year. Serguei Lvov(PI), Jorge Sofo, and James Kubicki.
* Penn State Research Experiences for Undergraduates and Teachers Program in Condensed Matter Physics and Interdisciplinary Materials Research. NSF Award DMR- 1062691. 5/1/11 ‑ 4/30/14. $446,193. Moses Chan, Ronald Redwing (PI), and Jorge O. Sofo.
* Seed grant Honda Research Institute, Columbus, Ohio. 05/01/2012-02/01/2013. $10,000. Milton W. Cole and Jorge O. Sofo.
* Kinetics of adsorption and photodesorption on carbon nanotubes. Honda Research Institute USA Inc. 07/01/2013-6/30/2014. $92,000. Milton W. Cole and Jorge O. Sofo (PI).
* Kinetics of adsorption and photodesorption on carbon nanotubes. Honda Research Institute USA Inc. 07/01/2014-8/30/2015. $95,000. Jorge O. Sofo (PI).
* Modeling Quartz Dissolution. Battelle, Oak Ridge National Laboratiory, DOE. 07/01/2013-06/30/2016. $216,250. James D. Kubicki and Jorge O. Sofo.
* REU/RET Site: Penn State REU and RET in Interdisciplinary Materials Physics. NSF DMR‑1460920. 05/01/2015-04/30/2018. $450,876. Kirstin Purdy Drew and Jorge O. Sofo (PI).
* NRT-DESE: Computational Materials Education and Training - Bridging Methods and Applications (COMET). NSF DGE-1449785. 04/01/2015-03/31/2021. $2,970,000. Kristen Fichthorn (Principal Investigator), Jorge Sofo (Co-Principal Investigator), Adri van Duin (Co-Principal Investigator), Michael Janik (Co-Principal Investigator)

Teaching Experience and Lectures

* Undergraduate Level:
  + Introduction to Solid State Physics. Instituto Balseiro.
  + Probability and Statistics. Instituto Balseiro.
  + Introduction to Scientific Computing. Instituto Balseiro.
  + Solid State Theory I. (PHYS412) Penn State.
  + Solid State Theory II. (PHYS413) Penn State.
* Graduate Level:
  + Parallel programming using PVM and MPI. Instituto Balseiro.
  + Density Functional Theory. Instituto Balseiro.
  + Bonding and Structure of Metals. Karl-Franzens Universität, Graz, Austria.
  + Application of Green’s functions to Density Functional Theory. Karl-Franzens Universität, Graz, Austria.
  + Computational Physics. (PHYS527) Penn State.
  + Computational Physics II. (PHYS597) Penn State.
  + Computer Simulation of Materials. Penn State.
  + Quantum Theory of Solids I. (PHYS512) Penn State, Fall 2015, Fall 2016.
  + Quantum Theory of Solids II. (PHYS513) Penn State, Spring 2016.
  + Density Functional Theory and Practice. (PHYS597) Penn State, Spring 2018.
  + Methods of Theoretical Physics I (PHYS525) Penn State, Fall 2018, Fall 2019
* Invited lectures
  + PHYS444: “Topics in Contemporary Physics”, Fall 2004, Spring 2007, Spring 2008, Spring 2010. Penn State.
  + PHYS590: “Current Research”, Spring 2003, Fall 2004, Spring 2005, Spring 2006, Fall 2006, Fall 2008, Fall 2009, Penn State.
  + ENGL202C: “Technical Writing”, Spring 2008, Fall 2008, Fall 2012, Penn State.

Graduate Students

Current:

* Brett Green, Optical response of 2D materials. Ph.D. Candidate, Physics, Penn State
* Jacob Robbins, Transport and gas sensing in 2D materials. Ph.D. Candidate, Physics, Penn State
* Mohamed Umar, Nanostructures of polar solids. Ph.D. Candidate, Physics, Penn State

Past:

* Juan Diego Suarez Fromm, Atomic Polarizability Effects in Solids. Co-directed with Prof. José Lorenzana. Master Thesis presented at Instituto Balseiro, University of Cuyo, Argentina. December 1997.
* Adrián Lew, Finite Element Methods in High Performance Computer Platforms. Co-directed with Prof. Gustavo Buscaglia. Master thesis presented at Instituto Balseiro, University of Cuyo, Argentina. July 1998. (Currently at Stanford University)
* Javier D. Fuhr, Electronic Structure of Surfaces and ion interaction with solids. Ph.D. Thesis presented at Instituto Balseiro, University of Cuyo, Argentina. September 2001. (Currently at Centro Atómico Bariloche, Argentina)
* Griselda N. García, On the Interaction of Hydrogen with Mg-Ni Alloys. Ph.D. thesis presented at Instituto Balseiro, University of Cuyo, Argentina. July 2002. (Currently at Pontificia Universidad Católica de Chile)
* Alexei Kisselev, Applications of the Lower Critical Solution Theory. Ph. D. in Physics, Penn State. September 2008. Co-advised with Evangelos Manias (Materials Science and Engineering).
* Ning Shen, Study of chemical doping of graphene on amorphous silica, electronic properties of the graphene-fluorine super-lattice and interactions of graphene with atomic fluorine. Ph.D. in Physics, Penn State. May 2011. (Currently a Postdoc at the group of Prof. Ward Thompson in the Department of Chemistry of the University of Kansas, USA)
* Nitin Kumar, Ab Initio Molecular Dynamics Study of Water Dissociation and Proton Dynamics on Rutile and Cassiterite Surfaces. Ph.D. in Physics, Penn State. February 2012. (Currently at Sandia National Lab, Albuquerque, NM)
* Alejandro Suarez, Theory and Simulation of Atomic Hydrogen, Fluorine, and Oxygen on Graphene. Ph.D. in Physics, Penn State. August 2012. (Currently Program Manager NSF)
* Ivan Iordanov, Theoretical Modeling of Photoelectron Spectroscopy of Transition Metal Clusters. Ph.D. in Physics, Penn State. August 2012. (Currently at Edgewood Chemical and Biological Center, Baltimore, Maryland).
* Piali Aditya, Direct Fluorination of Graphene: A Theoretical and Computational Study of its Formation and of the Resulting Magnetic and Electronic Properties. Ph.D. in Physics, Penn State. November 2015.
* Sangzi Liang, Electronic Transport in Functionalized Graphene: From Strong Chemisorption to Weakly Bonded Adsorbates. Ph.D. in Physics, Penn State. November 2015. (Currently at Dupont, Iowa.)
* Mark DelloStritto, Modelling The Structure And Dynamics Of H-Bond Networks At Oxide-Water Interfaces: From Neutron Spectroscopy To Sum Frequency Generation. Ph.D. in Physics, Penn State. November 2015. (Currently postdoc at Temple University.)
* Garrett DuCharme, Water-oxide interactions. Masters in Physics, Physics, Penn State. May 2019.

Undergraduate Students

Undergraduate Honors Thesis advisor of:

Adam Focht (2004)

George Malek (2007)

Kevin Ribicki (2009)

Robert Weldon (2013)

Patrick Thornton (2018)

Stephen Thornton (2019)

Research Experience for Undergraduate advisor of:

Woody Leed (2003).

Adam Focht (2003). He is currently working as a research programmer for ITS, Penn State.

Johanna Speare (2004). She is currently attending graduate school in de Department of Physics, University of Notre Dame.

Dennise Nemetz (2005).

Ben Winchester (2005). Currently attending graduate school in the Department of Materials Science and Engineering, Penn State

Robert Skarbek, Penn State Physics (2005). Currently Masters in Geoscience, Penn State 2008. Working in industry.

George Malek, Penn State Honors College (2006).

Kevin Ribicki, Penn State Honors College (2008).

Ryan Atwater, University of Maryland (2009)

Casey Robinson, Penn State Physcis(2009)

Ryan Maunu, University of Minnesota - Twin Cities (2010)

Chris Billman, Penn State Physics(2010)

Tyler Maunu, University of Minnesota – Twin Cities (2011)

Diego B. Carrasco, Engineering Physics, Universidad Iberoamericana, Mexico (2012)

Robert Weldon, Physics, Penn State (2012)

John Groh, Physics, Penn State (2012)

Michael O’Boyle, SUNY at Geneseo (summer 2013)

Nicholas Roman, Penn State (2013)

Patrick Thornton, Penn State (2013-2016)

Eric Stopper, Penn State (08/2015-08/2018)

Stephen Thornton (08/2016-4/2019)

Rachel Ratvasky (08/2017-08/2019)

Other Activities

* Consultant for Marlow Industries, Inc. Dallas, Texas. July 1994 - June 1995.
* Consultant for Allied Signal Corporation, Morristown, New Jersey. September 1997 - November 1999.
* Lecturer in the Workshop on the Physics of the Electronic Behavior in the Core Region: All-Electron LAPW Electronic Structure Calculations, Trieste, Italy, June 22 - July 4, 1998.
* Member of the organizing committee of the conference “Applied DFT2001,” Vienna, Austria, January 2001.
* Member of the organizing committee of the conference “DFTEM 2006 - bringing together two communities,” Vienna, Austria, April 2006.
* Reviewer for ACS Nano, Acta Materialia, Applied Physics Letters, Applied Surface Science, Calphad, Chemical Physics, Chemical Physics Letters, Chemistry of Materials, Computational Materials Science, Computer Physics Communications, Desalination, Europhysics Letters, Geochimica et Cosmochimica Acta, International Journal of Hydrogen Energy, Journal of Applied Physics, Journal of Chemical Physics, Journal of Chemical Theory and Computation, Journal of Physical Chemistry B, Journal of Physical Chemistry Letters, Journal of Physics and Chemistry of Solids, Langmuir, Materials Chemistry and Physics, Materials Science in Semiconductor Processing, Nanoletters, New Journal of Physics, Physica Status Solidi, Physical Review B, Physical Review Letters, Proceedings of the National Academy of Science of the U.S.A., Solid State Communications, Surface Science, The Petroleum Research Fund of the American Chemical Society, The Department of Energy, The National Science Foundation (U.S.A.), and the Austrian Research Promotion Agency (FFG).
* Guest Editor for the Proceedings of the National Academy of Sciences. April 2011.
* Member of the Board of Directors of Fundación José A. Balseiro, Inc. since September 2006.
* Member of the Advisory Council of the Delta Program. A special program of the State College Area School District for grades 7-12. September 2006-April 2009.
* Chair of the organizing committee of the Wien2k workshop series held in University Park, PA, U.S.A:
  + “WIEN2002: Wien2k workshop at Penn State,” July 22-25, 2002
  + “WIEN2004: Wien2k workshop at Penn State,” July 12-15, 2004
  + “WIEN2007: Wien2k workshop at Penn State,” June 12-15, 2007
  + “WIEN2009: Wien2k workshop at Penn State,” June 23-26, 2009
  + “WIEN2011: Wien2k workshop at Penn State,” June 28-July 1, 2011
  + “WIEN2013: Wien2k workshop at Penn State,” August 12-16, 2013
* Organizing committee of the Quantum Espresso Workshop series held in University Park, PA, U.S.A:
  + “Quantum Espresso Workshop 2012”, June 25-29, 2012.
  + “Quantum Espresso Workshop 2014”, June 16-20, 2014.
  + “Quantum Espresso Workshop 2018”, May 21-25, 2014.

Memberships

* American Association for the Advancement of Science
* American Physical Society
* American Chemical Society

Invited Talks and Lectures

* Corning Inc., Corning, New York, "The Hydrogen-Bond and Proton Dynamics at Surfaces," Presentations, Invited. (August 6, 2019).
* II Coloquio de Simulaciones Computacionales en Ciencias, Universidad Autonoma de Mexico, Ensenada, Baja California, Mexico, "The Hydrogen-Bond and Proton Dynamics at Surfaces," (August 15, 2019).
* Theoretical Physics Group Colloquium, Humboldt University of Berlin, Berlin, Germany, "The Hydrogen-Bond and Proton Dynamics at Surfaces," Lectures, (June 11, 2019).
* Physics Department Colloquium, Universidad de Chile, Santiago de Chile, Chile, "The Hydrogen-Bond and Proton Dynamics at Surfaces," (May 2, 2019).
* Millenium Cafe, Materials Research Institute - Penn State, University Park, PA, "The Hydrogen-Bond and Proton Dynamics at Surfaces," (April 2, 2019).
* Physics Club - State College Area High School, State College, PA, "Computational Alchemy: The transmutation of Quantum Mechanics into Gold," Lectures, Invited. (April 27, 2018).
* XXIII Latin American Symposium on Solid State Physics, Bariloche, Argentina, "Bilayer graphene under pressure: Electron-hole Symmetry Breaking, Valley Hall Eect, and Landau Levels," Lectures, Invited. (April 13, 2018).
* From the Schrödinger Equation to Materials: An Alchemist Dream. Interdisciplinary Physics and Materials REU, June 14, 2017. The Pennsylvania State University, University Park, Pennsylvania, U.S.A.
* Computational Challenges to Calculate the Non-Linear Optical Response of Water/Oxide Interfaces. Computational and Applied Mathematics Colloquium, 10/10/2016. Department of Mathematics, The Pennsylvania State University, University Park, Pennsylvania, U.S.A.
* Screening of charge impurities and defects: alternative mechanisms for the detection of gases on graphene and nanotubes. Invited talk at the Northeast Regional Meeting of the American Chemical Society, 10/07/2016. Binghamton, New York, U.S.A.
* Bilayer graphene under pressure is a material with multiple Dirac cones that are evident in the Valley Hall Effect and Landau Levels. Department of Physics Colloquium, 09/28/2016. Rensselaer Polytechnic Institute, Troy, New York, U.S.A.
* Optical excitations in bilayer graphene under pressure: Topological effects. Workshop on Excitations in Solids 2016, 8/04/2016, Humboldt-Universität zu Berlin, Germany.
* Bilayer graphene under pressure: Bands Structure, Anomalous Hall Effect, and Landau Levels. Brockhouse Institute for Materials Research Seminar Series, 04/11/2016. McMaster University, Hamilton, Canada.
* Bilayer graphene under pressure: Bands Structure, Anomalous Hall Effect, and Landau Levels. Condensed Matter, Atomic, and Molecular Physics Seminar, 12/01/2015. The Pennsylvania State University, Pennsylvania, U.S.A.
* Screening of charge impurities and defects: alternative mechanisms for the detection of gases on graphene and nanotubes. APS-Mid-Atlantic Section Annual Meeting. 10/24/2015. Morgantown, West Virginia, U.S.A.
* Vibration at the interface of water with metal oxides, a probe for bonding and reactivity. Colloquium Physics Department, 10/22/2015. The University of West Virginia, West Virginia, U.S.A.
* Numerical Renormalization Group Study of Magnetic Moments and Electronic Correlations in Chemically Functionalized Graphene. Condensed Matter Theory Seminar, 06/08/2015, Humboldt-Universität zu Berlin, Germany
* Numerical Renormalization Group Study of Magnetic Moments and Electronic Correlations in Chemically Functionalized Graphene. Theory Seminar, 06/04/2015, Fritz-Haber Institute of the Max Planck Society, Berlin, Germany
* Screening of charge impurities: an alternative mechanism for the detection of gases on graphene and nanotubes. Seminario de Struttura della Materia, 1/19/2015. Università di Roma "La Sapienza", Rome, Italy
* Graphene Functionalized with Hydrogen and Fluorine: Electronic Correlations, Magnetism, and Transport. Seminari Generali (Colloquium), 2/10/2015. Università di Roma "La Sapienza", Rome, Italy
* Screening of charged impurities as a possible mechanism for conductance change in graphene gas sensing, Hands-on Workshop on Excitations in Solids 2014, 8/01/2014, Humboldt-Universität zu Berlin, Germany.
* Apantallamiento de impurezas cargadas: un mecanismo alternativo para la detección de gases con grafeno, Seminario del Departamento de Física, 7/14/2014, Universidad de Buenos Aires, Argentina
* Apantallamiento de impurezas cargadas: un mecanismo alternativo para la detección de gases con grafeno, Coloquio, 7/03/2014, Instituto Balseiro and Centro Atómico Bariloche, Argentina.
* Correlaciones electrónicas y magnetismo en grafeno funcionalizado. Sexto Taller Mexico-Chile sobre el magnetismo, nanociencia, y sus aplicaciones. Cancun, Mexico, May 22, 2014.
* Electronic Correlations, Magnetism, Transport, and Gas Detection on Functionalized Graphene. Department of Physics Colloquium, Wake Forest University, Winston-Salem, NC, USA, February 26th, 2014.
* Thermoelectrics: A theoretical approach to the search for better materials. Workshop IV: Energy Conservation and Waste Heat Recovery, Institute for Pure and Applied Mathematics, UCLA, Los Angeles, California, November 20th, 2013.
* Electronic Correlations, Magnetism, and Transport in Functionalized Graphene. 2nd International Symposium on Nanoscience and Nanomaterials, Centro de Nanociencias y Nanotecnología, Universidad Autónoma de México, Ensenada, México. March 7th, 2013.
* Transport and doping in Single-Wall Carbon Nanotubes and Graphene. Honda Research Institute. Columbus, Ohio, U.S.A. January 16th, 2013.
* Electronic Correlations, Magnetism, and Transport in Functionalized Graphene. Department of Physics Colloquium, University of North Texas, Denton, Texas, U.S.A. November 27th, 2012.
* Thermoelectrics: The Search for Better Materials. CECAM Workshop - Vibrational coupling: most important, often ignored, and a challenge for ab-initio theory. CECAM, Lausanne, Switzerland. November 7, 2012.
* Materials for Thermoelectric Applications. Hand on Workshop on the Exciting Code. Humboldt University at Berlin, Germany. August 8th, 2012.
* Graphene, Graphane, and chemisorbed graphene: electron correlations and magnetism. Hand on Workshop on the Exciting Code. Humboldt University at Berlin, Germany. August 2nd, 2012.
* GraphEne, GraphAne, GraphEne Fluoride: materials for applications and a playground for physicists. Department of Physics Colloquium, Montana State University, Bozeman, Montana, U.S.A. October 7th, 2011.
* Equilibrium and Dynamics of Water Dissociation on the Surface of Oxides with the Rutile Structure. Invited talk at the Workshop “Materials by Design.” Center for Nanoscale Materials Science, Oak Ridge National Laboratory. September 21st, 2011.
* Applications of Density Functional Theory to Water Oxide Interfaces. Invited talk at the “First School of Computational Physics Applied to Nanoscience and Nanotechnology. Pontificia Universidad Católica de Chile, Santiago, Chile. August 19th, 2011.
* Magnetic Moment and Electronic Correlations in Chemically Functionalized Graphene. Invited talk in the 2011 March Meeting of the American Physical Society, Dallas, TX. March 25, 2011.
* Grafeno, grafano, y fluoruro de grafeno: Materiales para ingeniería y un parque de diversión para los físicos. Coloquio José A. Balseiro. Instituto Balseiro, Bariloche, Argentina. March 11, 2011.
* GraphEne, GraphAne, GraphEne Fluoride: materials for applications and a playground for physicists. Department of Physics and Astronomy Colloquium, North Carolina State University, Raleigh, North Carolina, U.S.A. February 21, 2011.
* GraphEne, GraphAne, GraphEne Fluoride: materials for applications and a playground for physicists. Department of Physics Colloquium, Indiana University Purdue University at Indianapolis, Indianapolis, Indiana, U.S.A. February 17, 2011.
* GraphEne, GraphAne, GraphEne Fluoride: materials for applications and a playground for physicists. Department of Physics Colloquium, The Pennsylvania State University, University Park, PA, U.S.A. August 26, 2010.
* Electronic States, Magnetism, and Transport in Graphane, Partially Fluorinated and Hydrogenated Graphene. Jorge O. Sofo, Alejandro M. Suarez, and Ning Shen. Symposium 2, Theory and Computer Simulation of Materials of the XIX International Materials Research Congress. Cancun, Mexico. August 15-19, 2010.
* Dynamics of Water Dissociation on Oxides Surfaces: Comparison between Rutile and Cassiterite. Jorge O. Sofo, Nitin Kumar, Paul R. C. Kent, Andrei Bandura, and James D. Kubicki. Goldschmidt 2010, Earth, Energy, and the Environment. Geochemical Society and the European Association of Geochemistry. Knoxville, TN, U.S.A. June 14, 2010.
* Electronic states, magnetism, and transport in partially fluorinated and hydrogenated graphene. Nano-10. Instituto Balseiro and Comisión Nacional de Energía Atómica, Bariloche, RN, Argentina. May 14, 2010.
* Electronic states, magnetism, and transport in partially fluorinated and hydrogenated graphene. Department of Physics Colloquium, Lehigh University, Bethlehem, PA, U.S.A. April 15, 2010.
* Electronic states, magnetism, and transport in partially fluorinated and hydrogenated graphene. Department of Physics, University of California Berkeley, Berkeley, CA, U.S.A. March 30, 2010.
* Electronic states, magnetism, and transport in partially fluorinated and hydrogenated graphene. UCLA Nanoscience Institute, University of California Los Angeles, Los Angeles, CA, U.S.A. March 29, 2010.
* Electronic states, magnetism, and transport in partially fluorinated and hydrogenated graphene. Quantum Simulations Group, Lawrence Livermore National Laboratory, Livermore, CA, U.S.A. March 25, 2010.
* Electronic states, magnetism, and transport in partially fluorinated and hydrogenated graphene. GLAM Special Seminar. Geballe Laboratory for Advanced Materials and Department of Physics, Stanford University, Palo Alto, CA, U.S.A. March 24, 2010.
* Electronic Properties of Graphane and Partially Hydrogenated Graphene Nanostructures. Solidos 09 (Chile-Argentina International Condensed Matter Conference), Valparaiso, Chile. November 11th, 2009.
* Graphane, a new hydrocarbon: from prediction to synthesis. Departmental Colloquium. Department of Electrical Engineering, Penn State, University Park, PA, U.S.A., November 5th, 2009.
* Graphane, a new hydrocarbon: from prediction to synthesis. Campuses Faculty Meeting. Department of Physics, Penn State, University Park, PA, U.S.A., October 24th, 2009.
* Fast dissociation dynamics of water on cassiterite SnO2 (110) surface. EDL Group Meeting. Department of Chemical Engineering, Vanderbilt University. Nashville, TN, U.S.A. August 19, 2009.
* Graphane, a new hydrocarbon: from prediction to synthesis. Physical-Chemistry Seminar, Department of Chemistry, Penn State, University Park, PA, U.S.A. Febrary 20th, 2009.
* Simulation of Materials with Density Functional Theory. Short graduate level course. Pontificia Universidad Católica de Chile. Santiago de Chile, Chile. November 24th to 28th, 2008
* The power of graphene for electronics and how to channel it. Condensed Matter, Atomic, and Molecular Physics Seminar, Department of Physics, Penn State, University Park, PA, U.S.A. October 28th, 2008.
* Two steps into the paradigm of all graphene electronics: The effect of substrates and a method to “draw” graphene channels. Condensed Matter Seminar. Department of Physics and Astronomy. Rutgers University. U.S.A. September 30th, 2008.
* Exchange and vibrational modes in bosonic quantum solids. Supersolids 2008, International Centre for Theoretical Physics, Trieste, Italy. August 22nd, 2008.
* Supersolids and the effect of particle exchange on the phonon spectra of quantum solids, Instituto Balseiro, Bariloche, Argentina. November 13th, 2007.
* Graphane, a two dimensional hydrocarbon. Solidos 07 (National Condensed Matter Conference), Huerta Grande, Córdoba, Argentina. November 8th, 2007.
* Graphane, a two dimensional hydrocarbon: Properties, synthesis, and applications. Physics Department, University of South Florida, Tampa, Florida, November 2nd, 2007.
* Graphane, a two dimensional hydrocarbon: Properties, synthesis, and applications. Colloquium, University of Leoben, Austria, July 2nd, 2007.
* Density Functional Theory for Atoms, Molecules, and Solids, Interdisciplinary Seminar on PDEs and their Applications, Department of Mathematics, Penn State, March 19th, 2007.
* Mapping dissociation activity on surfaces, Workshop on Recent Developments in Computer Simulational Studies in Condensed Matter Theory, University of Georgia, Athens, GA, U.S.A., February 23, 2006.
* Ab-initio Simulations of Water on the Surface of Oxides, Oak Ridge National Laboratory, Oak Ridge, TN, U.S.A., June 29, 2006.
* Mapping Water Reactivity at Oxide Surfaces, Water Festival IV, University of Delaware, Newark, DE, U.S.A., November 22, 2005.
* Pairing and Excitations in Bosonic Quantum Solids, Solidos 05 (National Condensed Matter Conference), Bariloche, Argentina. November 04, 2005.
* Water and Zn on TiO2(110): DFT molecular Dynamics, Annual meeting of the EDL group, Argonne National Laboratory, Argonne, IL, U.S.A., August 20, 2005.
* Mapping Water Reactivity at Oxide Surfaces, Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY, U.S.A., December 06, 2005.
* Effect of Quantum Correlations on the Vibrational Spectrum of Bosonic Quantum Solids, Physics Department, Brookhaven National Laboratory, Upton, NY, U.S.A., December 05, 2005.
* Water Dissociation on Silica and TiO2, Physical Chemistry Colloquium, Department of Chemistry. Penn State, October 21, 2005.
* Water on Oxide Surfaces: Application of the Reactivity Mapping Method, Physics Department Colloquium, Indiana University of Pennsylvania, Indiana, PA, U.S.A., April 8, 2005.
* Low temperature melting of ionic clusters: How small can a crystal be?, Physics Department Colloquium, Indiana University of Pennsylvania, Indiana, PA, U.S.A., October 31, 2003.
* Low temperature melting of ionic clusters: How small can a crystal be?, Pan-American Advanced Studies Institute on Physics at the Nanometer Scale. Bariloche, Argentina, June 18, 2003.
* Better Materials for Thermoelectric Applications, Frontiers in Condensed Matter Theory. University Park, Pennsylvania, April 12-13, 2003.
* Toward an ab-initio determination of transport coefficients, New Thermoelectric Materials Workshop Chemistry, Physics and Materials Science of Thermoelectric Materials: Beyond Bismuth Telluride. Traverse City, Michigan, August 20, 2002.
* The interaction of Pd with defects on the surface of MoS2. Department of Physics, Uppsala University, Sweden, October 23, 2000.
* Ab initio calculation of the c/a ratio of hexagonal Cu-Zn alloys, XXIV International Workshop on Condensed Matter Theories, Buenos Aires, Argentina, September 12-17, 2000.
* Thermoelectric properties of nanostructures, Karl-Franzes University of Graz, Graz, Austria, May 15, 2000.
* One-particle Excitations in Strongly Correlated Superconductors, ”Mini-workshop on Strongly Correlated Electronic Systems”, International Centre for Theoretical Physics, Trieste, Italy, June 8-July 27, 1990.

Publications in Refereed Journals

1. “Critical behavior of Young’s Modulus of two dimensional randomly holed metalized Mylar,” J. O. Sofo, J. G. Lorenzana and E. N. Martinez, Phys. Rev. B **36**, 3960-3962 (1987).
2. “Charge distribution in GaAs-(AlxGa1−x)As heterostructures under an external magnetic field,” J. O. Sofo, C. R. Proetto and C. A. Balseiro, Appl. Phys. Lett. **53**, 282-284 (1988).
3. “Electronic structure of BaPb1−xBixO3,” J. O. Sofo, A. A. Aligia and M. D. Nuñez Regueiro, Phys. Rev. B 39 (RC), 9701-9703 (1989).
4. “Effect of local charge disproportionation on the electronic structure of BaPb1−xBixO3,” J. O. Sofo, A. A. Aligia and M. D. Nuñez Regueiro, Phys. Rev. B **40**, 6955-6962 (1989).
5. “Intrinsic bistability in resonant-tunneling GaAs-AlxGa1−xAs double barrier structures: a self consistent calculation,” J. O. Sofo and C. A. Balseiro, Phys. Rev. B **42** (RC), 7292-7295 (1990).
6. “One particle excitations in strong coupling superconductors: a new realization of the t-J model,” A. G. Rojo, J. O. Sofo and C. A. Balseiro, Phys. Rev. B **42**, 10241-10244 (1990).
7. “Slave-Boson Mean Field Theory for the Negative-U Hubbard Model,” J. O. Sofo and C. A. Balseiro, Phys. Rev. B **45**, 377-382 (1992).
8. “Thermodynamic Properties of a 2D Electron Gas with Attractive Interactions,” J. O. Sofo and C. A. Balseiro, Phys. Rev. B **45** (RC), 8197-8200 (1992).
9. “Collective excitations in Strong Coupling Superconductors,” J. O. Sofo, C. A. Balseiro, and H. E. Castillo, Phys. Rev. B **45**, 9860-9864 (1992).
10. “Ground State of the Attractive Hubbard Model,” J. O. Sofo and C. A. Balseiro, Phys. Rev. Lett. **68**, 896-896 (1992).
11. “Resistivity and Superconductivity from Anharmonic Phonons,” G. D. Mahan and J. O. Sofo, Phys. Rev. B **47**, 8050-8055 (1993)
12. “Optimum Band Gap of a Thermoelectric Material,” J. O. Sofo and G. D. Mahan, Phys. Rev. B **49**, 4565-4570 (1994).
13. “Transport Coefficients and Thermoelectric Figure of Merit of n-Hg1−xCdxTe,” J. O. Sofo, G. D. Mahan, and J. Baars, J. Appl. Phys. **76**, 2249-2254 (1994).
14. “Thermoelectric Figure of Merit of Superlattices,” J. O. Sofo and G. D. Mahan, Appl. Phys. Lett. **65**, 2690-2692 (1994).
15. “Thermoelectric Figure of Merit of n-Hg1-xCdxSe” J. O. Sofo, J. Appl. Phys. **77**, 1561-1563 (1995).
16. “The Best Thermoelectric,” G. D. Mahan and J. O. Sofo, Proc. Natl. Acad. Sci. U.S.A. **93**, 7436-7439 (1996).
17. “Multilayer Thermionic Refrigerator and Generator,” G. D. Mahan, J. O. Sofo, and M. Bartkowiak, J. Appl. Phys. **83**, 4683-4689 (1998).
18. “Electronic Structure of CoSb3: A Narrow Band-Gap Semiconductor,” J. O. Sofo and G. D. Mahan, Phys. Rev. B **58**, 15620-15623 (1998).
19. “Calculation of the electronic and structural properties of cubic Mg2NiH4,” G. N. García, J. P. Abriata and J. O. Sofo, Phys. Rev. B **59**, 11746-11754 (1999).
20. “On the adsorption of Pd on MoS2(0001) :ab initio electronic structure calculations,” J. D. Fuhr, J. O. Sofo , and Andrés Saúl. Phys. Rev. B **60**, 8343-8347 (1999).
21. “Diffusion and transport coefficients in synthetic opals,” J. O. Sofo, and G. D. Mahan. Phys. Rev. B **62**, 2780-2785 (2000).
22. “Metal-insulator transition in the double perovskites,” A. A. Aligia, P. Petrone, J. O. Sofo, and B. Alascio. Phys. Rev. B **64**, 092414-4 (2001).
23. “Hydrogen movement in cubic Mg2NiH4,” G. N. García, J. P. Abriata, and J. O. Sofo. Phys. Rev. B **65**, 064306-9 (2002).
24. “Coverage dependence study of the adsorption of Pd on MoS2(0001),” J. D. Fuhr, J. O. Sofo, and Andrés Saúl, Surface Science **506**, 161-171 (2002).
25. “Electronic structure of the pyrochlore metals Cd2Os2O7 and Cd2Re2O7,” D. J. Singh, P. Blaha, K. Schwarz, and J. O. Sofo. Phys. Rev. B **65**, 155109-8 (2002).
26. “Photoemission study of the skutterudite compounds CoSb3 and RhSb3,” H. Ishii, K. Okazaki, A. Fujimori, Y. Nagamoto, T. Koyanagi, and J. O. Sofo. Journal of the Physical Society of Japan **71**, 2271-2275 (2002).
27. “Thermoelectric Properties of Sb2Te3 under Pressure and Uniaxial Stress,” T. Thonhauser, T. J. Scheidemantel, J. O. Sofo, J. V. Badding, and G. D. Mahan. Phys. Rev. B **68**, 085201‑8 (2003).
28. “Transport Coefficients from First-Principles Calculations,” T. J. Scheidemantel, C. Ambrosch-Draxl, T. Thonhauser, J. V. Badding, and J. O. Sofo. Phys. Rev. B **68**, 125210‑6 (2003).
29. “Stress induced defects in Sb2Te3,” T. Thonhauser, Gun Sang Jeon, G. D. Mahan, and J. O. Sofo. Phys. Rev. B. **68**, 205207-6 (2003).
30. “STM chemical signature of point defects on the MoS2(0001) surface,” J. D. Fuhr, Andrés Saúl, and J. O. Sofo. Phys. Rev. Lett. **92**, 026802-4 (2004).
31. “First-principles study of binary bcc alloys using Special Quasirandom Structures,” C. Jiang, C. Wolverton, J. O. Sofo, L.-Q. Chen, and Z.-K. Liu. Phys. Rev. B. **69**, 214202-10 (2004).
32. “Improved Thermoelectric Devices Using Bismuth Alloys,” T. Thonhauser, T. J. Scheidemantel, and J. O. Sofo. Appl. Phys. Lett. **85**, 588-590 (2004).
33. “An integrated framework for multiscale material simulation and design,” Z.K. Liu, L.Q. Chen, P. Raghavan, Q. Du, J. O. Sofo, S. Langer and C. Wolverton. Journal of Computer-Aided Materials Design **11**, 183-199 (2004).
34. “Linking First-Principles Energetics to the Calphad: An Application to thermodynamic Modeling of the Al-Ca Binary System,” K. Ozturk, Y. Zhong, L.-Q. Chen, C. Wolverton, J. O. Sofo, and Z.-K. Liu. Metallurgical and Materials Transactions A **36**, 5-13 (2005)
35. “Electronic Structure Calculations of Physisorption and Chemisorption on Oxide Glass Surfaces,” E. A. Leed, J. O. Sofo, and C. G. Pantano. Phys. Rev. B **72**, 155427-11 (2005).
36. “A density functional study of the structural, electronic, magnetic and vibrational properties of Ti8C12 metallocarbohedrynes.” M. A. Sobhy, A. W. Castleman, Jr., and J. O. Sofo. J. Chem. Phys. **123**, 154106-13 (2005).
37. “Static Polarizabilities of Dielectric Nanoclusters,” H. Kim, J. O. Sofo, D. Velegol, M. W. Cole and G. Mukhopadhyay. Phys. Rev. A **72**, 053201-8 (2005).
38. “How do insertions affect Green Fluorescent Protein?,” M. Cetinkaya, A. Zeytun, J. O. Sofo and M. Demirel. Chem. Phys. Lett. **419**, 48-54 (2005).
39. “First-principles investigation of laves phases in Mg-Al-Ca system,” Y. Zhong, A. A. Luo, J. O. Sofo and Z. Liu, Mater. Sci. Forum **488/9**, 169-175 (2005).
40. “van der Waals forces between nanoclusters: Importance of many body effects,” H. Kim, J. O. Sofo, D. Velegol, M. W. Cole and A. Lucas. J. Chem. Phys. **124**, 074504-4 (2006).
41. “Derivation of Force Field Parameters for SnO2-H2O Surface Systems from Plane-Wave Density Functional Theory Calculations,” A. V. Bandura, J. O. Sofo, and J. D. Kubicki. J. Phys. Chem. B **110**, 8386-8397 (2006).
42. “Linear optical properties of solids within the full-potential linearized augmented planewave method,” C. Ambrosch-Draxl and J. O. Sofo. Comput. Phys. Commun. **175**, 1-14 (2006).
43. “Contribution of First-Principles Energetics to the Ca-Mg Thermodynamic Modeling,” Y. Zhong, K. Ozturk, J. O. Sofo, and Z.-K. Liu. J. Alloys and Compounds **420**, 98-106 (2006).
44. “Thermodynamics Modeling of the Mg-Sr and Ca-Mg-Sr Systems,” Y. Zhong, J. O. Sofo, A. A. Luo, and Z.-K. Liu. J. Alloys and Compounds **421**, 172-178 (2006).
45. “Fully retarded van der Waals interaction between dielectric nanoclusters,” H. Kim, J. O. Sofo, D. Velegol and M. W. Cole, J. Chem. Phys. **125**, 174303-8 (2006).
46. “Structure of hydrated Zn2+ at the rutile TiO2 (110)-aqueous solution interface: Comparison of Xray standing wave, X-ray absorption spectroscopy, and density functional theory results,” Z. Zhang, P. Fenter, S. D. Kelly, J. G. Catalano, A. V. Bandura, J. Kubicki, J. O. Sofo, D. J. Wesolowski, M. L. Machesky, N. C. Sturchio and M. J. Bedzyk, Geochim. Cosmochim. Acta **70**, 4039-4056 (2006).
47. “Anion Photoelectron Spectroscopy and Density Functional Investigation of Vanadium Carbide Clusters,” K. L. Knappenberger, C. E. Jones, M. A. Sobhy, I. Iordanov, J. O. Sofo and W. Castleman, J. Phys. Chem. A **110**, 12814-12821, (2006).
48. “Van der Waals Dispersion Forces between Dielectric Nanoclusters,” H. Kim, J. O. Sofo, D. Velegol, M. W. Cole and A. Lucas, Langmuir **23**, 1735-1740, (2007).
49. “Graphane: a two dimensional hydrocarbon,” J. O. Sofo, A. S. Chaudhari, and G. D. Barber. Phys. Rev. B **75**, 153401-4 (2007).
50. “Theory of genus reduction in alkali-induced graphitization of nanoporous carbon,” Elena R. Margine, Aleksey N. Kolmogorov, Dragan Stojkovic, Jorge O. Sofo, Vincent H. Crespi. Phys. Rev. B **76**, 115436-5 (2007).
51. “Anion Photoelectron Spectroscopy and Density Functional Investigation of Diniobium−Carbon Clusters,” K. L. Knappenberger, P. A. Clayborne, J. U. Reveles, M. A. Sobhy, C. E. Jones, U. U. Gupta, S. N. Khanna, I. Iordanov, J. O. Sofo and W. Castleman. ACS Nano **1**, (2007) 319–326.
52. "Analysis of Periodic Schroedinger Operators: Regularity and Approximation of Eigenvalues," E. Hunsicker, V. Nistor and Jorge O. Sofo, J. Math. Phys. **49**, 083501-21 (2008)
53. "Surface Protonation at the Rutile (110) Interface: Explicit Incorporation of Solvation Structure within the Revised MUSIC Model Framework," M. L. Machesky, M. Predota, D. J. Wesolowski, L. Vlcek, P. T. Cummings, J. Rosenqvist, M. Ridley, J. Kubicki, A. V. Bandura, N. Kumar and Jorge O. Sofo, Langmuir **24**, 12331 – 12339 (2008)
54. "Comparison of the multilayer adsorption of H2O on the (110) surfaces of TiO2 and SnO2 with rutile structure," A. V. Bandura, Jorge O. Sofo and J. Kubicki, J. Phys. Chem. B **112**, 11616 – 11624 (2008)
55. "n-Type Behavior of Graphene Supported on Si/SiO2 Substrates," H. Romero, N. Shen, P. Joshi, H. R. Gutierrez, S. Tadigadapa, Jorge O. Sofo and P. C. Eklund, ACS Nano **2**, 2037 – 2044 (2008)
56. “Hydrogen Bonds and Vibrations of Water on (110) Rutile,” Nitin Kumar, Sanghamitra Neogi, Paul R. C. Kent, Andrei V. Bandura, James D. Kubicki, David J. Wesolowski, David Cole, and Jorge O. Sofo, J. Phys. Chem. C **113**, 13732-13740 (2009)
57. “Reversible fluorination of graphene: Evidence of a two-dimensional wide bandgap semiconductor,” S. Cheng, K. Zou, F. Okino, H. Rodriguez Gutierrez, A. Gupta, N. Shen, P. C. Eklund, J. O. Sofo and J. Zhu, Phys. Rev. B **81**, 205435-5 (2010)
58. "Structural, electronic, optical and vibrational properties of nanoscale carbons and nanowires: a colloquial review," M. W. Cole, V. H. Crespi, M. S. Dresselhaus, G. Dresselhaus, J. E. Fischer, H. Rodriguez Gutierrez, K. Kojima, G. Mahan, A. M. Rao, J. O. Sofo, M. Tachibana, K. Wako and Q. Xiong, J. Phys. Condens. Mat. **22**, 334201 (2010)
59. “Photoluminescence from nanocrystalline graphite monofluoride,” Bei Wang, Justin R. Sparks, Humberto R. Gutierrez, Fujio Okino, Qingzhen Hao, Youjian Tang, Vincent H. Crespi, Jorge O. Sofo and Jun Zhu. Appl. Phys. Lett. **97**, 141915 (2010)
60. “Faster Proton Transfer Dynamics of Water on SnO2 Compared to TiO2,” Nitin Kumar, Paul R. C. Kent, Andrei V. Bandura, James D. Kubicki, David J. Wesolowski, David Cole, and Jorge O. Sofo. J. Chem. Phys. **134**, 044706 (2011)
61. “Electrical Control of the Chemical Bonding of Fluorine on Graphene,” Jorge O. Sofo, Alejandro M. Suarez, Gonzalo Usaj, Pablo S. Cornaglia, Alexander D. Hernández-Nieves, Carlos A. Balseiro. Phys. Rev B (Rapid Communications) **83**, 081411 (2011)
62. “Gate Voltage Control of Oxygen Diffusion on Graphene,” Alejandro M. Suarez, Ljubisa R. Radovic, Ezra Bar-Ziv, and Jorge O. Sofo. Phys. Rev. Lett. **106**, 146802 (2011)
63. “Multiple Isomers in the Photoelectron Spectra of Small Mono-Niobium Carbide Clusters,” Ivan Iordanov and Jorge O. Sofo. J. Chem. Phys. **134**, 184310 (2011)
64. “Dispersion of edge states and quantum confinement of electrons in graphene channels drawn on graphene fluoride,” Ning Shen and Jorge O. Sofo. Phys. Rev. B **83**, 245424 (2011)
65. “Oxygen Migration on the Graphene Surface. 2. Thermochemistry of Basal-Plane Diffusion (Hopping),” Ljubisa R. Radovic, Alejandro M. Suarez, Fernando Vallejos-Burgos, and Jorge O. Sofo. Carbon **49**, 4226-4238 (2011)
66. "Periodic DFT Study of Water Adsorption on the α-Quartz (101) Surface," Andrei Bandura, James D. Kubicki, and Jorge O. Sofo. J. Phys. Chem. C **115**, 5756-5766 (2011)
67. “Adsorption of Zn2+ on the (110) surface of TiO2 (rutile): A density functional molecular dynamics study,” Andrei V. Bandura, Jorge O. Sofo, and James D. Kubicki. J. Phys. Chem. C **115**, 9608-9614 (2011)
68. "Magnetic structure of hydrogen-induced defects on graphene," Jorge O. Sofo, Gonzalo Usaj, Pablo S. Cornaglia, Alejandro M. Suarez, Alexander D. Hernández-Nieves and Carlos A. Balseiro, Phys. Rev. B **85**, 115405 (2012)
69. "Comment on “Structure and dynamics of liquid water on rutile TiO2(110)”," D. J. Wesolowski, Jorge O. Sofo, A. V. Bandura, Z. Zhang, E. Mamontov, M. Predota, N. Kumar, J. Kubicki, P. R. C. Kent, L. Vlcek, M. L. Machesky, P. Fenter, P. T. Cummings, A. A. Skelton and J. Rosenqvist, Phys. Rev. B **85**, 167401 (2012)
70. "Metal-substituted Ti8C12 metallocarbohedrynes: Toward less reactive clusters as building blocks of cluster-assembled materials," C. Berkdemir, W. Castleman and J. O. Sofo, Phys. Chem. Chem. Phys. **14**, 9642 – 9653 (2012)
71. "Broad photoelectron spectrum and lowered electron affinity due to Hydrogen in ZnOH: A joint experimental and theoretical study," I. Iordanov, K. Gunaratne, C. L. Harmon, Jorge O. Sofo and W. Castleman, J. Chem. Phys. **136**, 214314 (2012)
72. "The impurity state and variable range hopping conduction in graphene," S. Liang and J. O. Sofo, Phys. Rev. Lett. **109,** 256601 (2012)
73. "A New Hypothesis for the Dissolution Mechanism of Silicates," J. Kubicki, J. O. Sofo, A. A. Skelton and A. V. Bandura, J. Phys. Chem. C **116**, 17479 – 17491 (2012)
74. “The Electrical Conductivity of Strontium-Barium Niobate,” G. D. Mahan and J. O. Sofo, J. Electron. Mater. **42**, 1375 (2013)
75. “Development of a ReaxFF Reactive Force Field for Titanium Dioxide/Water Systems,” S. Kim, N. Kumar, P. Persson, J. O. Sofo, A. van Duin and J. Kubicki, Langmuir **29**, 7838‑7846 (2013)
76. “Analysis and optimization of carbon nanotubes and graphene sensors based on adsorption‑desorption kinetics,” Sang-Zi Liang, Gugang Chen, Avetik R. Harutyunyan, Milton W. Cole, and Jorge O. Sofo, Appl. Phys. Lett. **103**, 233108 (2013)
77. "Vibrational Density of States of Strongly H-Bonded Interfacial Water: Insights from Inelastic Neutron Scattering and Theory," H. Wang, M. Dellostritto, N. Kumar, P. R. C. Kent, A. Kolesnikov, J. Kubicki, D. J. Wesolowski and J. O. Sofo, J. Phys. Chem. C **118**, 10805 (2014)
78. "Density functional theory simulation of hydrogen-bonding structure and vibrational densities of states at the quartz (101)-water interface and its relation to dissolution as a function of solution pH and ionic strength," M. Dellostritto, J. Kubicki and J. O. Sofo, J. Phys. Condens. Mat. **26**, 244101 (2014)
79. "Screening of charged impurities as a possible mechanism for conductance change in graphene gas sensing," S. Liang, G. Chen, A. Harutyunyan and J. O. Sofo, Phys. Rev. B **90**, 115410 (2014)
80. "An Investigation of Machine Learning Methods Applied to Structure Prediction in Condensed Matter", W. J. Brouwer, J. Kubicki, J. O. Sofo and C. L. Giles, submitted to Comput. Phys. Commun. (2014)
81. "First-principles Studies of Lattice Dynamics and Thermal Properties of Mg2Si1-xSnx," X. Liu, Y. Wang, J. O. Sofo, T. Zhu, L. Chen and X. Zhao, J. Mater. Res. **30**, 2578 – 2584 (2015).
82. “Electrically tunable multiple Dirac cones in thin films of the (LaO)2(SbSe2)2 family of materials,” Xiao-Yu Dong, Jian-Feng Wang, Rui-Xing Zhang, Wen-Hui Duan, Bang-Fen Zhu, Jorge O. Sofo and Chao-Xing Liu, Nature Comm. **6**, 8517 (2015).
83. "Bilayer graphene under pressure: Electron-hole Symmetry Breaking, Valley Hall Effect, and Landau Levels," F. Munoz, H. P. Ojeda Collado, G. Usaj, J. O. Sofo and C. A. Balseiro, Phys. Rev. B **93**, 235443 (2016)
84. “Heavy Dirac fermions in a graphene/topological insulator hetero-junction,” W. Cao, R. Zhang, P. Tang, G. Yang, J. O. Sofo, W. Duan and C. X. Liu, 2D Materials **3**, 34006 (2016).
85. "Effect of Ions on H-Bond Structure and Dynamics at the Quartz(101)-Water Interface," M. J. Dellostritto, J. Kubicki and J. O. Sofo, Langmuir 32, 11353–11356 (2016).
86. "Bond Polarizability Model for Sum Frequency Generation at the Al2O3(0001)-H2O Interface," M. J. Dellostritto, and J. O. Sofo, accepted in Journal of Physical Chemistry A.
87. "Expansive strain increases temperature needed to defluorinate graphene", C. Junkermeier, S. Goverapet Srinivasan, P. Aditya, J. O. Sofo and A. van Duin, submitted to J. Phys. Chem. Lett. (2016).
88. “Effective Bond Polarizability Model for Sum Frequency Generation,” M. J. Dellostritto and J. O. Sofo, submitted to Journal of Physical Chemistry A (2016).
89. “Bending energy of 2D materials: graphene, MoS2, and imogolite,” González, R. I., Valencia, F. J., Rogan, J., Valdivia, J. A., Sofo, J. O. (Author), Kiwi, M., & Munoz, F. , RSC Advances, **8**, 4577 (2018).
90. “Low-Energy Phases of Bi Monolayer Predicted by Structure Search in Two Dimensions,” S. Singh, Z. Zanolli, M. Amsler, B. Belhadji, J. O. Sofo, M. J. Verstraete, and A. H. Romero, J. Phys. Chem. Lett. **10**, 7324 (2019).

Invited Contribution

1. “Viewpoint: Geodesic carbon nanodomes,” Jorge O. Sofo and Renee D. Diehl, Physics (APS), **2**, 84 (2009)
2. "Peter Clay Eklund: a scientific biography," Milton W. Cole, Vincent H. Crespi, Gene Dresselhaus, Mildred S. Dresselhaus, Gerald D. Mahan and Jorge O. Sofo, J. Phys. Condens. Mat. **22**, 330301 (2010)
3. "Book Review: Problems in Solid State Physics with Solutions," J. O. Sofo, Contemp. Phys. **54**, 73 (2013)

Publications in Conference Proceedings

1. “Superlattices in Thermoelectric Applications,” J. O. Sofo and G. D. Mahan, in Proceedings of the XIII International Conference on Thermoelectrics edited by B. Mathiprakasam y P. Heenan (American Institute of Physics, New York, 1994) p. 239-246.
2. “Evaluation of the Heat of Solution of Hydrogen in Metals Using the Jellium Model,” J. L. Gervasoni, M. J. Maresca, J. O. Sofo, and J. P. Abriata in Proceedings of the 12th World Hydrogen Energy Conference, edited by J. C. Bolcich and T. N. Veziroglu (Asoc. Arg. de Hidrógeno, Buenos Aires, 1998) pp. 997-1004.
3. “Electronic Structure and Transport Properties of CoSb3: A Narrow Band-Gap Semiconductor,” J. O. Sofo and G. D. Mahan in Thermoelectric Materials 1998 – The Next Generation Materials for Small- Scale Refrigeration and Power Generation Applications, edited by T. M. Tritt, M. G. Kanatzidis, G. D. Mahan, and H. B. Lyon, Jr., (Mater. Res. Soc. Proc. 545, Warrendale, PA, 1998) pp. 315-320.
4. “Transport in Opal Structures,” J. O. Sofo, and G. D. Mahan in Proceedings of the 18th International Conference on Thermoelectrics (ICT99) (IEEE, New York, 2000) pp. 626‑629.
5. “Ab-initio calculation of the c/a ratio of hexagonal Cu-Zn alloys,” J. O. Sofo and J. P. Abriata in Condensed Matter Theories, Vol. 16, ed. by Susana Hernández and John Clark (Nova Science Publishers, New York, 2001), pp. 101-108.
6. “Towards a First-Principles Determination of Transport Coefficients,” Thomas J. Scheidemantel and Jorge O. Sofo in Chemistry, Physics and Materials Science of Thermoelectric Materials: Beyond Bismuth Telluride, edited by M. G. Kanatzidis, T. P. Hogan, and S.D. Mahanti (Kluwer Academic/Plenum Publishers, New York, 2003), pp. 249-257.
7. “Protein simulations in confined environments,” Murat Cetinkaya, Jorge O. Sofo, Melik C. Demirel. Proceedings of SPIE, Nanomodeling; Akhlesh Lakhtakia, Sergey A. Maksimenko; Eds. Vol. 5509, (2004), pp. 133-137.
8. “Adsorption Sites on Silicate Glasses,” C. G. Pantano, E. A. Leed, V. A. Bakaev, and J. O. Sofo. Proceedings of the XXth International Conference on Glass, Kyoto, Japan. 2004. Published on CD, code I-09-020.
9. “New Phases in Mg-Al-Ca System,” Y. Zhong, A. A. Luo, J. F. Nie, J. O. Sofo and Z. Liu, in Magnesium Technology 2005, Ed.: N. R. Neelameggham, H. I. Kaplan, B. R. Powell (Minerals, Metals and Materials Soc./AIME, 2005) p. 185-190. February 13, 2007
10. “Comparison of TiO2 and SnO2 (100) and (110) hydrated surfaces via molecular modeling,” J. D. Kubicki, A. V. Bandura, and J. O. Sofo. Geochimica et Cosmochimica Acta **71** (15): A529-A529 Suppl. S. AUG 2007
11. “Hydrogen bonds and vibrations of water on (110) rutile,” N. Kumar, S. Neogi, J. O. Sofo, P. R. C. Kent, A. V. Bandura, J. D. Kubicki. Geochimica et Cosmochimica Acta **73** (13): A705-A705 Suppl. S. JUN 2009
12. “Atomistic origins of mineral-water interfacial phenomena and their relation to surface complexation models,” D. J. Wesolowski, A. V. Bandura, P. T. Cummings, P. A. Fenter, J. D. Kubicki, S. N. Lvov, M. L. Machesky, E. Mamontov, M. Predota, M. K. Ridley, J. Rosenqvist, J. O. Sofo, L. Vlcek, Z. Zhang. Geochimica et Cosmochimica Acta **73** (13): A1429-A1429 Suppl. S. JUN 2009
13. “GEOC 37-Density functional theory calculations combined with X-ray standing wave, EXAFS, neutron scattering, and NMR to examine the solid-water interface,” James D. Kubicki, Jorge O. Sofo, Andrei V. Bandura, Karl T. Mueller, Nancy M. Washton. Abstracts of Papers of the American Chemical Society **235,** 37-GEOC (2010)
14. “Ortho‐para conversion of H2 in crystalline silicon,” Roger M. Herman, Alejandro M. Suarez; Jorge O. Sofo; John Courtenay Lewis. AIP Conf. Proc. **1290**, 284 (2010)