Curriculum Vitae

IGOR VASILIEV

March 16, 2021

Department of Physics, MSC 3D
New Mexico State University
P.O. Box 30001, Las Cruces, NM 88003-8001

Phone: (575) 646-3710
Fax: (575) 646-1934
E-mail: vasiliev@nmsu.edu

Education

B. Sc.	Chemical Physics	Moscow Institute of Physics and Technology, Russia	1991
M. Sc.	Chemical Physics Academic advisor: Thesis title:	Moscow Institute of Physics and Technology, Russia Professor Victor A. Nadtochenko *Investigation of the Photophysical and Photochemical Properties of Fullerenes by Picosecond Laser Photolysis*	1993
Ph. D.	Materials Science Academic advisor: Dissertation title:	University of Minnesota, Minneapolis, Minnesota Professor James R. Chelikowsky *First Principles Calculations for Optical Absorption Spectra and Polarizabilities of Atomic Clusters*	2000

Employment

G. W. Gardiner Professor	Department of Physics, New Mexico State University, Las Cruces, New Mexico, USA	2019 – 2021
Professor	Department of Physics, New Mexico State University, Las Cruces, New Mexico, USA	2014 – Present
Associate Professor	Department of Physics, New Mexico State University, Las Cruces, New Mexico, USA	2008 – 2014
Assistant Professor	Department of Physics, New Mexico State University, Las Cruces, New Mexico, USA	2002 – 2008
Postdoctoral Associate	Department of Physics, University of Illinois at Urbana-Champaign, Urbana, Illinois, USA	2000 – 2002
Research Assistant	Department of Materials Science, University of Minnesota, Minneapolis, Minnesota, USA	1995 – 2000
Staff Member	Institute of Chemical Physics, Chernogolovka, Moscow region, Russia	1993 – 1994

Awards

George. W. Gardiner Professorship, New Mexico State University	2019 – 2021
J. Tinsley Oden Fellowship, University of Texas at Austin	2008 – 2009
Silver Medal Award, Materials Research Society	1999
Best Research Project Award, Institute of Chemical Physics	1993

Publications

Book Chapters

1. V. A. Nadtochenko, I. V. Vasiliev, N. N. Denisov, I. V. Rubtsov, A. S. Lobach, and A. P. Moravskii, *External Heavy Atom Effect on the Intersystem Crossing of Fullerenes. Picosecond Laser Photolysis Study*, in *Recent Advances in the Chemistry and Physics of Fullerenes and Related Materials*, edited by K. M. Kadish and R. S. Ruoff, pp. 1658−1669 (Electrochemical Society, Pennington, New Jersey, 1994) ISBN 1-56677-082-3.

2. J. R. Chelikowsky, S. Öğüt, I. Vasiliev, A. Stathopoulos, and Y. Saad, *Predicting the Properties of Semiconductor Clusters*, in *Theory of Atomic and Molecular Clusters*, edited by J. Jellinek, pp. 136−156 (Springer-Verlag, Berlin, 1999) ISBN 3-540-62000-1.

3. J. R. Chelikowsky, L. Kronik, I. Vasiliev, M. Jain, and Y. Saad, *Using Real Space Pseudopotentials for the Electronic Structure Problem*, in *Handbook of Numerical Analysis, Volume X: Computational Chemistry*, edited by P. G. Ciarlet and C. Le Bris, pp. 613−638 (Elsevier, Amsterdam, 2003) ISBN 0-444-51248-9.

4. J. R. Chelikowsky, Y. Saad, and I. Vasiliev, *Atoms and Clusters*, in *Time Dependent Density Functional Theory*, edited by M. Marques, F. Nogueira, A. Rubio, K. Burke, and E.K.U. Gross, Lect. Notes Phys. **706**, pp. 259−269 (Springer, Berlin, 2006) ISBN 3-540-35422-0.

5. I. Vasiliev, *Functionalization of Carbon Nanotubes for Assembly*, in *Handbook of Nanophysics: Nanotubes and Nanowires*, edited by K. Sattler, pp. 9.1−9.16 (CRC Press, Boca Raton, 2011) ISBN 978-1-4200754-2-7.

Journal Articles

6. V. A. Nadtochenko, I. V. Vasiliev, N. N. Denisov, I. V. Rubtsov, A. S. Lobach, A. P. Moravskii, and A. F. Shestakov, *Photophysical Properties of C_{60}: Picosecond Study of Intersystem Crossing*, J. Photochem. Photobiol. A **70**, 153−156 (1993).

7. I. V. Vasiliev, V. A. Nadtochenko, N. N. Denisov, A. S. Lobach, and A. P. Moravskii, *Photophysical Properties of C_{70} in Excited State. Picosecond Laser Photolysis*, Zh. Fizicheskoi Khimii **67**, 1880−1883 (1993).

8. V. A. Nadtochenko, N. N. Denisov, I. V. Vasiliev, I. V. Rubtsov, A. S. Lobach, and A. P. Moravskii, *Photophysical and Photochemical Properties of C_{60} and C_{70}. Intersystem Crossing and Photoionization in Solutions. Photooxidation of T_1 Excited C_{60} by Electron Acceptors in Solutions*, Mol. Cryst. Liq. Cryst. C **4**, 95−103 (1994).

9. I. Vasiliev, S. Öğüt, and J. R. Chelikowsky, *Ab Initio Calculations for the Polarizabilities of Small Semiconductor Clusters*, Phys. Rev. Lett. **78**, 4805−4808 (1997).

10. I. Vasiliev, S. Öğüt, and J. R. Chelikowsky, *Ab Initio Excitation Spectra and Collective Electronic Response in Atoms and Clusters*, Phys. Rev. Lett. **82**, 1919−1922 (1999).

11. I. Vasiliev, S. Öğüt, and J. R. Chelikowsky, *Ab Initio Absorption Spectra of Gallium Arsenide Clusters*, Phys. Rev. B **60**, R8477−R8480 (1999).

12. J. R. Chelikowsky, Y. Saad, S. Öğüt, I. Vasiliev, and A. Stathopoulos, *Electronic Structure Methods for Predicting the Properties of Materials: Grids in Space*, Phys. Stat. Sol. (b) **217**, 173−195 (2000).

13. L. Kronik, I. Vasiliev, and J. R. Chelikowsky, *Ab Initio Calculations for Structure and Temperature Effects on the Polarizabilities of Na_n ($n \leq 20$) Clusters*, Phys. Rev. B **62**, 9992−9995 (2000).

14. I. Vasiliev, S. Öğüt, and J. R. Chelikowsky, *Ab Initio Absorption Spectra and Optical Gaps in Nanocrystalline Silicon*, Phys. Rev. Lett. **86**, 1813−1816 (2001).

15. L. Kronik, I. Vasiliev, M. Jain and J. R. Chelikowsky, *Ab Initio Structures and Polarizabilities of Sodium Clusters*, J. Chem. Phys. **115**, 4322−4332 (2001); erratum: **115**, 8714 (2001).

16. I. Vasiliev, S. Öğüt, and J. R. Chelikowsky, *First-Principles Density-Functional Calculations for Optical Spectra of Clusters and Nanocrystals*, Phys. Rev. B **65**, 115416 (2002).

17. I. Vasiliev, R. M. Martin, and J. R. Chelikowsky, *Surface Oxidation Effects on the Optical Properties of Silicon Nanocrystals*, Phys. Rev. B **65**, 121302(R) (2002).

18. M. D. Deshpande, D. G. Kanhere, I. Vasiliev, and R. M. Martin, *Density-Functional Study of Structural and Electronic Properties of Na_nLi and Li_nNa ($1 \leq n \leq 12$) Clusters*, Phys. Rev. A **65**, 033202 (2002).

19. M. D. Deshpande, D. G. Kanhere, P. V. Panat, I. Vasiliev, and R. M. Martin, *Ground-State Geometries and Optical Properties of $Na_{8-x}Li_x$ ($x = 0 - 8$) Clusters*, Phys. Rev. A **65**, 053204 (2002).

20. I. Vasiliev and R. M. Martin, *Optical Properties of Hydrogenated Silicon Clusters with Reconstructed Surfaces*, Phys. Stat. Sol. (b) **233** 5−9 (2002).

21. M. D. Deshpande, D. G. Kanhere, I. Vasiliev, and R. M. Martin, *Ab Initio Absorption Spectra of Al_n ($n = 2 - 13$) Clusters*, Phys. Rev. B **68**, 035428 (2003).

22. I. Vasiliev, *Optical Excitations in Small Hydrogenated Silicon Clusters: Comparison of Theory and Experiment*, Phys. Stat. Sol. (b) **239** 19−25 (2003).

23. J. R. Chelikowsky, L. Kronik, and I. Vasiliev, *Time-Dependent Density-Functional Calculations for the Optical Spectra of Molecules, Clusters, and Nanocrystals*, J. Phys.: Condens. Matter **15**, R1517−R1547 (2003).

24. W. R. Burdick, Y. Saad, L. Kronik, I. Vasiliev, M. Jain, and J. R. Chelikowsky, *Parallel Implementation of Time-Dependent Density Functional Theory*, Comp. Phys. Comm. **156**, 22−42 (2003).

25. I. Vasiliev and R. M. Martin, *Time-Dependent Density-Functional Calculations with Asymptotically Correct Exchange-Correlation Potentials*, Phys. Rev. A **69**, 052508 (2004).

26. M. Lopez del Puerto, M. L. Tiago, I. Vasiliev, and J. R. Chelikowsky, *Real Space Pseudopotential Calculations of the Ground State and Excited State Properties of the Water Molecule*, Phys. Rev. A **72**, 052504 (2005).

27. I. Vasiliev and S. A. Curran, *Ab Initio Study of the Self-Assembly of Phenosafranin to Carbon Nanotubes*, Phys. Rev. B **73**, 165420 (2006).

28. B. Medasani, Y. H. Park, and I. Vasiliev, *Theoretical Study of the Surface Energy, Stress, and Lattice Contraction of Silver Nanoparticles*, Phys. Rev. B **75**, 235436 (2007).

29. I. Vasiliev and S. A. Curran, *Cross-Linking of Thiolated Carbon Nanotubes: An Ab Initio Study*, J. Appl. Phys. **102**, 024317 (2007).

30. A. Lugo-Solis and I. Vasiliev, *Ab Initio Study of K Adsorption on Graphene and Carbon Nanotubes: Role of Long-Range Ionic Forces*, Phys. Rev. B **76**, 235431 (2007).

31. B. Medasani and I. Vasiliev, *Computational Study of the Surface Properties of Aluminum Nanoparticles*, Surf. Sci. **603**, 2042−2046 (2009).

32. N. Al-Aqtash and I. Vasiliev, *Ab Initio Study of Carboxylated Graphene*, J. Phys. Chem. C **113**, 12970−12975 (2009).

33. I. Vasiliev, M. Lopez del Puerto, M. Jain, A. Lugo-Solis, and J. R. Chelikowsky, *Application of Time-Dependent Density-Functional Theory to Molecules and Nanostructures*, J. Mol. Struct.: THEOCHEM **914**, 115−129 (2009).

34. I. Vasiliev and J. R. Chelikowsky, *Real-Space Calculations of Atomic and Molecular Polarizabilities Using Asymptotically Correct Exchange-Correlation Potentials*, Phys. Rev. A **82**, 012502 (2010).

35. Z. Bao, S. Alnemrat, L. Yu, I. Vasiliev, Q. Ren, X. Lu, and S. Deng, *Kinetic Separation of Carbon Dioxide and Methane on a Copper Metal-Organic Framework*, J. Colloid Interface Sci. **357**, 504−509 (2011).

36. N. Al-Aqtash and I. Vasiliev, *Ab Initio Study of Boron- and Nitrogen-Doped Graphene and Carbon Nanotubes Functionalized with Carboxyl Groups*, J. Phys. Chem. C **115**, 18500−18510 (2011).

37. Z. Bao, S. Alnemrat, L. Yu, I. Vasiliev, Q. Ren, X. Lu, and S. Deng, *Adsorption of Ethane, Ethylene, Propane and Propylene on a Magnesium-Based Metal-Organic Framework*, Langmuir **27**, 13554−13562 (2011).

38. N. Al-Aqtash, K. M. Al-Tarawneh, T. Tawalbeh, and I. Vasiliev, *Ab Initio Study of the Interactions between Boron and Nitrogen Dopants in Graphene*, J. Appl. Phys. **112**, 034304 (2012).

39. S. Alnemrat, J. P. Hooper, I. Vasiliev, and B. Kiefer, *The Role of Equilibrium Volume and Magnetism on the Stability of Iron Phases at High Pressures*, J. Phys.: Condens. Matter **26**, 046001 (2014).

40. L. S. Abdallah, T. M. Tawalbeh, I. V. Vasiliev, S. Zollner, C. Lavoie, A. Ozcan, and M. Raymond, *Optical Conductivity of $Ni_{1-x}Pt_x$ Alloys ($0 < x < 0.25$) from 0.76 to 6.6 eV*, AIP Advances **4**, 017102 (2014).

41. S. Alnemrat, Y. H. Park, and I. Vasiliev, *Ab Initio Study of ZnSe and CdTe Semiconductor Quantum Dots*, Physica E **57**, 96−102 (2014).

42. L. V. Frolova, I. V. Magedov, A. Harper, S. K. Jha, M. Ovezmyradov, G. Chandler, J. Garcia, D. Bethke, E. A. Shaner, I. Vasiliev, and N. G. Kalugin, *Tetracyanoethylene Oxide-Functionalized Graphene and Graphite Characterized by Raman and Auger Spectroscopy*, Carbon **81**, 216−222 (2015).

43. M. Hammouri, S. K. Jha, and I. Vasiliev, *First-Principles Study of Graphene and Carbon Nanotubes Functionalized with Benzyne*, J. Phys. Chem. C **119**, 18719−18728 (2015).

44. M. Hammouri, E. Fohtung, and I. Vasiliev, *Ab initio study of magnetoelectric coupling in* $\mathrm{La_{0.66}Sr_{0.33}MnO_3/PbZr_{0.2}Ti_{0.8}O_3}$ *multiferroic heterostructures*, J. Phys.: Condens. Matter **28**, 396004 (2016).

45. M. Hammouri and I. Vasiliev, *Ab Initio Study of the Electronic and Transport Properties of Waved Graphene Nanoribbons*, Physica E **89**, 170−176 (2017).

46. S. K. Jha and I. Vasiliev, *Vibrational Signatures of Carboxylated Graphene: A First-Principles Study*, J. Phys. Chem. C **122**, 24996−25006 (2018).

47. I. Vasiliev, B. Ale Magar, J. Duay, T. N. Lambert, and B. Chalamala, *Ab Initio Studies of Hydrogen Ion Insertion into β-, R-, and γ-MnO_2 Polymorphs and the Implications for Shallow-Cycled Rechargeable Zn/MnO_2 Batteries*, J. Electrochem. Soc. **165**, A3517−A3524 (2018).

48. B. Paudel, I. Vasiliev, M. Hammouri, D. Karpov, A. Chen, V. Lauter, and E. Fohtung, *Strain vs. Charge Mediated Magnetoelectric Coupling Across the Magnetic Oxide/Ferroelectric Interfaces*, RSC Adv. **9**, 13033−13041 (2019).

49. B. Ale Magar, N. Paudel, T. N. Lambert, and I. Vasiliev *Ab Initio Studies of Discharge Mechanism of MnO_2 in Deep-Cycled Rechargeable Zn/MnO_2 Batteries*, J. Electrochem. Soc. **167**, 020557 (2020).

50. B. Ale Magar, N. Paudel, T. N. Lambert, and I. Vasiliev *Phase Transformations of MnO_2 Cathode Material in Rechargeable Zn/MnO_2 Batteries: An Ab Initio Study*, (in preparation).

51. N. Paudel, B. Ale Magar, T. N. Lambert, and I. Vasiliev *Influence of Surfaces and Structural Defects on the Electrochemical Properties of MnO_2 in Rechargeable Zn/MnO_2 Batteries: A First Principles Study*, (in preparation).

52. K. Acharya, M. Hammouri, and I. Vasiliev *Influence of Polarization, Strain, and Doping on the Magnetoelectric Properties of LSMO/PZT Interfaces*, (in preparation).

Conference Proceedings

53. I. Vasiliev, S. Öğüt, and J. R. Chelikowsky, *Optical Excitations in Nanostructures: Application of Time Dependent Density Functional Theory to Si_n ($n = 3 - 10$) Clusters*, in *Proceedings of the International Symposium on Clusters and Nanostructure Interfaces*, edited by P. Jena (World Scientific, 2000).

54. I. Vasiliev, S. Öğüt, and J. R. Chelikowsky, *Optical Absorption and Electronic Excitations in Hydrogenated Silicon Clusters*, Materials Research Society Symposium Proceedings **579**, 91−96 (2000).

55. I. Vasiliev and B. Medasani, *Surface Properties of Silver and Aluminum Nanoclusters*, in *Quantum Dots, Particles, and Nanoclusters V*, edited by K. G. Eyink, F. Szmulowicz, and D. L. Huffaker, Proceedings of SPIE **6902**, 690207 (2008).

56. N. Al-Aqtash and I. Vasiliev, *Carboxylation of Boron- and Nitrogen-Doped Graphene and Carbon Nanotubes*, Technical Proceedings of the 2010 NSTI Nanotechnology Conference and Expo **2**, 729−732 (2010).

57. I. Vasiliev, *Ab Initio Study of Group II-VI Semiconductor Nanocrystals*, in *Physical Chemistry of Interfaces and Nanomaterials IX*, edited by O. V. Prezhdo, Proceedings of SPIE **7758**, 77580N (2010).

Citations

Total number of citations in peer reviewed journals: $\sim$ **2870**, h-index: **23**

Articles with over **200** citations:

Ab Initio Calculations for the Polarizabilities of Small Semiconductor Clusters: **260**

Ab Initio Absorption Spectra and Optical Gaps in Nanocrystalline Silicon: **256**

Surface Oxidation Effects on the Optical Properties of Silicon Nanocrystals: **240**

Ab Initio Excitation Spectra and Collective Electronic Response in Atoms and Clusters: **230**

Adsorption of Ethane, Ethylene, Propane & Propylene on a Magnesium-Based Metal-Organic Framework: **217**

First-Principles Density-Functional Calculations for Optical Spectra of Clusters and Nanocrystals: **210**

Presentations

Colloquia and Seminars

1. *Density-Functional Calculations for the Optical Properties of Clusters and Nanocrystals*, Lawrence Livermore National Laboratory (Livermore, California, February 14, 2002).

2. *Optical Properties of Semiconductor Clusters and Nanostructures*, Department of Physics, New Mexico State University (Las Cruces, New Mexico, March 13, 2002).

3. *First Principles Calculations for the Structural, Electronic, and Optical Properties of Nanoclusters*, Department of Mechanical Engineering, New Mexico State University (Las Cruces, New Mexico, October 17, 2002).

4. *Optical Properties of Nanostructured Materials*, Department of Physics, University of Texas at El Paso (El Paso, Texas, February 11, 2004).

5. *Modeling and Simulation of Nanostructured Materials*, Department of Mathematical Sciences, New Mexico State University (Las Cruces, New Mexico, September 22, 2004).

6. *Optical Properties of Nanoscale Structures*, Kansas Center for Advanced Scientific Computing, University of Kansas (Lawrence, Kansas, October 8, 2004).

7. *Electronic and Optical Properties of Self-Assembled Nanostructures*, Los Alamos National Laboratory (Los Alamos, New Mexico, March 10, 2005).

8. *Optical Excitations in Nanoscale Materials*, Departments of Mathematical Sciences, New Mexico State University (Las Cruces, New Mexico, November 2, 2006).

9. *Theoretical Modeling of Complex Nanosystems*, Department of Physics, University of Texas at El Paso (El Paso, Texas, February 22, 2008).

10. *First Principles Studies of Nanoscale Structures*, Department of Physics, University of Texas at Austin (Austin, Texas, April 21, 2009).

11. *Exchange-Correlation Functionals for Density-Functional Calculations*, Departments of Physics, New Mexico State University (Las Cruces, New Mexico, October 22, 2009).

12. *Theoretical Characterization of Electronic Nanomaterials*, Department of Physics, Texas State University at San Marcos (San Marcos, Texas, October 3, 2012).

13. *Theoretical Modeling of Nanoscale Materials*, Materials Department, New Mexico Tech (Socorro, New Mexico, November 15, 2012).

14. *Theoretical Studies of Doped and Functionalized Carbon Nanostructures*, Department of Physics, University of Texas at El Paso (El Paso, Texas, September 25, 2015).

15. *Ab Initio Theoretical Studies of Nanoscale Materials*, Sandia National Laboratories (Albuquerque, New Mexico, April 21, 2016).

16. *Computational Modeling of Complex Nanostructures*, CUNY Energy Institute (New York City, New York, December 13, 2016).

17. *Discharge Mechanism of MnO_2 in Rechargeable Alkaline Zn/MnO_2 Batteries*, Apple Inc. (San Jose, California, December 16, 2019).

Invited Talks

18. *Time-Dependent LDA: Computing the Optical Properties of Clusters*, Workshop on New Methods in Electronic Structure (Urbana-Champaign, Illinois, May 21−24, 1999).

19. *TDLDA Optical Spectra of Large Clusters and Nanocrystals*, 11^{th} Lakeview Conference on Computational Research on Materials (Morgantown, West Virginia, May 9−11, 2001).

20. *Optical Properties of Silicon Nanoclusters*, 3^{rd} Motorola Workshop on Computational Materials and Electronics (Tempe, Arizona, November 12−14, 2001).

21. *Efficient Exchange-Correlation Functionals for Time-Dependent Density Functional Calculations*, 4^{th} Motorola Workshop on Computational Materials and Electronics (Tempe, Arizona, November 14−15, 2002).

22. *Time-Dependent Density Functional Calculations for Optical Excitations in Nanoscale Materials*, APS 2006 March Meeting (Baltimore, Maryland, March 13−17, 2006).

23. *Theoretical Modeling of Clusters, Nanoparticles, and Quantum Dots*, SPIE Photonics West, Conference OE17: Quantum Dots, Particles, and Nanoclusters V (San Jose, California, January 19−24, 2008).

24. *Ab Initio Study of Group II-VI Semiconductor Nanocrystals*, SPIE Nanoscience + Engineering, Conference OP106: Physical Chemistry of Interfaces and Nanomaterials IX (San Diego, California, August 1−5, 2010).

25. *Electronic and Transport Properties of Functionalized Carbon Nanostructures*, Telluride Science Research Center, Workshop on Nanomaterials: Computation, Theory, and Experiment (Telluride, Colorado, June 29−July 4, 2015).

26. *Real-Space TDDFT Studies of the Optical Properties of Nanoscale Structures*, CECAM Workshop on DFT and TDDFT in the Real-Space Formalism within the PARSEC Code: Perspectives and Future Development (Tel Aviv, Israel, December 13−17, 2015).

27. *Ab Initio Density Functional Studies of Nanoscale Materials*, APS Joint Four Corners and Texas Sections Meeting (Las Cruces, New Mexico, October 21−22, 2016).

28. *Ab Initio Study of Electrochemical Properties of MnO_2*, Workshop on Practical Quantum Mechanics for Electronic Materials (Austin, Texas, June 2, 2018).

Contributed Talks

29. *Ab Initio Calculations for the Polarizabilities of Semiconductor Clusters*, APS 1997 March Meeting (Kansas City, Kansas, March 17−21, 1997).

30. *Ab Initio Calculations for Collective Electronic Response*, APS 1998 March Meeting (Los Angeles, California, March 16−20, 1998).

31. *Ab Initio Calculations for the Absorption Spectra of Gallium Arsenide Clusters*, APS 1999 March Meeting (Atlanta, Georgia, March 20−26, 1999).

32. *Application of the Time-Dependent Local Density Approximation to the Optical Properties of Atoms and Clusters*, MRS 1999 Fall Meeting (Boston, Massachusetts, November 29 − December 3, 1999).

33. *Ab Initio Calculations for the Optical Properties of Nanocrystalline Silicon*, APS 2000 March Meeting (Minneapolis, Minnesota, March 20−24, 2000).

34. *TDLDA Absorption Spectra and Optical Gaps in Silicon Nanoclusters*, CMSN Workshop on Excited State Properties and Response Functions for Materials (Minneapolis, Minnesota, November 13−14, 2000).

35. *The Effect of Oxygen Contamination on the Optical Gap of Nanocrystalline Silicon*, APS 2001 March Meeting (Seattle, Washington, March 12−16, 2001).

36. *Optical Properties of Silicon Nanoclusters with Oxidized and Reconstructed Surfaces*, CMSN Workshop on Excited State Properties and Response Functions for Materials (Berkeley, California, October 18−19, 2001).

37. *Efficient Algorithms for Time-Dependent Density-Functional Calculations with Asymptotically Corrected Potentials*, APS 2002 March Meeting (Indianapolis, Indiana, March 18−22, 2002).

38. *Absorption Spectra and Optical Gaps of Small Hydrogenated Silicon Dots: Comparison of Theory and Experiment*, APS 2003 March Meeting (Austin, Texas, March 3−7, 2003).

39. *Time-Dependent Density-Functional Calculations with Asymptotically Correct Exchange-Correlation Potentials*, CMSN Workshop on Excited State Properties and Response Functions for Materials (Gaithersburg, Maryland, December 19, 2003).

40. *Time-Dependent Density-Functional Calculations for the Optical Properties of Self-Assembled Nanostructures*, CMSN Workshop on Excited State Properties and Response Functions for Materials (Seattle, Washington, October 15−16, 2004).

41. *Ab Initio Calculations for the Optical Properties of Self-Assembled Nanostructures*, APS 2005 March Meeting (Los Angeles, California, March 21−25, 2005).

42. *Electronic and Optical Properties of Self-Assembled Nanostructures*, Workshop on Nanoengineered Materials and Macro-Molecular Technologies (Santa Fe, New Mexico, October 3−7, 2005).

43. *Ab Initio Study of Crosslinking of Functionalized Carbon Nanotubes*, APS 2007 March Meeting (Denver, Colorado, March 5−9, 2007).

44. *Surface Stress and Energy of Metal Nanoclusters*, APS 2008 March Meeting (New Orleans, Louisiana, March 10−14, 2008).

45. *First Principles Studies of Nanoscale Structures*, Workshop on Pseudopotentials and Complex Materials (Austin, Texas, April 9−11, 2008).

46. *Ab Initio Study of Atomic and Molecular Polarizabilities*, APS 2009 March Meeting (Pittsburgh, Pennsylvania, March 16−20, 2009).

47. *First Principles Study of Core-Shell Semiconductor Nanocrystals*, APS 2011 March Meeting (Dallas, Texas, March 21−25, 2011).

48. *Ab Initio Study of the Interactions between Dopant Atoms in Graphene*, APS 2012 March Meeting (Boston, Massachusetts, February 27 − March 2, 2012).

49. *Discharge Mechanism of MnO_2 in Deep-Cycle Rechargeable Zn/MnO_2 Batteries*, DOE OE Energy Storage Peer Review 2019 (Albuquerque, New Mexico, September 23−26, 2019).

50. *Phase Transformations of the MnO_2 Cathode Material in Rechargeable Zn/MnO_2 Batteries: An Ab Initio Study*, APS 2021 March Meeting (Online Meeting, March 15−19, 2021).

Co-Authored Talks and Abstracts

51. V. A. Nadtochenko, I. V. Vasiliev, I. V. Rubtsov, A. S. Lobach, and A. P. Moravskii, *Photophysical Properties of Fullerenes. Picosecond and Nanosecond Transient Absorption Spectra of C_{60} and C_{70}. New Bands in the Near IR*, Fullerenes '93: 1st International Interdisciplinary Colloquium on the Science and Technology of the Fullerenes (Santa Barbara, California, June 27−30, 1993).

52. V. A. Nadtochenko, I. V. Vasiliev, I. V. Rubtsov, A. S. Lobach, and A. P. Moravskii, *Photophysical and Photochemical Properties of C_{60} and C_{70}. Study by the Picosecond and Nanosecond Laser Photolysis Techniques*, International Workshop on Fullerenes and Atomic Clusters (St. Petersburg, Russia, October 4−9, 1993).

53. L. Kronik, I. Vasiliev, and J. R. Chelikowsky, *Gradient-Corrected Density Functional Pseudopotentials Applied to the Electronic and Structural Properties of Sodium Clusters*, APS 2000 March Meeting (Minneapolis, Minnesota, March 20−24, 2000).

54. L. Kronik, I. Vasiliev, M. Jain, and J. R. Chelikowsky, *Temperature Dependent Polarizabilities in Sodium Clusters*, APS 2001 March Meeting (Seattle, Washington, March 12−16, 2001).

55. G. F. Bertsch, I. Vasiliev, and J. R. Chelikowsky, *Comparison of Algorithms for Time-Dependent Density-Functional Theory*, APS 2001 March Meeting (Seattle, Washington, March 12−16, 2001).

56. J. R. Chelikowsky, S. Öğüt, I. Vasiliev, S. Ismail-Beigi, and S. G. Louie, *Comparison of Time Dependent Local Density Approximation and Bethe-Salpeter Methods for the Optical Properties of Covalent and Ionic Systems*, APS 2001 March Meeting (Seattle, Washington, March 12−16, 2001).

57. A. Lugo-Solis and I. Vasiliev, *Ab initio Studies of Potassium Adsorption on Graphite and Carbon Nanotubes*, Workshop on Nanoengineered Materials and Macro-Molecular Technologies (Santa Fe, New Mexico, October 3−7, 2005).

58. A. Lugo-Solis and I. Vasiliev, *Ab initio Studies of Potassium Adsorption on Graphite and Carbon Nanotubes*, APS 2006 March Meeting (Baltimore, Maryland, March 13−17, 2006).

59. B. Medasani, Y. H. Park, and I. Vasiliev, *Ab Initio Calculations for the Surface Energy of Silver Nanoparticles*, APS 2007 March Meeting (Denver, Colorado, March 5−9, 2007).

60. N. Al-Aqtash and I. Vasiliev, *Ab Initio Study of Covalent Functionalization of Defective Carbon Nanotubes by Carboxyl Group*, APS Four Corners Section Meeting (Flagstaff, Arizona, October 19−20, 2007).

61. A. Lugo-Solis and I. Vasiliev, *First-Principles Studies of Metal-Graphene and Metal-Nanotube Heterostructures*, APS 2008 March Meeting (New Orleans, Louisiana, March 10−14, 2008).

62. N. Al-Aqtash and I. Vasiliev, *Role of Surface Defects in the Carboxylation of Carbon Nanotubes: An Ab Initio Study*, APS 2008 March Meeting (New Orleans, Louisiana, March 10−14, 2008).

63. N. Al-Aqtash and I. Vasiliev, *First-Principles Studies of Covalent Functionalization of Graphene by Carboxyl Groups*, APS 2009 March Meeting (Pittsburgh, Pennsylvania, March 16−20, 2009).

64. N. Al-Aqtash and I. Vasiliev, *Functionalization of Boron- and Nitrogen-Doped Graphene and Carbon Nanotubes: An Ab Initio Study*, APS 2010 March Meeting (Portland, Oregon, March 15−19, 2010).

65. N. Al-Aqtash and I. Vasiliev, *Ab Initio Study of Interaction between Boron and Nitrogen Dopants in Graphene*, APS Four Corners Section Meeting (Ogden, Utah, October 15−16, 2010).

66. T. Tawalbeh and I. Vasiliev, *Ab Initio Study of the Interaction between Dopant Atoms and Point Defects in Graphene*, APS Four Corners Section Meeting (Tucson, Arizona, October 21−22, 2011).

67. T. Tawalbeh and I. Vasiliev, *Ab Initio Study of the Interactions between Dopant Atoms and Point Defects in Graphene*, APS 2012 March Meeting (Boston, Massachusetts, February 27 − March 2, 2012).

68. L. Abdallah, S. Zollner, T. Tawalbeh, I. Vasiliev, C. Lavoie, A. Ozcan, and M. Raymond, *Dielectric Function of Ni-Pt Alloys from 0.6 to 6.6 eV by Spectroscopic Ellipsometry*, APS 2012 March Meeting (Boston, Massachusetts, February 27 − March 2, 2012).

69. M. Hammouri and I. Vasiliev, *Ab Initio Study of Single and Double Vacancies in Graphene*, APS Four Corners Section Meeting (Socorro, New Mexico, October 26−27, 2012).

70. L. Abdallah, S. Zollner, T. Tawalbeh, I. Vasiliev, C. Lavoie, A. Ozcan, and M. Raymond, *Composition Dependence of the Optical Conductivity of NiPt Alloys Determined by Spectroscopic Ellipsometry*, APS Four Corners Section Meeting (Socorro, New Mexico, October 26−27, 2012).

71. L. Abdallah, S. Zollner, T. Tawalbeh, I. Vasiliev, C. Lavoie, A. Ozcan, and M. Raymond, *Compositional Dependence of the Dielectric Function and Optical Conductivity of NiPt Alloy Thin Films*, AVS 2012 International Symposium (Tampa, Florida, October 28 − November 2, 2012).

72. M. Hammouri and I. Vasiliev, *Ab Initio Study of the Interactions between Single Vacancies in Graphene*, APS 2013 March Meeting (Baltimore, Maryland, March 18−22, 2013).

73. T. Tawalbeh and I. Vasiliev, *Ab Initio Study of the Interactions between Dopant Atoms and Vacancies in Graphene*, APS 2013 March Meeting (Baltimore, Maryland, March 18−22, 2013).

74. L. Abdallah, T. Tawalbeh, I. Vasiliev, S. Zollner, C. Lavoie, A. Ozcan, and M. Raymond, *Optical Constants of Ni-Pt and Ni-Pt-Si thin films*, AVS 2013 New Mexico Symposium (Albuquerque, New Mexico, May 21, 2013).

75. S. K. Jha, I. V. Magedov, L. V. Frolova, N. G. Kalugin, and I. Vasiliev, *Ab Initio Study of Graphene Functionalized with Benzyne*, APS Four Corners Section Meeting (Denver, Colorado, October 18−19, 2013).

76. S. K. Jha, M. Hammouri, I. V. Magedov, L. V. Frolova, N. G. Kalugin, and I. Vasiliev, *Ab Initio Study of Covalently Functionalized Graphene and Carbon Nanotubes*, APS 2014 March Meeting (Denver, Colorado, March 3−7, 2014).

77. M. Hammouri and I. Vasiliev, *Transport Properties of p-n Junctions Formed in Boron/Nitrogen Doped Carbon Nanotubes and Graphene Nanoribbons*, APS 2014 March Meeting (Denver, Colorado, March 3−7, 2014).

78. S. K. Jha, I. V. Magedov, L. V. Frolova, N. G. Kalugin, and I. Vasiliev, *Ab Initio Study of Graphene Functionalized with Carboxyl Groups and Tetracyanoethylene Oxide*, APS Four Corners Section Meeting (Orem, Utah, October 17−18, 2014).

79. M. Hammouri and I. Vasiliev, *Electronic and Transport Properties of Waved Graphene Nanoribbons*, APS Four Corners Section Meeting (Orem, Utah, October 17−18, 2014).

80. S. K. Jha and I. Vasiliev, *First Principles Study of Chemically Functionalized Graphene*, APS 2015 March Meeting (San Antonio, Texas, March 2−6, 2015).

81. M. Hammouri and I. Vasiliev, *Tuning Magnetism of Zirconium Disulfide Nanoribbons by Strain*, APS Four Corners Section Meeting (Tempe, Arizona, October 16−17, 2015).

82. M. Hammouri, D. Karpov, E. Fohtung, and I. Vasiliev, *Magnetoelectric Coupling Characteristics of the $La_{0.67}Sr_{0.33}MnO_3/PbZr_{0.2}Ti_{0.8}O_3$ (001) Interface*, APS 2016 March Meeting (Baltimore, Maryland, March 14−18, 2016).

83. M. Hammouri, E. Fohtung, R. Harder, V. Lauter, and I. Vasiliev, *First-Principles Study of the $La_{0.67}Sr_{0.33}MnO_3/PbZr_{0.2}Ti_{0.8}O_3$ (001) Interface*, APS Joint Four Corners and Texas Sections Meeting (Las Cruces, New Mexico, October 21−22, 2016).

84. B. Ale Magar, T. N. Lambert, J. Duay, B. Chalamala, and I. Vasiliev, *First-Principles Study of Hydrogen Trapping in Electrolytic Manganese Dioxide*, APS Four Corners Section Meeting (Fort Collins, Colorado, October 20−21, 2017).

85. B. Ale Magar, T. N. Lambert, J. Duay, B. Chalamala, and I. Vasiliev, *Discharge Mechanism of the γ-MnO_2 Electrode in Shallow-Cycled Zn/MnO_2 Batteries: An Ab Initio Study*, APS 2018 March Meeting (Los Angeles, California, March 5−9, 2018).

86. B. Paudel, I. Vasiliev, M. Hammouri, and E. Fohtung, *Ferroelectric Polarization Switching Induced Charge versus Strain Mediated Interfacial Magnetic Phases in Oxide Heterostructures*, APS Four Corners Section Meeting (Salt Lake City, Utah, October 12−13, 2018).

87. T. N. Lambert, J. Duay, M. Kelly, B. Ale Magar, I. Vasiliev, M. B. Lim, D. Arnot, I. V. Kolesnichenko, B. R. Chalamala, *Advances in Alkaline Storage Batteries and their Potential Impact for Society*, World Materials Research Institute Forum (WMRIF Symposium and General Assembly (Budapest, Hungary, June 17−20, 2019).

88. N. Paudel, B. Ale Magar, T. N. Lambert, and I. Vasiliev, *Theoretical Studies of Zinc Contamination of γ-MnO_2 in Deep-Cycled Rechargeable Zn/MnO_2 Batteries*, APS Four Corners Section Meeting (Prescott, Arizona, October 11−12, 2019).

89. K. Acharya and I. Vasiliev, *Ab Initio Studies of Magnetoelectric Coupling at $PbZr_{0.2}Ti_{0.8}O_3$/$La_{0.8}Sr_{0.2}MnO_3$ and $PbZr_{0.2}Ti_{0.8}O_3$/$La_{0.5}Sr_{0.5}MnO_3$ Multiferroic Interfaces*, APS Four Corners Section Meeting (Prescott, Arizona, October 11−12, 2019).

90. N. Paudel, B. Ale Magar, T. N. Lambert, and I. Vasiliev, *Ab Initio Study of the Influence of Structural Defects on the Electrochemical Properties of MnO_2 in Rechargeable Zn/MnO_2 Alkaline Batteries*, APS Four Corners Section Meeting (Albuquerque, New Mexico, October 23−24, 2020).

91. K. Acharya and I. Vasiliev, *Influence of Polarization, Strain, and Doping on the Magnetoelectric Properties of LSMO/PZT Interfaces: An Ab Initio Study*, APS 2021 March Meeting (Online Meeting, March 15−19, 2021).

92. B. Ale Magar, N. Paudel, T. N. Lambert, and I. Vasiliev, *First Principles Studies on the Cycling Mechanism of MnO_2 Modified with Bi, Cu, and Mg in Rechargeable Zn/MnO_2 Batteries*, APS 2021 March Meeting (Online Meeting, March 15−19, 2021).

93. N. Paudel, B. Ale Magar, T. N. Lambert, and I. Vasiliev, *Influence of Surfaces on the Electrochemical Properties of MnO_2 in Rechargeable Zn/MnO_2 Batteries*, APS 2021 March Meeting (Online Meeting, March 15−19, 2021).

Poster Presentations

94. I. Vasiliev, S. Öğüt, and J. R. Chelikowsky, *Ab Initio Optical Excitation Spectra of Quantum Dots*, 10^{th} International Symposium on Small Particles and Inorganic Clusters (Atlanta, Georgia, October 11−15, 2000).

95. I. Vasiliev and R. M. Martin, *Optical Properties of Silicon Dots: the Role of Surfaces*, NSF/DMR Computational Program Review (Urbana-Champaign, Illinois, June 19−20, 2002).

96. N. Al-Aqtash and I. Vasiliev, *Ab Initio Study of Carboxylated Graphene*, APS Four Corners Section Meeting (Golden, Colorado, October 23−24, 2009).

97. N. Al-Aqtash and I. Vasiliev, *Carboxylation of Boron- and Nitrogen-Doped Graphene and Carbon Nanotubes*, NSTI Nanotechnology Conference and Expo 2010 (Anaheim, California, June 21−24, 2010).

98. S. Alnemrat, I. Vasiliev, and H. Wang, *Ab Initio Molecular Metadynamics Study of the Base-Catalyzed Hydrolysis of N-Methylacetamide*, APS Four Corners Section Meeting (Ogden, Utah, October 15−16, 2010).

99. M. Hammouri and I. Vasiliev, *Electronic and Transport Properties of Waved Graphene Nanoribbons*, Penn State University Workshop on 2D Materials, Graphene and Beyond: From Atoms to Applications (University Park, Pennsylvania, May 11−12, 2015)

100. B. Ale Magar, I. Vasiliev, J. Duay, and T. N. Lambert, *Ab Initio Studies of Electrolytic MnO_2 in Shallow-Cycled Rechargeable Zn/MnO_2 Batteries*, DOE OE Energy Storage Peer Review 2018 (Santa Fe, New Mexico, September 25−27, 2018).

101. B. Ale Magar, T. N. Lambert, J. Duay, and I. Vasiliev, *Ab Initio Studies of the Electrochemical Properties of β-, R-, and γ-MnO_2 Polymorphs*, APS Four Corners Section Meeting (Salt Lake City, Utah, October 12−13, 2018).

102. B. Ale Magar, N. Paudel, I. Vasiliev, and T. N. Lambert, *Theoretical Studies of the Electrochemical Properties of Bi- and Cu-Modified delta-MnO_2 Electrodes in Rechargeable Zn/MnO_2 Batteries*, DOE OE Energy Storage Peer Review 2019 (Albuquerque, New Mexico, September 23−26, 2019).

103. B. Ale Magar, N. Paudel, T. N. Lambert, and I. Vasiliev, *Bi- and Cu-Modified δ-MnO_2 Electrodes in Rechargeable Zn/MnO_2 Batteries: An Ab Initio Study*, APS Four Corners Section Meeting (Prescott, Arizona, October 11−12, 2019).

104. B. Ale Magar, N. Paudel, T. N. Lambert, and I. Vasiliev, *Ab Initio Studies of the Cycling Mechanism of MnO_2 Cathodes Modified with Bi, Cu, and Mg in Rechargeable Zn/MnO_2 Batteries*, DOE OE Energy Storage Peer Review 2020 (Albuquerque, New Mexico, September 29 − October 1, 2020).

105. N. Paudel, B. Ale Magar, T. N. Lambert, and I. Vasiliev, *Influence of Surfaces and Structural Defects on the Electrochemical Properties of MnO_2 in Rechargeable Zn/MnO_2 Batteries*, DOE OE Energy Storage Peer Review 2020 (Albuquerque, New Mexico, September 29 − October 1, 2020).

106. B. Ale Magar, N. Paudel, T. N. Lambert, and I. Vasiliev, *Ab Initio Studies of the Phase Transition Mechanism of MnO_2 Modified with Bi, Cu, and Mg in Rechargeable Zn/MnO_2 Batteries*, APS Four Corners Section Meeting (Albuquerque, New Mexico, October 23−24, 2020).

107. K. Acharya and I. Vasiliev, *Ab Initio Study of the Effects of Strain and Doping on the Properties of LSMO/PZT Multiferroic Interfaces*, APS Four Corners Section Meeting (Albuquerque, New Mexico, October 23−24, 2020).

Research Grants and Contracts

Funded Proposals

1. *Agile Response Chameleon Coatings* (with S. A. Curran), U.S. Air Force, 4/2005 − 3/2006, total NMSU award: $430,709, I. Vasiliev's subaward: **$77,099**.

2. *Multiscale Modeling of the Mechanical and Elastic Properties of Nanocrystalline Materials* (with Y. H. Park), NMSU Council of Research Centers Mini-Grant, 9/2005 − 12/2006, **$24,480**.

3. *Effect of Chemical Functionalization on the Raman and Optical Spectra of Carbon Nanotubes* (individual grant), Petroleum Research Fund of the American Chemical Society, 9/2005 − 8/2007, **$35,000**.

4. *Theoretical Characterization of Interfacial Bonding in Self-Assembled Carbon Nanotubes* (individual grant), National Science Foundation, 7/2005 − 6/2008, **$200,000**.

5. *Multiscale Modeling of Core-Shell Nanostructures* (with Y. H. Park), NMSU Interdisciplinary Research Grant, 1/2007 − 12/2007, **$49,814**.

6. *Development of High-Performance Nanomaterials Using Multiscale Modeling* (with Y. H. Park and P. Hynes), U.S. Department of Defense, 9/2007 – 8/2008, **$79,081**.

7. *High Efficiency Cascade Solar Cells* (with S. Deng, R. Schoenmackers, and S. A. Curran), U.S. Department of Energy, 7/2008 – 6/2010, total NMSU award: $974,000, I. Vasiliev's subaward: **$91,952**.

8. *Quantum Dynamics Study of Enzymatic and Non-enzymatic Hydrolysis Reactions* (with H. Wang, A. Piryatinski, and T. C. Germann), NMSU/LANL MOU Program, 8/2008 – 9/2010, **$67,500**.

9. *Core-Shell Heterostructures: Application to Energy Conversion and Solar Power* (individual grant), Petroleum Research Fund of the American Chemical Society, 7/2008 – 8/2011, **$99,701**.

10. *Theoretical Characterization of Functionalized Carbon Nanostructures* (individual grant), National Science Foundation, 7/2011 – 6/2016, **$160,000**.

11. *Nanoscale Semiconductor Heterostructures for Photovoltaic Energy Conversion* (with Y. H. Park), National Aeronautics and Space Administration, 2/2012 – 5/2013, **$44,505**.

12. *Real-Space TDDFT Studies of the Optical Properties of Nanoscale Structures* (individual grant), NMSU College of Arts and Sciences Travel Grant, 12/2015 – 12/2016, **$1,000**.

13. *Theoretical Studies of the Electrochemical Behavior of γ-MnO_2 Cathode Material in Rechargeable Zn/MnO_2 Batteries* (individual grant), Sandia National Laboratories, 8/2017 – 9/2019, **$69,804**.

14. *Theoretical Studies of the Electrochemical Behavior of Solid-State Cathode Materials in Rechargeable Alkaline Zn/MnO_2 and Zn/Cu_2S Batteries* (individual grant), Sandia National Laboratories, 10/2019 – 9/2022, **$167,115**.

Courses Taught

Undergraduate Courses

Physics 454 *Intermediate Modern Physics I*
Physics 461 *Intermediate Electricity and Magnetism I*
Physics 462 *Intermediate Electricity and Magnetism II*
Physics 480 *Thermodynamics*
Physics 488 *Introduction to Condensed Matter Physics*

Graduate Courses

Physics 551 *Classical Mechanics*
Physics 561 *Electromagnetic Theory I*
Physics 562 *Electromagnetic Theory II*
Physics 584 *Statistical Mechanics*
Physics 588 *Condensed Matter Physics*
Physics 688 *Advanced Condensed Matter Physics*

Special courses

Physics 450 *Selected Topics: Condensed Matter Physics*
Physics 620 *Advanced Topics in Density Functional Theory*

Supervised Graduate Students

1. Bharat Medasani — *Ph.D. 2010, Theoretical Calculation of Surface Properties of Silver and Aluminum Nanoparticles*.
2. Nabil Al-Aqtash — *Ph.D. 2011, First Principles Studies of Functionalization and Substitutional Doping of Graphene and Carbon Nanotubes*.
3. Alejandro Lugo-Solis — *Ph.D. 2011, Ab Initio Density Functional Study of the Adsorption of K Atoms and Clusters on Graphene and Carbon Nanotubes*.
4. Tarek Tawalbeh — *Ph.D. 2014, Ab Initio Study of Dopant-Defect Interactions in Graphene Sheets and Graphene Nanoribbons*.
5. Sanjiv Jha — *Ph.D. 2015, First Principles Study of Covalently Functionalized Graphene*.
6. Mahmoud Hammouri — *Ph.D. 2016, First Principles Study of Carbon Nanostructures*.
7. Meera Mohana Varier — *M.S. 2018*
8. Birendra Ale Magar
9. Nirajan Paudel
10. Krishna Acharya

Affiliations and Memberships

American Physical Society
Materials Research Society
The Electrochemical Society

Conferences and Workshops Organized

- Chair of the Focused Session *Application of Pseudopotentials* at the 2003 March Meeting of the American Physical Society (Austin, Texas, March 3–7, 2003).
- Co-organizer of the Fall Teacher Nanotechnology Workshop at New Mexico State University under the New Mexico EPSCoR Nanoscience Initiative K-12 Community Outreach Program (Las Cruces, New Mexico, November 13–15, 2003).
- Chair of the Focused Session *Computational Nanoscience IV: Nanocrystals* at the 2008 March Meeting of the American Physical Society (New Orleans, Louisiana, March 10–14, 2008).
- Chair of the Focused Session *Computational Physics I* at the 2016 Joint Four Corners and Texas Sections Meeting of the American Physical Society (Las Cruces, New Mexico, October 21–22, 2016).

Review and Editorial Work

Journal Referee

Chemical Physics Letters
Journal of Chemical Physics
Journal of Computational Chemistry
Journal of Physical Chemistry
Journal of Physics: Condensed Matter
Journal of Physics D: Applied Physics
Journal of the Electrochemical Society
MRS Communications
New Journal of Physics
Physical Chemistry Chemical Physics
Physical Review A
Physical Review Applied
Physical Review B
Physical Review Letters
Physica Status Solidi
Solid State Communications

Proposal Reviewer

National Science Foundation (Programs: DMR, CHE, CAREER)
U.S. Department of Energy (Program: BES)
American Chemical Society, Petroleum Research Fund
U.S.-Israel Binational Science Foundation

University, College, and Departmental Service

New Mexico State University

Faculty Senate, member, 2012−2015
Faculty Affairs Committee, member, 2013−2015
Scholastic Affairs Committee, member, 2012−2013

College of Arts and Sciences

A & S Faculty Affairs Committee, chair, 2019−2020
A & S Faculty Affairs Committee, member, 2017−2019
ABET and UG Assessment Committee, member, 2020−2021
Engineering Physics Committee, member, 2010−2020
Department Head Search Committee, member, 2009−2010

Physics Department

Curriculum Committee, chair, 2009−2021
Tenure and Promotion Committee, chair, 2015−2016
Tenure and Promotion Committee, member, 2008−2021
Graduate Affairs Committee, member, 2008−2021
Computer Committee, chair, 2002−2012
Computer Committee, member, 2014−2021
Colloquium Committee, chair, 2012
Colloquium Committee, member, 2003−2004
Graduate Recruiting Committee, member, 2002−2005
Faculty Search Committees (3), member, 2002−2003, 2014−2015