Biographical Sketch: N. A. W. Holzwarth (updated 1/8/2017)

Address

Mail: Wake Forest University, Department of Physics, Winston-Salem, NC 27109-7507
Email: natalie@wfu.edu
Phone: (336)-758-5510 (Office) (336)-758-6241 (Fax)
Web: www.wfu.edu/~natalie

Professional Preparation

Undergraduate: M. I. T. 1964-1967; BS degree in Chemical Physics, June 1967.
Graduate: U. Chicago 1967-1974; PhD degree in Physics, June 1975.

Appointments

1983-Present: Professor of Physics, Wake Forest University (joined faculty in 9/83 as Assistant Professor of Physics)
1982–1983: Postdoctoral research under Professor Melvin Lax, Department of Physics, City College of New York
1980-1982: Research Physicist, Theoretical Sciences Group, Exxon Research and Engineering Company
1975-1980: Postdoctoral research under Professors L. A. Girifalco, S. Rabii, P. Soven, and S. G. Louie in the Departments of Metallurgy and Materials Science, Physics, and Electrical Engineering at the University of Pennsylvania
1974-1975: Postdoctoral research under Professor M. J. G. Lee, Department of Physics, University of Toronto

Publications (since 2003)

1. N.A.W. Holzwarth, "Li_4SnS_4: Simulations of Its Structure and Electrolyte Properties" Electrochemical Society Transactions **73** 231-240 (2016); dx.doi.org/10.1149/07301.0231ecst
2. Jason Howard and N.A.W. Holzwarth, "First principles simulations of the porous layered calcogenides $Li_{2+x}SnO_3$ and $Li_{2+x}SnS_3$", Phys. Rev. B **94**, 064198 (2016); http://dx.doi.org/10.1103/PhysRevB.94.064108
3. Ahmad Al-Qawasmeh and N.A.W. Holzwarth, " Computational Study of Li Ion Electrolytes Composed of Li_3AsS_4 Alloyed with Li_4GeS_4", Journal of the Electrochemical Society **163**, A2079-A2088 (2016); http://dx.doi.org/10.1149/2.1131609jes
4. Larry E. Rush Jr. and N. A.W. Holzwarth, "First principles investigation of the Structural and electrolyte properties of $Na_4P_2S_6$ and $Li_4P_2S_6$", Solid State Ionics **286**, 45-50 (2016)
5. N. D. Lepley and N. A. W. Holzwarth, "Modeling interfaces between solids: Application to Li battery materials", Phys. Rev. B **92** 214201 (2015)
6. Zachary D. Hood, Cameron Kates, Melanie Kirkham, Shiba Adhikari, Chengdu Liang, and N. A. W. Holzwarth, "Structural and electrolyte properties of $Li_4P_2S_6$" Solid State Ionics **284**, 61-70 (2015)
7. M. D. Johannes and N. A. W. Holzwarth, "Crystalline Inorganic-Solid Electrolytes: Computer Simulations and comparisons with experiment" in Chapter 6, pp. 191 - 232 of **Handbook of Solid State Batteries**, 2nd Edition, Nancy J. Dudney, William C. West, and Jagjit Nanda

Editors, World Scientific (2016); ISBN 978-981-4651-89-9
8. Jacilynn A. Brant, Danielle M. Massi, N. A. W. Holzwarth, Joseph H. MacNeil, Alexios P. Douvalis, Thomas Bakas, Steve W. Martin, Michael D. Gross, and Jennifer A. Aitken, -- "Fast Lithium Ion Conduction in Li_2SnS_3: Synthesis, Physicochemical Characterization, and Electronic Structure" *Chemistry of Materials* **27**, 189-196 (2015) http://pubs.acs.org/doi/10.1021/cm5037524
9. N. A. W. Holzwarth, -- "First Principles Modeling of Electrolyte Materials in All-Solid-State Batteries" *Physics Procedia* **57** 29-37 (2014) http://dx.doi.org/10.1016/j.phpro.2014.08.127
10. Chaochao Dun, N. A. W. Holzwarth, Yuan Li, Wenxiao Huang, and David L. Carroll, -- "$Cu_2ZnSnS_xO_{4-x}$ and $Cu_2ZnSnS_xSe_{4-x}$: First principles simulations of optimal alloy configurations and their energies" -- *Journal of Applied Physics* **115**, 193513 (2014) http://scitation.aip.org/content/aip/journal/jap/115/19/10.1063/1.4876447
11. François Jollet and Marc Torrent (CEA, France) and Natalie Holzwarth, -- "Generation of Projector Augmented-Wave atomic data: A 71 element validated table in the XML format" -- *Computer Physics Communications* **185**, 1246-1254 (2014) http://www.sciencedirect.com/science/article/pii/S0010465513004359
12. Nicholas Lepley, Yaojun A. Du, and N. A. W. Holzwarth, "Structures, Li^+ mobilities, and interfacial properties of solid electrolytes Li_3PS_4 and Li_3PO_4 from first principles" -- *Phys. Rev. B* **88**, 104103 (2013) http://link.aps.org/doi/10.1103/PhysRevB.88.104103
13. Keerthi Senevirathne, Cynthia S. Day, Michael D. Gross, Abdessadek Lachgar, and N. A. W. Holzwarth, "A new crystalline LiPON electrolyte: Synthesis, properties, and electronic structure" -- *Solid State Ionics* **233**, 95-101 (2013) http://dx.doi.org/10.1016/j.ssi.2012.12.013
14. N. D. Lepley and N. A. W. Holzwarth, "Computer Modeling of Crystalline Electrolytes -- Lithium Thiophosphates and Phosphates" -- *J. Electrochem. Soc.* **159**, A538-A547 (2012) http://dx.doi.org/10.1149/2.jes113225
15. Xiao Xu and N. A. W. Holzwarth, "Adaptation of the Projector Augmented Wave (PAW) formalism to the treatment of orbital-dependent exchange-correlation functionals" - *Phys. Rev. B* **84** 155113 (16 pages) (2011) http://link.aps.org/doi/10.1103/PhysRevB.84.155113
16. N. A. W. Holzwarth and Xiao Xu, "Analysis of numerical methods for evaluating the Fock exchange integral in a plane wave basis" -- *Phys. Rev. B* **84** 113102 (4 pgs; brief report) (2011) http://link.aps.org/doi/10.1103/PhysRevB.84.113102
17. N. D. Lepley and N. A. W. Holzwarth, "Computer Modeling of Crystalline Electrolytes -- Lithium Thiophosphates and Phosphates" -- *ECS Transactions* **35** (14) 39-51 (2011) http://dx.doi.org/10.1149/1.3644902
18. N. A. W. Holzwarth, N. D. Lepley, and Yaojun A. Du, "Computer Modeling of Lithium Phosphate and Thiophosphate Electrolyte Materials " -- *Journal of Power Sources* **196** 6870-6876 (2011) http://dx.doi.org/10.1016/j.jpowsour.2010.08.042
19. Marc Torrent, N. A. W. Holzwarth, Francois Jollet, David Harris, Nicholas Lepley, and Xiao Xu, "Electronic structure packages: Two implementations of the projector augmented wave (PAW) formalism" -- *Computer Physics Communications* **181** 1862-1867 (2010) http://dx.doi.org/10.1016/j.cpc.2010.07.036
20. Yaojun A. Du and N. A. W. Holzwarth, "First-principles study of LiPON and related solid

electrolytes" -- *Phys. Rev. B*, **81** 184106 (15pp) (2010) http://prb.aps.org/abstract/PRB/v81/i18/e184106

21. Xiao Xu and N. A. W. Holzwarth, "A projector augmented wave (PAW) formulation of Hartree-Fock calculations of electronic structure" -- *Phys. Rev. B* **81** 245105 (14pp) (2010) http://link.aps.org/doi/10.1103/PhysRevB.81.245105
22. Yaojun A. Du and N. A. W. Holzwarth, "First principles simulations of Li ion migration in materials related to LiPON electrolytes" -- *ECS Transactions* **25** (36) 27-36 (2010) http://dx.doi.org/10.1149/1.3393837
23. Yaojun A. Du and N. A. W. Holzwarth, "Effects of O vacancies and N or Effects of O vacancies and N or Si substitutions on Li^+ migration in Li_3PO_4 electrolytes from first principles" -- *Phys. Rev. B* **76**, 174301 (2008) http://link.aps.org/abstract/PRB/v78/e174301
24. Yaojun A. Du and N. A. W. Holzwarth, "Li ion migration in Li_3PO_4 electrolytes: Effects of O vacancies and N substitutions" -- *ECS Transactions* **13** (26) 75-82 (2008) http://dx.doi.org/10.1149/1.3050379
25. Yaojun A. Du and N. A. W. Holzwarth, "Mechanisms of Li^+ diffusion in crystalline γ- and β-Li_3PO_4 electrolytes from first principles" -- *Phys. Rev. B* **76**, 174302 (2007) http://link.aps.org/abstract/PRB/v76/e174302
26. Yaojun A. Du and N. A. W. Holzwarth, "Li ion diffusion mechanisms in the crystalline electrolyte γ-Li_3PO_4" -- *Journal of the Electrochemical Society* **155**, A999 (2007) http://dx.doi.org/10.1149/1.3050379
27. Ping Tang, N. A. W. Holzwarth, and Yaojun A. Du, "Comparison of the electronic structures of four crystalline phases of $FePO_4$" -- *Phys. Rev. B.* **76**, 174118 (2007) http://link.aps.org/abstract/PRB/v76/e174118
28. Yonas Abraham and N. A. W. Holzwarth, "A method for calculating electronic structures near surfaces of semi-infinite crystals" -- *Phys. Rev. B* **73**, 035412 (2006) http://prb.aps.org/abstract/PRB/v73/i3/e035412
29. Ping Tang and N. A. W. Holzwarth, "Electronic structure of $FePO_4$, $LiFePO_4$, and related materials" -- Phys. Rev. B **68**, 165107 (2003) http://prb.aps.org/abstract/PRB/v68/i16/e165107

Invited presentations (since 2003)

1. Talk presented by N. A. W. Holzwarth at the International Material Research Congress, August 15-19, 2016 Cancun, Mexico. "Simulations of Idealized Solid Electrolytes"
2. Talk presented by N. A. W. Holzwarth at Sandia National Laboratory in Albuquerque, NM at the invitation of Kevin Leung -- June 3, 2015 "Simulations of Idealized Solid Electrolytes for Solid State Battery Designs"
3. Talk presented by N. A. W. Holzwarth at the Joint School of Nanoscience and Nanoengineering in Greensboro at the invitation of professor Sung-Jin Cho -- January 16, 2015 "Overview of Computer Simulation Methods Used to Study and Design New Materials: Examples from the Study of Solid Electrolytes"
4. Invited talk by N. A. W. Holzwarth at the 27th Annual CSP Workshop February 24-28, 2014 in Athens, GA, USA – "First principles modeling of electrolyte materials in all-solid-state batteries"
5. Presentation by N. A. W. Holzwarth at the CFCAM meeting "Pseudopotentials and PAW

atomic data: beyond a ""black art""?" January 28-29, 2014 at the Ecole National Superieure de Chimie de Paris, Paris, France; organized by F. Jollet, J. J. Mortensen, and G. Rignanese. -- Introduction to generating PAW Atomic Datasets

6. Invited talk presented by N. A. W. Holzwarth at the 6th International ABINIT Developer Workshop in Dinard, France April 15-18, 2013 -- Comments on Generating and Testing PAW Datasets
7. Talk presented by N. A. W. Holzwarth at Oak Ridge National Laboratory at the invitation of Dr. Paul Kent -- March 11, 2013 "Design and Synthesis of a Crystalline LiPON Electrolyte"
8. Talk presented by N. A. W. Holzwarth at the Duquesne University at the invitation of Professor Jennifer Aitken, Department of Chemistry and Biochemistry -- October 19, 2012 "Solid electrolytes for battery applications -- a theoretical perspective"
9. Talk presented by N. A. W. Holzwarth at the University of Louisville at the invitation of Professor Yongsheng Lian, Mechanical Engineering Department and the Conn Center for Renewable Energy Research -- April 6, 2012 -- "Solid electrolytes for battery applications -- a theoretical perspective"
10. Talk presented by N. A. W. Holzwarth for WFU's Center for Energy, Environment, and Sustainability -- Renewable Energy Research (CEES-RER) Sept. 30, 2011 -- Solid electrolytes for battery applications -- a theoretical perspective
11. Invited talk presented by N. A. W. Holzwarth at the 5th International Abinit Developer Workshop in Han-sur-Lesse, Belgium April 11-15, 2011 -- The ATOMPAW Generator
12. Invited talk presented by N. A. W. Holzwarth at 7th Canadian Computational Chemistry Conference July 20-24, 2009 , Dalhousie University in Halifax, Nova Scotia -- A Projector Augmented Wave Formulation of the Optimized Effective Potential Formalism
13. Invited talk presented by N. A. W. Holzwarth at "Workshop on Pseudopotentials and the Quantum Theory of Materials" in Austin, TX Apr. 9-11 2008 in honor of J. R. Chelikowsky -- Simulations of Li ion diffusion in the electrolyte material -- Li_3PO_4
14. Invited talk presented by N. A. W. Holzwarth at 74th Annual Meeting of the Southeastern Section of the APS in Nashville, November 2007 -- Simulations of Li ion diffusion in the electrolyte Li_3PO_4
15. Invited talk presented by N. A. W. Holzwarth at the CEACAM workshop -- Lyon, France -- June 12-14, 2006: State of the art, developments and perspectives of electronic structure calculations in the frame of the Projector Augmented-Wave (PAW) method

Seminar or colloquium presentations and contributed presentations at meetings and workshops by N. A. W. Holzwarth and collaborators (from last 10 years)

1. Poster presented by N. A. W. Holzwarth at the 18th International Meeting on Lithium Batteries, June 19-24, 2016 in Chicago, IL. Li_4SnS_4: Simulations of Its Structure and Electrolyte Properties
2. Talk presented by Larry Rush, Jr. at the March 2016 Meeting of the American Physical Society, March 14-18, 2016 in Baltimore, MD. First principles investigation of the structural and electrochemical properties of $Na_4P_2S_6$ and $Li_4P_2S_6$
3. Talk presented by Jason Howard at the March 2016 Meeting of the American Physical Society, March 14-18, 2016 in Baltimore, MD. Computational study of $Li_{2+x}SnO_3$ and

$Li_{2+x}SnS_3$

4. Talk presented by Ahmad Al-Qawasmeh at the March 2016 Meeting of the American Physical Society, March 14-18, 2016 in Baltimore, MD. Computational study of Li ion electrolytes composed of Li_3AsS_4 alloyed with Li_4GeS_4
5. Talk presented by N. A. W. Holzwarth (based on work of Nicholas Lepley) at the March 2016 Meeting of the American Physical Society, March 14-18, 2016 in Baltimore, MD. A formalism for modeling solid electrolyte/electrode interfaces using first principles methods
6. Talk presented by Jason Howard at the 228th ECS Meeting, October 11-15, 2015 in Phoenix, AZ. "Computational Study of Li_2SnO_3 and Li_2SnS_3".
7. Talk presented by N. A. W. Holzwarth at the 228th ECS Meeting, October 11-15, 2015 in Phoenix, AZ. "Electrolyte properties of $Li_4P_2S_6$ -- Simulations and comparison with experiment; Constrast with simulations of Na analog", in collaboration with Z. D. Hood, M. J. Kirkham, and L. E. Rush, Jr..
8. Undergraduate honors thesis by Hannah Zhang, in partial fulfillment of the Wake Forest University requirements for graduation with Honors in Physics (May 2015) -- "Computational Modeling of Li Diffusion Using Molecular Dynamics" .
9. Contributed talk presented by Nicholas Lepley at the March Meeting 2015 of the American Physical Society March 2-6, 2015 in San Antonio, Texas. Modeling Electrolyte-Electrode interfaces with co-author N. A. W. Holzwarth
10. Contributed talk presented by N. A. W. Holzwarth at the March Meeting 2015 of the American Physical Society March 2-6, 2015 in San Antonio, Texas. Structure and interface properties of the electrolyte material $Li_4P_2S_6$ with co-authors Zachary D. Hood (Oak Ridge National Laboratory) and Cameron M. Kates (currently at Duke U.).
11. Contributed poster presented by Nicholas Lepley at 2014 summer school on Transformational Technologies in Molecular Simulations held at University of Wisconsin-Madison, Madison, WI May 19-22, 2014 -- Modeling the Interface of Lithium Metal and Lithium Solid Electrolytes with First Principles calculations.
12. Contributed poster presented by Chaochao Dun at the 26th Annual Workshop on Recent Developments in Electronic Structure Methods held at the University of North Texas, May 18-21, 2014 -- First principles simulations of $Cu_2ZnSnS_xO_{4-x}$ alloys.
13. Undergraduate honors thesis by James Drewery, in partial fulfillment of the Wake Forest University requirements for graduation with Honors in Physics -- Modeling Materials: Comparison of Two Projector-Augmented Wave (PAW) Datasets.
14. Undergraduate honors thesis by Cameron Kates, in partial fulfillment of the Wake Forest University requirements for graduation with Honors in Physics -- Computational Modeling of Surface Energy and Structural Behavior of $Li_4P_2S_6$ Electrolytic Solid Interfacing with Lithium Anodes.
15. Contributed talk presented by Chaochao Dun (in collaboration with N. A. W. Holzwarth, Y. Li, W. Huang, and D. Carroll) APS March Meeting 2014, Denver, Colorado Mar. 3 - 7, 2014 -- $Cu_2ZnSnS_xO_{4-x}$ and $Cu_2ZnSnS_xSe_{4-x}$: First principles simulations of optimal alloy configurations and their energies
16. Contributed talk presented by N. A. W. Holzwarth (with content from N. D. Lepley, A. Al-

Qawasmeh, and C. Kates) at the APS March Meeting 2014, Denver, Colorado Mar. 3 - 7, 2014 -- First principles modeling of lithium (thio) phosphate solid electrolytes and lithium metal anodes

17. Contributed talk presented by N. A. W. Holzwarth (with content from N. D. Lepley and A. Al-Qawasmeh) at the 224th ECS Meeting, in San Francisco, CA, Oct. 27-Nov. 1, 2013 -- First principles modeling of electrolyte/anode interfaces in an all-solid state battery -- γ-Li_3PS_4/Li
18. Contributed poster presented by N. A. W. Holzwarth (with content from N. D. Lepley) at the The 25th Annual Workshop on Recent Developments in Electronic Structure Methods held at the College of William and Mary, June 11-14, 2013 -- First principles modeling of the interface between a solid state lithium thiophosphate electrolyte and a lithium metal anode
19. Contributed talk presented by N. A. W. Holzwarth (in collaboration with K. Senevirathne, C. Day, A. Lachgar, and M. Gross) at the APS March Meeting 2013 in Baltimore, MD, Mar. 18 - Mar. 22, 2013 -- Design and synthesis of a crystalline LiPON electrolyte
20. Contributed talk presented by Nicholas Lepley (in collaboration with N. A. W. Holzwarth) at the APS March Meeting 2013 in Baltimore, MD, Mar. 18 - Mar. 22, 2013 -- Surface Structure and Stability in Li_3PS_4 and Li_3PO_4 Electrolytes from First Principles
21. Poster presented by N. Lepley at the ES12: 24th Annual Meeting of the Electronic Structure Workshop -- June 5-8, 2012 -- Computer Modeling of Crystalline Electrolytes - Lithium Thiophosphates and Phosphates.
22. Poster presented by N. Holzwarth at the ES12: 24th Annual Meeting of the Electronic Structure Workshop -- June 5-8, 2012 -- First Principles Computer Simulations of $Li_{10}GeP_2S_{12}$ and Related Lithium Superionic Conductors.
23. Contributed talk presented by N. A. W. Holzwarth at the APS March Meeting 2012 in Boston, MA, Feb. 27 - Mar. 2, 2012 -- First principles computer simulations of $Li_{10}GeP_2S_{12}$ and related lithium superionic conductors
24. Contributed talk presented by Nicholas Lepley at the APS March Meeting 2012 in Boston, MA, Feb. 27 - Mar. 2, 2012 -- First principles investigation of the superionic electrolyte $Li_7P_3S_{11}$
25. Contributed talk presented by Xiao Xu at the APS March Meeting 2012 in Boston, MA, Feb. 27 - Mar. 2, 2012 -- Projector Augmented Wave formulation of orbital-dependent exchange-correlation functionals
26. Poster presented by N. A. W. Holzwarth and N. Lepley at The 15th International Meeting on Lithium Batteries in Montreal, Canada June 27 - July 2, 2010 -- Computer Modeling of Lithium Phosphate and Thiophosphate Electrolyte Materials
27. Poster presented by Xiao Xu at 22nd Annual Workshop on Electronic Structure Methods at the University of Texas - Austin, June 7-10, 2010 -- Projector augmented wave (PAW) formulation of Hartree-Fock calculations of electronic structure -- HF-PAW
28. Poster presented by N. A. W. Holzwarth at 22nd Annual Workshop on Electronic Structure Methods at the University of Texas - Austin, June 7-10, 2010 -- Two implementations of the Projector Augmented Wave (PAW) formalism
29. Talk presented by N. A. W. Holzwarth at 2010 APS March Meeting in Portland, OR March 2010 -- "Prediction of a New Material -- Lithium Phosphorus Oxynitride Li_2PO_2N"
30. Talk presented by N. A. W. Holzwarth at 216th Biannual Meeting of the Electrochemical Society Meeting October 4-9, 2009 in Vienna, Austria -- First principles simulations of Li ion migration in materials related to LiPON electrolytes
31. Poster presented by N. A. W. Holzwarth at 21th Annual Workshop on Recent

Developments in Electronic Structure Methods at the University of California Davis campus, June 22-25, 2009 -- Simulations of Li-ion migration in LiPON electrolytes

32. Talk presented by Yaojun Du at 2009 APS March Meeting in Pittsburgh, PA, March 2009 -- First-principles simulations of extended structures in the lithium phosphorous oxynitride electrolytes
33. Talk presented by Xiao Xu at 2009 APS March Meeting in Pittsburgh, PA, March 2009 -- Implementation of the Optimized Effective Potential Method within the Projector Augmented Wave Scheme
34. Poster presented by Xiao Xu at 20th Annual Workshop on Recent Developments in Electronic Structure Methods in the University of Illinois at Urbana-Champaign, June 17-20, 2008 -- "Projector Augmented Wave Formulation of Optimized Effect Potential Density Functional Theory -- PAW-OEP"
35. Talk presented by Yaojun Du at 213th Biannual Meeting of the Electrochemical Society in Phoenix, AZ May 18-22, 2008 -- "Li ion migration in Li_3PO_4 electrolytes: Effects of O vacancies and N substitutions"
36. Talk presented by N. A. W. Holzwarth at 2008 APS March Meeting in New Orleans, LA, March 2008 -- Simulation of Li ion diffusion near electrolyte-metal interface -- Li_3PO_4 and Li
37. Poster presented by William Hodge at 2008 APS March Meeting in New Orleans, LA, March 2008 -- The One-Hole, One-Dimensional Hubbard Model at $U = \infty$
38. Poster presented by Xiao Xu at 19th Annual Workshop on Recent Developments in Electronic Structure Methods in Raleigh, NC June 2007 -- Projector Augmented Wave Formulation of Exact Exchange Density Functional Theory -- PAW-EXX
39. Poster presented by Yaojun Du at 19th Annual Workshop on Recent Developments in Electronic Structure Methods in Raleigh, NC June 2007 -- Li ion diffusion mechanisms in Li_3PO_4 electrolytes
40. Talk presented by Xiao Xu at March 2007 APS meeting in Denver -- Simulated electrolyte-metal interfaces -- Li_3PO_4 and Li
41. Talk presented by Dr. Yaojun Du at March 2007 APS meeting in Denver -- Li-ion diffusion mechanisms in crystalline Li_3PO_4 electrolytes
42. Poster presented by William Hodge at March 2007 APS meeting in Denver -- Pair State Analysis of the Hubbard Hamiltonian in One-Dimension

Ph. D. Thesis Students (from last 10 years)

1. Nicholas D. Lepley – Ph. D. December 2015 – "First Principles Investigations of Solid-Solid Interfaces in Lithium Battery Materials"
2. Xiao Xu – Ph. D. August 2011 – "Orbital Dependent Functionals: An Atom Projector Augmented Wave Method Implementation"
3. William Hodge – Ph. D. August 2008 (also mentored by W. C. Kerr) – "Exact and variational investigations of Hubbard rings"
4. Kevin Conley – Ph. D. May 2008 – "A Dirac all-electron basis and spin-orbit coupled project implementation of the projector augmented wave method for atomic systems"
5. Ping Tang – Ph. D. August 2006 – "Computational research on lithium ion battery materials"
6. Yonas Abraham – Ph. D. December 2004 (also mentored by R. T. Williams) – "Electronic states near surfaces – a)Analysis of calculation methods using semi-infinite boundary conditions; b) Sensitive detection using laser photoelectron spectroscopy

Other professional activities

1. Together with colleagues Timo Thonhauser and Akbar Salam formed the local organizing committee for ES12: The *24th Annual Workshop on Recent Developments in Electronic Structure Theory*, held June 5-8, 2012 at Wake Forest University in Winston-Salem, NC 27109.

Grant funding (from last 10 years)

1. NSF DMR-1507942: Computational studies of solid electrolytes – 09/01/2015-08/31/2018 -- $300,000 (projected)
2. NSF DMR-1105485: First principles simulations of battery materials -- 09/01/2011-08/31/2015 -- $300,000
3. NSF DMR-0705239: First Principles Simulations of Battery Materials -- 12/15/2007-11/30/2011 -- $225,000
4. NSF DMR-0427055: ITR - Computational Tools for Detailed Simulations of Materials -- 09/01/2004-08/31/2010 -- $336,000
5. NSF DMR-0405456: Computational Study of Transition Metal Phosphate Materials -- 08/01/2004- 07/31/2008 -- $143,000