Biographical Sketch: N. A. W. Holzwarth (updated 8/22/2021)

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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. "Computational study of Li_3BO_3 and Li_3BN_2 I: Electrolyte properties of pure and doped crystals and II: Stability analysis of pure phases and of model interfaces with Li anodes", Yan Li, Zachary D. Hood, and N.A.W. Holzwarth, Physical Review Materials 5 , 085402 (2021) (I) and Physical Review Materials 5 , 085403 (2021) (II) https://doi.org/10.1103/PhysRevMaterials.5.085402 and https://doi.org/10.1103/PhysRevMaterials.5.085403
2. N. Brouwer, V. Recoules, N. Holzwarth, and M. Torrent, "Calculation of optical properties with spin-orbit coupling for warm dense matter", Computer Physics Communications 266, 108029 (2021) https://doi.org/10.1016/j.cpc.2021.108029
3. Yan Li, Zachary D. Hood, and N.A.W. Holzwarth, "Computational and experimental (re)investigation of the structural and electrolyte properties of $Li_4P_2S_6$, and $Na_4P_2S_6$, and $Li_2Na_2P_2S_6$", Physical Review Materials **4**, 045406 (2020) https://link.aps.org/doi/10.1103/PhysRevMaterials.4.045406
4. Yan Li, W. C. Kerr, and N. A. W. Holzwarth, "Continuity of phonon dispersion curves in layered ionic materials", J. Phys.: Condens. Matter **32**, 055402 (2020); https://iopscience.iop.org/article/10.1088/1361-648X/ab4cc1/pdf
5. N. A. W. Holzwarth, "Updated comments on projector augmented wave (PAW)

implementations within various electronic structure code packages", *Computer Physics Communications* **234**, 25-29 (2019); https://doi.org/10.1016/j.cpc.2019.05.009

6. Jason David Howard and N. A. W. Holzwarth, "First-principles estimation of partition functions representing disordered lattices such as the cubic phases of Li2OHCl and Li_2OHBr", *Physical Review B* **99,** 014109 (2019); https://doi.org/10.1103/PhysRevB.99.014109
7. Jason David Howard and N. A. W. Holzwarth "Analysis of the statistical and convergence properties of ionic transport coefficients with application to the solid electrolyte Li_2OHCl", *Solid State Ionics* **325** 80-89 (2018); https://doi.org/10.1016/j.ssi.2018.07.025
8. Jason Howard, Zachary D. Hood, and N. A. W. Holzwarth, "Fundamental aspects of the structural and electrolyte properties of Li_2OHCl from simulations and experiment", *Physical Review Materials* **1** 075406 (2017); https://link.aps.org/doi/10.1103/PhysRevMaterials.1.075406
9. Larry E. Rush, Jr., Zachary D. Hood, and N. A. W. Holzwarth, "Unraveling the electrolyte properties of Na_3SbS_4 through computation and experiment", *Physical Review Materials* **1** 075405 (2017); https://link.aps.org/doi/10.1103/PhysRevMaterials.1.075405
10. Ahmad Al-Qawasmeh and N.A.W. Holzwarth, "$Li_{14}P_2O_3N_6$ and Li_7PN_4: Computational study of two nitrogen rich crystalline LiPON electrolyte materials" *Journal of Power Sources* **364** 410-419 (2017); https://doi.org/10.1016/j.jpowsour.2017.08.025
11. Ahmad Al-Qawasmeh, Jason Howard, and N.A.W. Holzwarth, "Li_4SnS_4 and Li_4SnSe_4: Simulations of Their Structure and Electrolyte Properties", J. Electrochem. Soc. **164** A6386-A6394 (2017); http://dx.doi.org/10.1149/2.0581701jes
12. 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
13. 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
14. 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
15. 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)
16. N. D. Lepley and N. A. W. Holzwarth, "Modeling interfaces between solids: Application to Li battery materials", Phys. Rev. B **92** 214201 (2015)
17. 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)

18. 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
19. 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
20. 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
21. 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
22. 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
23. 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
24. 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
25. 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
26. 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
27. 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
28. 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
29. 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

30. 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
31. 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
32. 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
33. 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
34. 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
35. 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
36. 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
37. 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
38. 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
39. 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
40. 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. Presentation by N. A. W. Holzwarth at the Electronic Structure Discussion Group at Cambridge University invited by WFU alum Angela Harper -- June 9, 2021 -- First principles simulations of electrolyte materials with a view toward all solid-state battery

technology -- $Li_4P_2S_6$, $Na_4P_2S_6$, and possible alloys

2. Invited presentation by N. A. W. Holzwarth at Wake's CFM (Center for Functional Materials) Seminar Series, Dec. 4, 2019 -- "First principles simulations of idealized known and unknown crystalline materials".
3. Invited presentation by N. A. W. Holzwarth at Duke University's MEMS Seminar Series, invited by Olivier Delaire, " Nov. 6, 2019 -- "Computational Investigation of the Structural and Electrolyte Properties of $Li_4P_2S_6$, $Na_4P_2S_6$, and $Li_2Na_2P_2S_6$"
4. Presentation by N. A. W. Holzwarth at the Workshop on Precision Quantification in DFT May 23-24, 2019 in Louvain la Neuve, Belgium – "Assessment of Accuracy and Efficiency of PAW Datasets in Materials Simulations"
5. Presentation by N. A. W. Holzwarth at the HybriD^3 Theory Training Workshop at Duke University, organized by Volker Blum (Duke) and Yosuke Kanai (UNC) Sept. 28-29, 2018 -- "Practical Density Functional Theory with Plane Waves"
6. Invited talk presented by N. A. W. Holzwarth at the 2018 Electronic Structure Workshop, at the University of Pennsylvania, Philadelphia PA. June 10-14, 2018 -- "Perspectives on the Projector Augmented Wave Method (PAW)"
7. Invited talk presented by N. A. W. Holzwarth at the SSI: 21st International Conference on Solid State Ionics, Padua, Italy, June 18-23,2017 -- "Simulations of Idealized Solid Electrolytes"
8. Invited talk presented by N. A. W. Holzwarth at the EMCMRE-4: 4th Euro-Mediterranean Conference on Materials and Renewable Energies, Marrakech, Morocco May 8-11, 2017. "Simulations of Idealized Solid Electrolytes"
9. Talk presented by N. A. W. Holzwarth at the International Material Research Congress, August 15-19, 2016 Cancun, Mexico. "Simulations of Idealized Solid Electrolytes"
10. 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"
11. 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"
12. 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"
13. 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
14. 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
15. 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"
16. 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"

17. 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"
18. 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
19. 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
20. 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
21. 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
22. 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
23. 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. Presentation by N. A. W. Holzwarth at the 10th ABINIT International Developer Workshop May 31-June 4, 2021 -- Progress on self-consistent meta-gga PAW datasets from ATOMPAW (PP slides)
2. Presentation by Yan Li at the March 2021 APS meeting -- "Li_3BO_3 and Li_3BN_2: Computational study of structural and electrolyte properties of pure and doped crystals" (link to abstract)
3. Annotated slides that would have been presented by Yan Li at the cancelled March 2020 APS meeting -- "Prediction and analysis of a sodium ion electrolyte: $Li_2Na_2P_2S_6$"
4. Annotated slides that would have been presented by N. A. W. Holzwarth at the cancelled March 2020 APS meeting -- "Continuity of Phonon Dispersion Curves of Anisotropic Ionic Materials"
5. Presentation by Yan Li at the 236th Meeting of the Electrochemical Society in Atlanta, Ga Oct. 13-17, 2019. Computational (Re)investigation of the Structural and Electrolyte Properties of $Li_4P_2S_6$, $Na_4P_2S_6$, and $Li_2Na_2P_2S_6$
6. Poster by Yan Li at the 2019 Workshop on Recent Developments in Electronic Structure at the University of Illinois in Champaign-Urbana, Illinois May 20-22, 2019 Computational Reinvestigation of the Structural and Electrolyte Properties of $Li_4P_2S_6$ and $Na_4P_2S_6$
7. Contributed talk presented by Yan Li at the March 2019 Meeting of the American Physical Society, March 4-8, 2019 in Boston, MA Computational and experimental investigation of

$Na_4P_2S_6$ as a promising solid electrolyte material for sodium metal batteries

8. Contributed talk presented by Jason Howard at the March 2018 Meeting of the American Physical Society, March 6-9, 2018 in Los Angeles, CA Understanding the phase properties of Li_2OHCl, $Li_2(OH)_{1-x}F_xCl$, and Li_2OHBr with first principles simulations.
9. Contributed talk presented by N. A. W. Holzwarth on behalf of Ahmad Al-Qawasmeh at the March 2018 Meeting of the American Physical Society, March 6-9, 2018 in Los Angeles, CA Computational Study of the Solid Electrolyte Li_4PS_4I and Related Materials
10. Eight minute talk presented by Natalie Holzwarth at the New Ideas Series from the Dean of the College of Wake Forest University, February 22, 2018 in the WFU Library Auditorium -- "Simulations of materials -- focusing on electrolytes for all solid state batteries"
11. Poster contributed by Jason Howard and Zachary Hood at the 232nd Meeting of the Electrochemical Society Oct. 1-5, 2017 in National Harbor, MD -- Structural and Electrolyte Properties of Li_2OHCl
12. Poster contributed by Jason Howard at the 29th Annual Workshop on Recent Developments in Electronic Structure Methods June 25-28, 2017 at Princeton University -- First Principles Simulations of $Li_2(OH)Cl$
13. Poster contributed by Ahmad Al-Qawasmeh at the 29th Annual Workshop on Recent Developments in Electronic Structure Methods June 25-28, 2017 at Princeton University -- $Li_{14}P_2O_3N_6$: Computational study of a possible new electrolyte for Li ion batteries
14. Talk presented by Jason Howard at the March 2017 Meeting of the American Physical Society, March 13-17, 2017 in New Orleans, LA DFT simulations of Li-ion conductor $Li_2(OH)Cl$
15. Talk presented by Ahmad N. Al-Qawasmeh at the March 2017 Meeting of the American Physical Society, March 13-17, 2017 in New Orleans, LA $Li_{14}(PON_3)_2$: Computational study of a possible new electrolyte for Li ion batteries.
16. Talk presented by Larry Rush, Jr. at the March 2017 Meeting of the American Physical Society, March 13-17, 2017 in New Orleans, LA Computational Study of Ideal Electrolyte/Anode Interface for Na_3SbS_4/Na.
17. 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
18. 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 $Li_4P_2S_6$
19. 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 $Li_{2+x}SnS_3$
20. 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
21. 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

22. 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".
23. 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..
24. 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" .
25. 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
26. 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.).
27. 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.
28. 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.
29. 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.
30. 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.
31. 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
32. 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
33. 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

34. 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
35. 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
36. 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
37. 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.
38. 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.
39. 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
40. 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 $Li_7P_3S_{11}$
41. 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
42. 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
43. 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
44. 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
45. 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"
46. 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
47. 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
48. 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
49. 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

50. 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"
51. 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"
52. 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
53. Poster presented by William Hodge at 2008 APS March Meeting in New Orleans, LA, March 2008 -- The One-Hole, One-Dimensional Hubbard Model at $U = \infty$
54. 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
55. 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
56. Talk presented by Xiao Xu at March 2007 APS meeting in Denver -- Simulated electrolyte-metal interfaces -- Li_3PO_4 and Li
57. Talk presented by Dr. Yaojun Du at March 2007 APS meeting in Denver -- Li-ion diffusion mechanisms in crystalline Li_3PO_4 electrolytes
58. Poster presented by William Hodge at March 2007 APS meeting in Denver -- Pair State Analysis of the Hubbard Hamiltonian in One-Dimension

Thesis Students (from last 15 years)

1. Ahmad Al-Qawasmeh -- Ph. D. August 2018 – "Ab Initio Simulations of Idealized Solid Electrolytes in Lithium Ion Batteries"
2. Jason Howard -- Ph. D. May 2018 – "First-Principles Simulations of Solid State Battery Materials"
3. Larry E. Rush Jr – M. S. May 2017 – "First-Principles Investigation of Electronic Properties in Sodium-ion Electrolytes for Solid-state Battery Materials"
4. Nicholas D. Lepley – Ph. D. December 2015 – "First Principles Investigations of Solid-Solid Interfaces in Lithium Battery Materials"
5. Nicholas D. Lepley – M. S. December 2013 – "An investigation of lithium solid electrolyte materials with first principles calculations"
6. Xiao Xu – Ph. D. August 2011 – "Orbital Dependent Functionals: An Atom Projector Augmented Wave Method Implementation"
7. William Hodge – Ph. D. August 2008 (also mentored by W. C. Kerr) – "Exact and variational investigations of Hubbard rings"
8. 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"
9. Ping Tang – Ph. D. August 2006 – "Computational research on lithium ion battery materials"
10. 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. Since 2017, together with Richard Hennig (University of Florida) and Francois Gygi (University of California at Davis) and a few others, have served on the advisory board for the Center for Predictive Simulation of Functional Materials, directed by Paul Kent (Oak Ridge National Laboratory), participating in a yearly review and preparing a short report.
2. 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-1940324: Computational Studies of Solid Electrolytes -- 04/15/2020-03/31/2022 -- $200,000 (projected)
2. NSF DMR-1507942: Computational studies of solid electrolytes – 09/01/2015-08/31/2019 -- $300,000
3. NSF DMR-1105485: First principles simulations of battery materials -- 09/01/2011-08/31/2015 -- $300,000
4. NSF DMR-0705239: First Principles Simulations of Battery Materials -- 12/15/2007-11/30/2011 -- $225,000
5. NSF DMR-0427055: ITR - Computational Tools for Detailed Simulations of Materials -- 09/01/2004-08/31/2010 -- $336,000
6. NSF DMR-0405456: Computational Study of Transition Metal Phosphate Materials -- 08/01/2004- 07/31/2008 -- $143,000