

Biographical Sketch: N. A. W. Holzwarth

Address

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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 (5 most closely related to project)

1. N. A. W. Holzwarth, N. D. Lepley, and Yaojun A. Du, in press: *J. Power Sources* (2010): "Computer Modeling of Lithium Phosphate and Thiophosphate Electrolyte Materials"
<http://dx.doi.org/10.1016/j.jpowsour.2010.08.042>
2. Yaojun A. Du and N. A. W. Holzwarth, *Phys. Rev. B*, **81** 184106 (15pp) (2010): "First-principles study of LiPON and related solid electrolytes" <http://prb.aps.org/abstract/PRB/v81/i18/e184106>
3. Xiao Xu and N. A. W. Holzwarth, *Phys. Rev. B* **81** 245105 (14pp) (2010): "A projector augmented wave (PAW) formulation of Hartree-Fock calculations of electronic structure"
<http://link.aps.org/doi/10.1103/PhysRevB.81.245105>
4. Yaojun A. Du and N. A. W. Holzwarth, *Phys. Rev. B* **76**, 174301 (2008): "Effects of O vacancies and N or Effects of O vacancies and N or Si substitutions on Li⁺ migration in Li₃PO₄ electrolytes from first principles" <http://link.aps.org/abstract/PRB/v78/e174301>
5. Yaojun A. Du and N. A. W. Holzwarth, *Phys. Rev. B* **76**, 174302 (2007): "Mechanisms of Li⁺ diffusion in crystalline Li₃PO₄ electrolytes from first principles"
<http://link.aps.org/abstract/PRB/v76/e174302>

Publications (5 additional publications)

1. Marc Torrent, N. A. W. Holzwarth, Francois Jollet, David Harris, Nicholas Lepley, and Xiao Xu, *Computer Physics Communications* **181** 1862-1867 (2010): "Electronic structure packages: Two implementations of the projector augmented wave (PAW) formalism"
<http://dx.doi.org/10.1016/j.cpc.2010.07.036>
2. Yaojun A. Du and N. A. W. Holzwarth, *Journal of the Electrochemical Society* **155**, A999 (2007): "Li ion diffusion mechanisms in the crystalline electrolyte γ -Li₃PO₄"
<http://dx.doi.org/10.1149/1.3050379>

3. Ping Tang, N. A. W. Holzwarth, and Yaojun A. Du, *Phys. Rev. B.* **76**, 174118 (2007): “Comparison of the electronic structures of four crystalline phases of FePO₄”
<http://link.aps.org/abstract/PRB/v76/e174118>
4. Y. Abraham, N. A. W. Holzwarth, R. T. Williams, G. Eric Matthews, and Alan R. Tackett, *Phys. Rev. B* **64**, (245109) (2001): ”The Electronic Structure of Oxygen Related Defects in PbWO₄ and CaMoO₄” <http://link.aps.org/abstract/PRB/v64/e245109>
5. A. R. Tackett, N. A. W. Holzwarth, and G. E. Matthews, *Computer Physics Communications* **135**, 329-376 (2001): ”A Projector Augmented Wave (PAW) code for electronic structure calculations, Part I: atompaw for generating atom-centered functions and PartII: pwpaw for periodic solids in a plane wave basis” (<http://pwpaw.wfu.edu>) [http://dx.doi.org/10.1016/S0010-4655\(00\)00244-7](http://dx.doi.org/10.1016/S0010-4655(00)00244-7)
[http://dx.doi.org/10.1016/S0010-4655\(00\)00241-1](http://dx.doi.org/10.1016/S0010-4655(00)00241-1)

Synergistic activities

1. Invited to speak at 7th Canadian Computational Chemistry Conference at Dalhousie University in Halifax, Nova Scotia, July 20-24,2009.
2. Invited to speak at 74th annual meeting of SESAPS in Nashville, TN, November 8-10, 2007.
3. Invited to speak at CEACAM workshop: “State of the art, developments and perspectives of electronic structure calculations in the frame of the Projector Augmented-Wave (PAW) method” in Lyon, France, June 12-14 2006.
4. Membership in American Physical Society, Electrochemical Society, Materials Research Society.
5. Member of several university and departmental committees, including Committee for Wake Forest University Fellowship program for undergraduate research, Women in Science Committee, and organizer of Physics Department Colloquium Series for more than 10 years.

Collaborators & Other Affiliations

Collaborators:

K. J. Cho (University of Texas at Dallas), Adri C. T. Duin (Pennsylvania State University), O. Jurchescu (Wake Forest University), W. C. Kerr (Wake Forest University), A. Lachgar (Wake Forest University), G. E. Matthews (Wake Forest University), Normand Modine (Sandia National Laboratory), Francisco Muñoz (CSIC, Spain), F. R. Salsbury (Wake Forest University), A. R. Tackett (Vanderbilt University), T. Thonhauser (Wake Forest University), Marc Torrent (CEA-DIF, France), R. T. Williams (Wake Forest University), Alan Wright (Sandia National Laboratory)

Graduate and Post Doctoral Advisors:

J. Bernholc (North Carolina State University), L. A. Girifalco (University of Pennsylvania), Melvin Lax (City College of the City University of New York), M. J. G. Lee (University of Toronto), S. G. Louie (University of California-Berkeley), S. Rabii (University of Pennsylvania)

Current and former students and post-doctoral associates:

Nicholas Lepley (current Ph. D. student), Xiao Xu (current Ph. D. student), Yaojun Du (post doctoral associate 2006-2009, currently at ICAMS, Germany), W. B. Hodge (Ph. D. 2008, supervised jointly with W. C. Kerr, currently visiting faculty at Davidson College), K. Conley (Ph. D. 2008, currently faculty member at Forsyth Tech), P. Tang (Ph. D. 2006, working as software engineer in Florida), Y. Abraham (Ph. D. December 2004 supervised jointly with R. T. Williams – currently working for Financial Company in Texas), Y. Zhang (Ph. D. 2001, supervised jointly with R. T. Williams – currently working for Sara Lee Corporation), A. R. Tackett (Ph. D. 1998 supervised jointly with G. E. Matthews; also post-doctoral associate – currently Research Assistant Professor at Vanderbilt University), Y. Zeng (Ph. D. 1997 – currently at Imaging Diagnostic Systems, Inc. in Plantation, FL)