

Biographical Sketch: N. A. W. Holzwarth

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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

1. Ping Tang, N. A. W. Holzwarth, Freddie Salsbury, Jr. and Jeremy Qualls, submitted to *Phys. Rev. B* (2004): "The electronic structures of BEDT-TTF·PF₆ crystals; a comparison of self-consistent field and Hubbard model analyses"
2. P. Tang and N. A. W. Holzwarth, *Phys. Rev. B* **68**, (165107) (2003): "Electronic structure of FePO₄, LiFePO₄, and related materials"
(<http://www.wfu.edu/~natalie/papers/LiFePO4/>)
3. 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://www.wfu.edu/~natalie/papers/ovacancy/>)
4. 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>)
5. Y. Abraham, N. A. W. Holzwarth, and R. T. Williams, *Phys. Rev. B* **62**, 1733-1741 (2000): "Electronic Structure and Optical Properties of CdMoO₄ and CdWO₄",
(<http://www.wfu.edu/~natalie/papers/cdwo/man.html>)
6. Y. Zhang, N. A. W. Holzwarth, and R. T. Williams, *Phys. Rev. B* **57**, 12738-12750 (1998): "Electronic band structures of the scheelite materials CaMoO₄, CaWO₄, PbMoO₄, and PbWO₄"
(<http://www.wfu.edu/~natalie/papers/cmo/man.html>)
7. N. A. W. Holzwarth, G. E. Matthews, A. R. Tackett, and R. B. Dunning, *Phys. Rev. B* **57**, 11827-11830 (1998); "Orthogonal polynomial projectors for the projector augmented wave method of electronic structure calculations"

8. N. A. W. Holzwarth, G. E. Matthews, R. B. Dunning, A. R. Tackett, and Y. Zeng, *Phys. Rev. B* **55**, 2005-2017 (1997): "Comparison of the PAW, pseudopotential, and LAPW formalisms for density functional calculations of solids"
(<http://www.wfu.edu/~natalie/papers/pawman/man.html>)
9. N. A. W. Holzwarth and Y. Zeng, *Phys. Rev. B* **51**, 13653-13659 (1995): "Density functional calculation of the bulk and surface geometry of beryllium"
10. Y. Zeng and N. A. W. Holzwarth, *Phys. Rev. B* **50**, 8214-8220 (1994): "Density functional calculation of the electronic structure and equilibrium geometry of iron pyrite (FeS₂)"
11. N. A. W. Holzwarth and Y. Zeng, *Phys. Rev. B* **49**, 2351-2361 (1994) (Erratum: PRB **50**, 2047 (1994): "Core-cancellation functions for evaluating exchange-correlation functions in first-principles pseudopotential calculations"
12. N. A. W. Holzwarth, J. A. Chervenak, C. J. Kimmer, Y. Zeng, Wei Xu, and James Adams, *Phys. Rev. B* **48**, 12136 (1993): "Multilayer relaxation geometry and electronic structure of a W (111) surface"
13. N. A. W. Holzwarth, in H. Zabel and S. A. Solin, Eds., **Graphite Intercalation Compounds II: Transport and Electronic Properties**, *Springer series in materials science Vol. 18*, Springer-Verlag, 1992, pgs. 7-51: "Electronic band structure of graphite intercalation compounds"
14. Q. S. Wang and N. A. W. Holzwarth, *Phys. Rev. B* **41**, 3211-3225 (1990): "Electronic structure of vacancy defects in MgO Crystals"
15. N. A. W. Holzwarth, S. Azhar, and T. J. Kerr, *Phys. Rev. B* **38**, 9409-9419 (1988): "'Singular factor' method for electronic-structure calculations"
16. N. A. W. Holzwarth, Q. Wang, and S. D. Had, *Phys. Rev. B* **38**, 3722-3732 (1988): "Electronic structure of KHgC₈"
17. C. Gao, A. L. Ritter, J. R. Dennison, and N. A. W. Holzwarth, *Phys. Rev. B* **37**, 3914-3923 (1988): "Spectral momentum density of graphite from (e,2e) spectroscopy: Comparison with first-principles calculation"
18. Jeffrey R. Gardner and N. A. W. Holzwarth, *Phys. Rev. B* **33**, 7139 (1986): "Pseudopotential inversion scheme"
19. N. A. W. Holzwarth, S. Harris, and K. C. Liang, *Phys. Rev. B* **32**, 3745 (1985): "Electronic structure of RuS₂"
20. N. A. W. Holzwarth, S. G. Louie, and S. Rabii, *Phys. Rev. B* **30**, 2219-2222 (1984): "Interlayer states in graphite and in alkali-metal-graphite intercalation compounds"
21. M. Y. Chou, S. G. Louie, M. L. Cohen, and N. A. W. Holzwarth, *Phys. Rev. B* **30**, 1062-1064 (1984): "Electron momentum distribution in graphite and lithium-intercalated graphite"
22. N. A. W. Holzwarth, S. G. Louie, and S. Rabii, *Phys. Rev. B* **28**, 1013-1025 (1983): "Lithium-intercalated graphite: Self-consistent electronic structures for stages one, two, and three"
23. J. Bernholc and N. A. W. Holzwarth, *Phys. Rev. B* **27**, 2458-2469 (1983): "Local spin-density description of multiple metal-metal bonding: Mo₂ and Co₂"
24. D. P. DiVincenzo, E. J. Mele, and N. A. W. Holzwarth, *Phys. Rev. B* **27**, 2458-2469 (1983): "Density-functional study of interplanar binding in graphite"
25. N. A. W. Holzwarth, S. G. Louie, and S. Rabii, *Phys. Rev. B* **26**, 5382-5390 (1982): "X-ray form factors and the electronic structure of graphite"
26. N. A. W. Holzwarth, S. G. Louie, and S. Rabii, *Phys. Rev. Letters* **47**, 1318-1321 (1981): "Electronic structure of third-stage lithium intercalated graphite"

27. E. W. Plummer, B. Tonner, N. A. W. Holzwarth, and A. Liebsch, *Phys. Rev. B* **21**, 4306-4321 (1980): "Electronic structure of ordered sulfur overlayers on Ni(001)"
28. N. A. W. Holzwarth, S. G. Louie, and S. Rabii, *Phys. Rev. B* **28**, 1013-1025 (1983): "Lithium intercalated graphite: Self-consistent electronic structures for stages one, two, and three"
29. N. A. W. Holzwarth, *Phys. Rev. B* **21**, 3665-3674 (1980): "Graphite intercalation compounds: A simple model of Fermi surface and transport properties"
30. B. R. Weinberger, J. Kaufer, A. J. Heeger, J. E. Fischer, M. Moran, and N. A. W. Holzwarth, *Phys. Rev. Letters* **41**, 1417-1421 (1978) "Magnetic spin susceptibility of AsF₅-intercalated graphite: Determination of density of states at Fermi energy"
31. N. A. W. Holzwarth and M. J. G. Lee, *Phys. Rev. B* **18**, 5350-5364 and 5365-5378 (1978): "Surface electronic wave functions of a semi-infinite muffin-tin lattice I. The spherical-wave method and II. Application to Cu (001) and (110)"
32. N. A. W. Holzwarth, L. A. Girifalco, and S. Rabii, *Phys. Rev. B* **18**, 5206-5216 (1978): "Theoretical study of lithium graphite. II. Spatial distribution of valence electrons"
33. N. A. W. Holzwarth, S. Rabii, and L. A. Girifalco, *Phys. Rev. B* **18**, 5190-5205 (1978): "Theoretical study of lithium graphite. I. Band structure, density of states, and Fermi-surface properties"
34. M. J. G. Lee, N. A. W. Holzwarth, and P. T. Coleridge, *Phys. Rev. B* **13**, 3249-3260 (1976): "Electronic states of impurity atoms in noble-metal lattices"
35. N. A. W. Holzwarth and M. J. G. Lee, *Phys. Rev. B* **13**, 2331-2341 (1976): "Effects of spin-orbit interaction on impurity scattering in dilute alloys"
36. N. A. W. Holzwarth, *Phys. Rev. B* **11**, 3718-3738 (1976): "Theory of impurity scattering in dilute metal alloys based on the muffin-tin model" (PhD thesis paper)
37. N. A. W. Holzwarth and M. J. G. Lee, *Physics of Condensed Matter* **19**, 161 (1975): "Theory of impurity scattering: interstitial impurities"
38. P. T. Coleridge, N. A. W. Holzwarth, and M. J. G. Lee, *Phys. Rev. B* **10**, 1213-1229 (1974): "Nonrelativistic phase-shift analysis of impurity scattering in noble metal hosts"
39. N. A. W. Holzwarth, M. J. G. Lee, and P. T. Coleridge, *Journal of Physics F-Metal Physics* **4**, L129 (1974): "Backscattering in dilute silver alloys"

Synergistic activities

1. Invited to speak at the International Workshop on Tungstate Crystals in Rome, Italy, Oct. 12-14, 1998 – "Electronic structure of scheelite tungstates and consequences for materials properties".
2. Membership in American Physical Society and Materials Research Society.
3. 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:

Alan Wright (Sandia National Laboratory), A. R. Tackett (Vanderbilt University), W. C. Kerr (Wake Forest University), F. R. Salsbury (Wake Forest University), R. T. Williams (Wake Forest University), G. E. Matthews (Wake Forest University),

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)

Former students and post-doctoral associates within the past 5 years:

P. Tang (current Ph. D. student), W. B. Hodge (current Ph. D. student working jointly with W. C. Kerr), K. Conley (current part-time Ph. D. student), Y. Abraham (Ph. D. December 2004 supervised jointly with R. T. Williams – currently working at Targarcept, Inc.), 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), Aaron Clausett (REU summer student – currently attending graduate school in computer science after graduating from Haverford College), Y. Zeng (Ph. D. 1997 – currently at Imaging Diagnostic Systems, Inc. in Plantation, FL), C. J. Kimmer (undergraduate research student – currently at Sandia National Laboratories at Livermore, Ca. after completing Ph. D. in Physics from Cornell University)

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1. NSF grant – DMR-0427055 “ITR - Computational Tools for Detailed Simulations of Materials”, Sept. 1, 2004 - Aug. 21, 2009 (\$336,000)
2. NSF grant – DMR-0405456 “Computational Study of Transition Metal Phosphate Materials”, Aug. 1, 2004 - July 31, 2007 (\$143,000)