

Tom Berlijn

Research Staff Member
Nanomaterials Theory Institute
Center For Nanophase Materials Sciences
Computer Science & Mathematics Division
Oak Ridge National Laboratory (ORNL)
(865) 576-8793
tberlijn@gmail.com



Education

University of Amsterdam Higher Energy Physics M.S. 2005 *cum laude*
Stony Brook University Condensed Matter Physics Ph.D. 2011

Professional Experience

2013-present, Research Staff Member, Oak Ridge National Laboratory
2011-2013, Research Associate, Brookhaven National Laboratory/ University of Florida

Awards

2016 Best Scientific Paper Award, Computer Science and Mathematics Division Oak Ridge National Laboratory
2013 Eugene Wigner Fellowship, Oak Ridge National Laboratory

Research Synopsis

My research focuses on studying the influence of disorder on the electronic, vibrational and magnetic structure from first principles calculations. To this end I, together with my collaborators, have developed accurate and efficient methods to study how dopants and defects can be used to manipulate the properties of functional materials such as superconductors, dilute magnetic semiconductors and thermoelectrics.

Publications

- 1) “Tip-induced local strain on MoS₂/graphite detected by inelastic electron tunneling spectroscopy”, Wonhee Ko, Saban M. Hus, Xufan Li, Tom Berlijn, Giang D. Nguyen, Kai Xiao, An-Ping Li, under review with Phys. Rev. B
- 2) “Visualization and manipulation of magnetic domains in the quasi-two-dimensional material Fe₃GeTe₂”, Giang D. Nguyen, Jinhwan Lee, Tom Berlijn, Qiang Zou, Saban M. Hus, Jewook Park, Zheng Gai, Changgu Lee, and An-Ping Li, Phys. Rev. B 97, 014425 (2018)
- 3) “Lattice dynamics of ultrathin FeSe films on SrTiO₃”, Shuyuan Zhang, Jiaqi Guan, Yan Wang, Tom Berlijn, Steve Johnston, Xun Jia, Bing Liu, Qing Zhu, Qichang An, Siwei Xue, Yanwei Cao, Fang Yang, Weihua Wang, Jiandi Zhang, E. W. Plummer, Xuetao Zhu, and Jiandong Guo, Phys. Rev. B 97, 035408 (2018)

- 4) "Universality of scanning tunneling microscopy in cuprate superconductors", P. Choubey, A. Kreisel, T. Berlijn, B. M. Andersen, P.J. Hirschfeld, Phys. Rev B 96, 174523 (2017)
- 5) "Localization of phonons in mass-disordered alloys: A typical medium dynamical cluster approach", W. R. Mondal, NS Vidhyadhiraja, T. Berlijn, J. Moreno, M. Jarrell, Phys. Rev. B 96, 014203 (2017)
- 6) "Uniaxial pressure effect on the magnetic ordered moment and transition temperatures in $\text{BaFe}_{2-x}\text{TxA}_2$ (T=Co, Ni)", D. W. Tam, Y. Song, H. Man, S. C. Cheung, Z. Yin, X. Lu, W. Wang, B. A. Frandsen, L. Liu, Z. Gong, T. U. Ito, Y. Cai, M. N. Wilson, S. Guo, K. Koshiishi, W. Tian, B. Hitti, A. Ivanov, Y. Zhao, J. W. Lynn, G. M. Luke, T. Berlijn, T. A. Maier, Y. J. Uemura, P. Dai, Phys. Rev. B 95, 060505 (2017)
- 7) "Itinerant Antiferromagnetism in RuO_2 " T. Berlijn, P. C. Snijders, O. Delaire, H.-D. Zhou, T. A. Maier, H.-B. Cao, S.-X. Chi, M. Matsuda, Y. Wang, M. R. Koehler, P. R. C. Kent, H. H. Weitering, Phys. Rev. Lett. 118, 077201 (2017)
- 8) "Giant Spin Gap and Magnon Localization in the Disordered Heisenberg Antiferromagnet $\text{Sr}_2\text{Ir}_{1-x}\text{Ru}_x\text{O}_4$ " Yue Cao, Xuerong Liu, Wenhui Xu, Weiguo Yin, D. Meyers, Jungho Kim, Diego Casa, Mary Upton, Thomas Gog, Tom Berlijn, Gonzalo Alvarez, Shujuan Yuan, Jasminka Terzic, J. M. Tranquada, John P. Hill, Gang Cao, Robert M. Konik, M. P. M. Dean, Phys. Rev. B 95 (12), 121103 (2017)
- 9) "Atomic-scale observation of structural and electronic orders in the layered compound $\alpha\text{-RuCl}_3$ ", M. Ziatdinov, A. Banerjee, A. Maksov, T. Berlijn, W. Zhou, H. B. Cao, J-Q. Yan, C.A. Bridges, D.G. Mandrus, S.E. Nagler, A.P. Baddorf, S.V. Kalinin, Nature Comm. 7 13774 (2016)
- 10) "Towards a quantitative description of tunneling conductance of superconductors: application to LiFeAs ", A. Kreisel, R. Nelson, T. Berlijn, W. Ku, Ramakrishna Aluru, Shun Chi, Haibiao Zhou, Udai Raj Singh, Peter Wahl, Ruixing Liang, Walter N. Hardy, D. A. Bonn, P. J. Hirschfeld, Brian M. Andersen, Phys. Rev. B 94, 224518 (2016)
- 11) "Experimental elucidation of the origin of the 'double spin resonances' in $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ ", Meng Wang, M. Yi, H. L. Sun, P. Valdivia, M. G. Kim, Z. J. Xu, T. Berlijn, A. D. Christianson, Songxue Chi, M. Hashimoto, D. H. Lu, X. D. Li, E. Bourret-Courchesne, Pengcheng Dai, D. H. Lee, T. A. Maier, R. J. Birgeneau, Phys. Rev. B 93, 205149 (2016)
- 12) "Impact of Iron-site defects on Superconductivity in LiFeAs ", Shun Chi, Ramakrishna Aluru, Udai Raj Singh, Ruixing Liang, Walter N. Hardy, D. A. Bonn, A. Kreisel, Brian M. Andersen, R. Nelson, T. Berlijn, W. Ku, P. J. Hirschfeld, Peter Wahl, Phys. Rev. B 94, 134515 (2016)
- 13) "Generalized Multiband Typical Medium Dynamical Cluster Approximation: Application to $(\text{Ga,Mn})\text{N}$ ", Yi Zhang, R. Nelson, Elisha Siddiqui, K.-M. Tam, U. Yu, T. Berlijn, W. Ku, N.S. Vidhyadhiraja, J. Moreno, M. Jarrell, Phys. Rev. B 94,

224208 (2016)

- 14) “Ab initio Study of Cross-Interface Electron-Phonon Couplings in FeSe Thin Films on SrTiO₃ and BaTiO₃”, Y. Wang, A. Linscheid, T. Berlijn, S. Johnston, Phys. Rev. B 93, 134513 (2016)
- 15) “Aspects of electron-phonon interactions with strong forward scattering in FeSe Thin Films on SrTiO₃ substrates”, Y. Wang, K. Nakatsukasa, L. Rademaker, T. Berlijn, S. Johnston, Supercond. Sci. Technol. 29, 054009 (2016)
- 16) “Enhanced superconductivity due to forward scattering in FeSe thin films on SrTiO₃ substrates”, L. Rademaker, Y. Wang, T. Berlijn, S. Johnston, New J. Phys. 18, 022001 (2016)
- 17) “Study of multiband disordered systems using the typical medium dynamical cluster approximation”, Y. Zhang, H. Terletska, C. Moore, C. Ekuma, K.-M. Tam, T. Berlijn, W. Ku, J. Moreno, M. Jarrell, Phys. Rev. B 92, 205111 (2015)
- 18) “What is the valence of Mn in Ga_{1-x}Mn_xN?”, R. Nelson, T. Berlijn, J. Moreno, M. Jarrell, W. Ku, Phys. Rev. Lett. 115, 197203 (2015)
- 19) “Influence of interstitial Mn on magnetism in room-temperature ferromagnet Mn(1+ δ)Sb” A. E. Taylor, T. Berlijn, S. E. Hahn, A. F. May, T. J. Williams, L. Poudel, S. Calder, R. S. Fishman, M. B. Stone, A. A. Aczel, H. B. Cao, M. D. Lumsden, A. D. Christianson, Phys. Rev. B 91, 224418 (2015)
- 20) “Heavy-impurity resonance, hybridization, and phonon spectral functions in Fe_{1-x}M_xSi, M=Ir,Os”, O. Delaire, I. I. Al-Qasir, A. F. May, C. W. Li, B. C. Sales, J. L. Niedziela, J. Ma, M. Matsuda, D. L. Abernathy, T. Berlijn, Phys. Rev. B 91, 094307 (2015)
- 21) “Glide-Plane Symmetry and Superconducting Gap Structure of Iron-Based Superconductors”, Y. Wang, T. Berlijn, P. J. Hirschfeld, D. J. Scalapino, T. A. Maier, Phys. Rev. Lett. 114, 107002 (2015)
- 22) “On the role of chalcogen vapor annealing in inducing bulk superconductivity in Fe_{1+y}Te_{1-x}Se_x”, W. Lin, P. Ganesh, A. Gianfrancesco, J. Wang, T. Berlijn, T. A. Maier, S. V. Kalinin, B. C. Sales, M. Pan, Phys. Rev. B 91, 060513(R) (2015)
- 23) “First-principles studies in Fe-based superconductors”, W. Ku, T. Berlijn, L. Wang and C.-C. Lee, in “Iron-Based Superconductivity”, Editors: P. D. Johnson, G.-Y. Xu, W.-G. Yin, Springer Series in Materials Science 211 (2015)
- 24) “Interpretation of scanning tunneling quasiparticle interference and impurity states in cuprates”, A. Kreisel, Peayush Choubey, T. Berlijn, W. Ku, B. M. Andersen, P. J. Hirschfeld, Phys. Rev. Lett. 114, 217002 (2015)
- 25) “Orbital occupancy and charge doping in iron-based superconductors”, C. Cantoni, J. E. Mitchell, A. F. May, M. A. McGuire, J.-C. Idrobo, T. Berlijn, E. Dagotto, M. F.

- Chisholm, W. Zhou, S. J. Pennycook, A. S. Sefat, B. C. Sales, *Advanced Materials* 26, 6193 (2014)
- 26) “Visualization of atomic-scale phenomena in superconductors: application to FeSe”, Peayush Choubey, T. Berlijn, A. Kreisel, C. Cao, P. J. Hirschfeld, *Phys. Rev. B* 90, 134520 (2014)
- 27) “Doping effects of Se vacancies in monolayer FeSe”, T. Berlijn, H.-P. Cheng, P. J. Hirschfeld, W. Ku, *Phys. Rev. B* 89, 020501(R) (2014)
- 28) “Unfolding the electronic structure of $\text{Ca}_{10}(\text{Fe}_{1-x}\text{Pt}_x\text{As})_{10}(\text{Pt}_n\text{As}_8)$ ”, T. Berlijn, *Phys. Rev. B* 89, 104511 (2014)
- 29) “Lifshitz Transition and Superconductivity Enhancement in High Pressure c116 Li ”, C.-H. Lin, T. Berlijn, Wei Ku, arXiv:1311.4005
- 30) “Recovering hidden Bloch character: Unfolding Electrons, Phonons, and Slabs” P. B. Allen, T. Berlijn, D. A. Casavant, J. M. Soler, *Phys. Rev. B* 87, 085322 (2013)
- 31) “Effects of Disordered Ru Substitution in BaFe_2As_2 : Possible Realization of Superdiffusion in Real Materials”, L. Wang, T. Berlijn, Y. Wang, C.-H. Lin, P. J. Hirschfeld and W. Ku, *Phys. Rev. Lett.* 110, 037001 (2013)
- 32) “Thermal evolution of the full three-dimensional magnetic excitations in the multiferroic BiFeO_3 ”, Zhijun Xu, Jinsheng Wen, Tom Berlijn, Peter M. Gehring, Christopher Stock, M. B. Stone, Wei Ku, Genda Gu, Stephen M. Shapiro, R. J. Birgeneau, and Guangyong Xu, *Phys. Rev. B* 86, 174419 (2012)
- 33) “Effective doping and suppression of Fermi surface reconstruction via Fe vacancy disorder in $\text{KxFe}_{2-y}\text{Se}_2$ ”, T. Berlijn, P. Hirschfeld and Wei Ku, *Phys. Rev. Lett.* 109, 147003 (2012)
- 34) “Do Transition Metal Substitutions Dope Carriers in Iron Based Superconductors?”, T. Berlijn, C.-H. Lin, W. Garber and Wei Ku, *Phys. Rev. Lett.* 108, 207003 (2012)
- 35) “Relevance of the Heisenberg-Kitaev Model for the Honeycomb Lattice Iridates A_2IrO_3 ”, Y. Singh, S. Manni, J. Reuther, T. Berlijn, R. Thomale, W. Ku, S. Trebst, and P. Gegenwart, *Phys. Rev. Lett.* 108, 127203 (2012)
- 36) “One-Fe versus Two-Fe Brillouin Zone of Fe-Based Superconductors: Creation of the Electron Pockets by Translational Symmetry Breaking”, C.-H. Lin, T. Berlijn, L. Wang, C.-C. Lee, W.-G. Yin, and W. Ku, *Phys. Rev. Lett.* 107, 257001 (2011)
- 37) “Long range magnetic ordering in Na_2IrO_3 ”, X. Liu, T. Berlijn, W.-G. Yin, W. Ku, A. Tsvelik, J. P. Hill, et al, *Phys. Rev. B* 83, 220403 (2011)
- 38) “Can disorder alone destroy the eg' hole pockets of $\text{Na}_{0.3}\text{CoO}_2$?”, Tom Berlijn, Dmitri Volja, and Wei Ku, *Phys. Rev. Lett.* 106, 077005 (2011)

- 39) “Room-Temperature Ferromagnetism of Cu-Doped ZnO Films Probed by Soft X-Ray Magnetic Circular Dichroism” T. S. Heng, D.-C. Qi, T. Berlijn, W. Ku et al, Phys. Rev. Lett. 105, 207201 (2010)
- 40) “Unfolding First-Principles Band Structures”, Wei Ku, Tom Berlijn and Chi-Cheng Lee, Phys. Rev. Lett. 104, 216401 (2010)

Talks

- 1) “Simulating Disorder in Functional Materials”, University of Tennessee Knoxville, Department of Physics and Astronomy Colloquium, Dec 4 2017.
- 2) “Simulating Disorder in Functional Materials”, University of Memphis, Department of Physics and Materials Science Colloquium, Sep 22 2017.
- 3) “On the Origin of Charge Order in RuCl₃”, The American Physical Society (APS), March Meeting 2017, New Orleans, USA
- 4) “Itinerant Antiferromagnetism in RuO₂”, invited talk August 10 2016, Collective Phenomena in Layered and 2D Materials Workshop, Oak Ridge National Laboratory, TN USA
- 5) “Antiferromagnetism in Bulk Rutile RuO₂”, The American Physical Society (APS), March Meeting 2016, Baltimore, USA
- 6) “Investigation of magnetism in RuO₂”, February 3 2016, Quantum Theory Project Seminar, University of Florida, Gainesville FL, USA
- 7) “A first principles method for simulating phonons in strongly disordered materials”, The American Physical Society (APS), March Meeting 2015, San Antonio, USA
- 8) “Do Se vacancies electron dope monolayer FeSe?”, October 20 2014, Condensed Matter Seminar: Department of Physics and Astronomy, University of Tennessee, Knoxville TN, USA
- 9) “Do Se vacancies electron dope monolayer FeSe?”, April 21 2014, Condensed Matter Seminar: Department of Physics and Astronomy, Louisiana State University, Baton Rouge LA, USA
- 10) “Do Se vacancies electron dope monolayer FeSe?”, American Physical Society (APS), March Meeting 2014, Denver CO, USA
- 11) “Do Se vacancies electron dope monolayer FeSe?”, Sanibel Symposium 2014, St. Simons Island GA, USA
- 12) “Role of Disorder in Iron-based superconductors”, DCMP symposium on Fe-based superconductors March 2013, Baltimore, USA
- 13) “Effects of disordered substitutions and vacancies in Fe based superconductors from first principles”, Condensed Matter Seminar, January 28 2013, University of British Columbia, Vancouver, Canada

- 14) “Wannier Function Based First Principles Method for Disordered Systems”, Official Coffee Talk, January 14 2013, The Fritz Haber Institute of the Max Planck Society, Berlin, Germany
- 15) “Wannier Function Based First Principles Method for Disordered Systems”, Rappe Group Meeting, August 10 2012, University of Pennsylvania, Philadelphia, USA
- 16) “Wannier Function Based First Principles Method for Disordered Systems”, Center for Computational Material Science Seminar, August 6 2012, Navy Research Laboratory, Washington D.C., USA
- 17) “Effective doping and suppression of Fermi surface reconstruction via Fe vacancy disorder in $KxFe_{2-y}Se_2$ ”, Villa Conference on Iron-based Superconductors, April 20 2012, Orlando, USA.
- 18) “Do Transition Metal Substitutions Dope Carriers in Iron Based Superconductors?”, The American Physical Society (APS), March Meeting 2012, Boston, USA.
- 19) “Wannier Function Based First Principles Method for Disordered Systems”, International Computational Materials Science Seminar Series, Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA), December 14 2011, Baton Rouge, Louisiana
- 20) “Observation of room-temperature ferromagnetism in Cu:ZnO films part II; a theoretical study”, The American Physical Society (APS), March Meeting 2011, Dallas, USA.
- 21) “Wannier Function Based First Principles Method for Disordered Systems”, Computational Material Science Network, March 20 2011, Dallas
- 22) “Wannier Function Based First Principles Method for Disordered Systems”, seminar UC Louvain, August 25 2010, PCPM Louvain-la-Neuve
- 23) “Effect of disorder on electronic structure CaC_6 A first-principles study”, The American Physical Society (APS), March Meeting 2010, Portland, USA.
- 24) “Wannier Function Based First Principles Method for Disordered Systems”, Excitations in Condensed Matter: From Basic Concepts to Real Materials, November 23 2009, KITP Santa Barbara
- 25) “Wannier Function Based First Principles Method for Disordered Systems”, International Workshop on: Frontiers in Density Functional Theory, September 14 2009, Montauk
- 26) “Does disorder destroy eg’ pockets in $Na_{0.3}CoO_2$?, A new ab initio method for disorder”, The American Physical Society (APS), March Meeting 2009, Pittsburgh, USA.
- 27) “A new ab initio approach for disordered systems. Case study: Influence of disorder on Fermi-surface $NaxCoO_2$.”, Computational Material Science Network, November 16 2008, Oak Ridge National Laboratory, Tennessee
- 28) “Phonon softening & displacement pattern of commensurate charge density wave in

2H-TaSe₂ (DFT calculations)", The American Physical Society (APS), March Meeting 2008, New Orleans, USA.

Professional Activities

2018, Organizing committee member of the international conference: "New Developments in STM on Superconducting Surfaces", Tsung-Dao Lee Institute, Shanghai

2017, HEATER workshop, Lawrence Berkeley National Laboratory , Identifying key research directions to enable technological breakthroughs towards the theoretical limits of thermal efficiency in energy systems

2015, Science Judge, "da Vinci Arts & Science Fair", Oak Ridge

2012, Chair "APS Focus Session: Physics of Energy Storage Materials - Advanced Materials", Boston

2009, Local Organizer "International Workshop on: Frontiers in Density Functional Theory", Montauk

2008-now, Referee for Nature Physics, Physical Review Letters, Physical Review B, Physics Letters A, Physica E, Europhysics Letters and Materials Chemistry and Physics