Tom Berlijn

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Education

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

Professional Experience

2015-present, Research Staff Member, Oak Ridge National Laboratory
2013-2015, Eugene P. Wigner Fellow, Oak Ridge National Laboratory
2011-2013, Research Associate, Brookhaven National Laboratory/ University of Florida

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) "Atomic-scale observation of structural and electronic orders in the layered compound alpha-RuCl3", 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 (2016, accepted in Nature Communications)

2) "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, arXiv:1610.00619 (2016)

3) "Giant Spin Gap and Magnon Localization in the Disordered Heisenberg Antiferromagnet Sr2Ir1-xRuxO4" Yue Cao, Xuerong Liu, Wenhu 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, arXiv:1608.04640 (2016)

4) "Experimental elucidation of the origin of the `double spin resonances' in Ba(Fe$_{1-x}$Co$_x$)$_2$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)

5) "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, arXiv:1607.03192 (2016, accepted in Phys. Rev. B)

6) "Generalized Multiband Typical Medium Dynamical Cluster Approximation: Application to (Ga,Mn)N", Yi Zhang, R. Nelson, Elisha Siddiqui, K.-M. Tam, U. Yu, T. Berlijn, W. Ku, N.S. Vidhyadhiraja, J. Moreno, M. Jarrell, arXiv:1607.02778 (2016)

7) "Ab initio Study of Cross-Interface Electron-Phonon Couplings in FeSe Thin Films on SrTiO$_3$ and BaTiO$_3$", Y. Wang, A. Linscheid, T. Berlijn, S. Johnston, Phys. Rev. B 93, 134513 (2016)

8) "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)

9) "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)

10) "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)

11) "What is the valence of Mn in Ga$_{1-x}$Mn$_x$N?", R. Nelson, T. Berlijn, J. Moreno, M. Jarrell, W. Ku, Phys. Rev. Lett. 115, 197203 (2015)

12) "Influence of interstitial Mn on magnetism in room-temperature ferromagnet Mn(1+delta)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)

13) "Heavy-impurity resonance, hybridization, and phonon spectral functions in Fe1-xMxSi, 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)

14) "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)

15) "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)

16) "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)

17) "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)

18) "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)

19) "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)

20) "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)

21) "Unfolding the electronic structure of Ca10(Fe1-xPtxAs)10(PtnAs8)", T. Berlijn, Phys. Rev. B 89, 104511 (2014)

22) "Lifshitz Transition and Superconductivity Enhancement in High Pressure cI16 Li", C.-H. Lin, T. Berlijn, Wei Ku, arXiv:1311.4005

23) "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)

24) "Effects of Disordered Ru Substitution in BaFe2As2: 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)

25) "Thermal evolution of the full three-dimensional magnetic excitations in the multiferroic BiFeO3", 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)

26) "Effective doping and suppression of Fermi surface reconstruction via Fe vacancy disorder in KxFe2-ySe2" , T. Berlijn, P. Hirschfeld and Wei Ku, Phys. Rev. Lett. 109, 147003 (2012)

27) "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)

28) "Relevance of the Heisenberg-Kitaev Model for the Honeycomb Lattice Iridates A2IrO3" , Y. Singh, S. Manni, J. Reuther, T. Berlijn, R. Thomale, W. Ku, S. Trebst,

and P. Gegenwart, Phys. Rev. Lett. 108, 127203 (2012)

29) "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)

30) "Long range magnetic ordering in Na2IrO3", X. Liu, T. Berlijn, W.-G. Yin, W. Ku, A. Tsvelik, J. P. Hill, et al, Phys. Rev. B 83, 220403 (2011)

31) "Can disorder alone destroy the eg' hole pockets of Na0.3CoO2?", Tom Berlijn, Dmitri Volja, and Wei Ku, Phys. Rev. Lett. 106, 077005 (2011)

32) "Room-Temperature Ferromagnetism of Cu-Doped ZnO Films Probed by Soft X-Ray Magnetic Circular Dichroism" T. S. Herng, D.-C. Qi, T. Berlijn, W. Ku et al, Phys. Rev. Lett. 105, 207201 (2010)

33) "Unfolding First-Principles Band Structures", Wei Ku, Tom Berlijn and Chi-Cheng Lee, Phys. Rev. Lett. 104, 216401 (2010)

Talks

1) "Investigation of magnetism in RuO2", February 3 2016, Quantum Theory Project Seminar, University of Florida. Gainesville FL, USA

2) "A first principles method for simulating phonons in strongly disordered materials", The American Physical Society (APS), March Meeting 2015, San Antonio, USA

3) "Do Se vacancies electron dope monolayer FeSe?", October 20 2014, Condensed Matter Seminar: Department of Physics and Astronomy, University of Tennessee, Knoxville TN, USA

4) "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

5) "Do Se vacancies electron dope monolayer FeSe?", American Physical Society (APS), March Meeting 2014, Denver CO, USA

6) "Do Se vacancies electron dope monolayer FeSe?", Sanibel Symposium 2014, St. Simons Island GA, USA

7) "Role of Disorder in Iron-based superconductors", DCMP symposium on Fe-based superconductors March 2013, Baltimore, USA

8) "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

9) "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

10) "Wannier Function Based First Principles Method for Disordered Systems", Rappe Group Meeting, August 10 2012, University of Pennsylvania, Philadelphia, USA

11) "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

12) "Effective doping and suppression of Fermi surface reconstruction via Fe vacancy disorder in KxFe2-ySe2", Villa Conference on Iron-based Superconductors, April 20 2012, Orlando, USA.

13) "Do Transition Metal Substitutions Dope Carriers in Iron Based Superconductors?", The American Physical Society (APS), March Meeting 2012, Boston, USA.

14) "Observation of room-temperature ferromagnetism in Cu:ZnO films part II; a theoretical study", The American Physical Society (APS), March Meeting 2011, Dallas, USA.

15) "Wannier Function Based First Principles Method for Disordered Systems", Computational Material Science Network, March 20 2011, Dallas

16) "Wannier Function Based First Principles Method for Disordered Systems", seminar UC Louvain, August 25 2010, PCPM Louvain-la-Neuve

17) "Effect of disorder on electronic structure CaC6 A first-principles study", The American Physical Society (APS), March Meeting 2010, Portland, USA.

18) "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

19) "Wannier Function Based First Principles Method for Disordered Systems", International Workshop on: Frontiers in Density Functional Theory, September 14 2009, Montauk

20) "Does disorder destroy eg' pockets in Na0.3CoO2?, A new ab initio method for disorder" , The American Physical Society (APS), March Meeting 2009, Pittsburgh, USA.

21) "A new ab initio approach for disordered systems. Case study: Influence of disorder on Fermi-surface NaxCoO2.", Computational Material Science Network, November 16 2008, Oak Ridge National Laboratory, Tennessee

22) "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

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 B, Physical Review Letters, Physica E and Europhysics Letters