

Tom Berlijn

Senior Research Scientist
Nanomaterials Theory Institute
Center For Nanophase Materials Sciences Computer
Science & Mathematics Division
Oak Ridge National Laboratory (ORNL)
(865) 576-8793
berlijnt@ornl.gov



Education

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

Professional Experience

2023-present, Senior Research Scientist, Oak Ridge National Laboratory
2013-2023, 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. I am also working on the derivation of microscopic interactions in Kitaev quantum spin liquid materials via first principles calculations.

Selected Publications from:

- 68 peer reviewed articles with 3543 citations & h-index 26 (Google Scholar)
 - 22 high impact journal publications (impact factor > 7)
- 1) “Breaking Rayleigh’s Law with Spatially Correlated Disorder to Control Phonon Transport”, S. Thébaud, L. Lindsay, and T. Berlijn [Phys. Rev. Lett. 131, 026301 \(2023\)](#).
 - 2) “Role of the third dimension in searching for Majorana fermions in α -RuCl₃ via

- phonons”, S. Mu, K. D. Dixit, X. Wang, D. L. Abernathy, H. Cao, S. E. Nagler, J. Yan, P. Lampen-Kelley, D. Mandrus, C. A. Polanco, L. Liang, G. B. Halász, Y. Cheng, A. Banerjee, and T. Berlijn, [Phys. Rev. Research 4, 013067 \(2022\)](#).
- 3) “Simulating Spin Waves in Entropy Stabilized Oxides”, T. Berlijn, G. Alvarez, D. S. Parker, R. P. Hermann, R. S. Fishman, [Phys. Rev. Research 3, 033273 \(2021\)](#).
 - 4) “Interlayer magnetism in $\text{Fe}_{3-x}\text{GeTe}_2$ ”, Xiangru Kong, Giang D. Nguyen, Jinhwan Lee, Changgu Lee, Stuart Calder, Andrew F. May, Zheng Gai, An-Ping Li, Liangbo Liang, and Tom Berlijn, [Phys. Rev. Materials 4, 094403 \(2020\)](#).
 - 5) “Deriving models for the Kitaev spin-liquid candidate material $\alpha\text{-RuCl}_3$ from first principles”, Casey Eichstaedt, Yi Zhang, Pontus Laurell, Satoshi Okamoto, Adolfo G. Eguiluz, and Tom Berlijn, [Phys. Rev. B 100, 075110 \(2019\)](#).
 - 6) “Origin of localization in Ti-doped Si”, Yi Zhang, R Nelson, K-M Tam, W Ku, U Yu, NS Vidhyadhiraja, H Terletska, J Moreno, M Jarrell, T Berlijn, [Physical Review B 98 \(17\), 174204 \(2018\)](#).
 - 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) “Effective doping and suppression of Fermi surface reconstruction via Fe vacancy disorder in $\text{K}_x\text{Fe}_{2-y}\text{Se}_2$ ”, T. Berlijn, P. Hirschfeld and Wei Ku, [Phys. Rev. Lett. 109, 147003 \(2012\)](#)
 - 9) “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 \(2012\)](#)
 - 10) “Can disorder alone destroy the e_g ’ hole pockets of $\text{Na}_{0.3}\text{CoO}_2$?”, Tom Berlijn, Dmitri Volja, and Wei Ku, [Phys. Rev. Lett. 106, 077005 \(2011\)](#).

Selected Presentations (from 22 invited talks):

- 1) “Searching Majorana Fermions in $\alpha\text{-RuCl}_3$ via Phonons: The Role of the Third Dimension”, CNMS User Meeting, August 8 2022, Center for Nanophase Materials Sciences, Oak Ridge, USA.
- 2) “Understanding Disordered Materials via Unbiased Simulations”, Louisiana State University, Louisiana Consortium for Neutron Scattering Seminar, Mar 19 2018.
- 3) “Role of Disorder in Iron-based superconductors”, DCMP symposium on Fe-based superconductors March 2013, Baltimore, USA