THOMAS A. MAIER – CURRICULUM VITAE

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Computational Materials Sciences
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RESEARCH INTERESTS

- Many-body theory of correlated electron systems
- Quantum materials, unconventional superconductors, multi-layers and nanostructures
- Computational physics

EDUCATION

University of Regensburg, Germany	Physics	Diploma, highest honors, 1997
University of Regensburg, Germany	Physics	Dr. rer. nat. (Ph.D.), summa cum laude, 2001
University of Cincinnati	Physics	Postdoctoral Fellow, 2001–2003

APPOINTMENTS

Distinguished Research Staff	Computational Science and Engineering Division Oak Ridge National Laboratory	since 4/2017
Joint Faculty Associate Professor	Department of Physics and Astronomy, University of Tennessee, Knoxville	since 10/2013
Senior Research Staff	Computer Science and Math Division and Center for Nanophase Materials Sciences, ORNL	since 1/2010
Research Staff	Computer Science and Math Division and Center for Nanophase Materials Sciences, ORNL	since 4/2005
Wigner Fellow	Computer Science and Math Division, ORNL	2003–2005

SIGNIFICANT AWARDS AND HONORS

American Physical Society Outstanding Referee	2018
Fellow of the Americal Physical Society	2015
ACM Gordon Bell award for first petascale simulations	2008
Wigner Fellowship – Oak Ridge National Laboratory	2003
W.C. Röntgen prize for successful young scientists	2001
OBAG Kulturpreis – Cultural award for outstanding dissertation	2001

PROFESSIONAL SERVICE

- Associate Editor for de Gruyter Open Access Journal "Novel Superconducting Materials"

- Member of Oak Ridge Leadership Computing Facility User Group Executive Board
- Contributor to ORNL's computational nanoscience end-station, a multi-institutional project to provide scalable plug-and-play tools for nanoscience optimized for leadership class machines.
- Referee for Science, Nature Physics, APS Journals, IOP Journals and Journal of the Physical Society of Japan. Reviewer for NSF, DOE, NSERC, Swiss National Science Foundation and Swiss National Supercomputing Center (CSCS) grant applications.

GRADUATE AND POSTDOCTORAL ADVISORS

Prof. T. Pruschke	University of Göttingen, Germany (deceased)
Prof. M. Jarrell	Louisiana State University

PUBLICATION SUMMARY

Publications: 100 total, 98 in refereed journals
Total citations (ISI Web of Science, April 2018): 4377
Hirsch index (ISI Web of Science, April 2018): 34

PUBLICATION LIST – Thomas A. Maier

[1] F. Ming, S. Johnston, D. Mulugeta, T. S. Smith, P. Vilmercati, G. Lee, T. A. Maier, P. C. Snijders, and H. H. Weitering,*Realization of a Hole-Doped Mott Insulator on a Triangular Silicon Lattice*, Phys. Rev. Lett. **119**, 266802 (2017).

[2] F. Lin, T. A. Maier, and V. W. Scarola, *Disordered Supersolids in the Extended Bose-Hubbard Model*, Sci. Rep. **7**, 12752 (2017).

[3] B. Pan, Y. Shen, D. Hu, Y. Feng, J. T. Park, A. D. Christianson, Q. Wang, Y. Hao, H. Wo, Z. Yin, T. A. Maier, and J. Zhao, *Structure of Spin Excitations in Heavily Electron-Doped $Li_{0.8}Fe_{0.2}ODFeSe$ Superconductors*, Nat. Comms. **8**, 855 (2017).

[4] E. W. Huang, D. J. Scalapino, T. A. Maier, B. Moritz, and T. P. Devereaux, *D-Wave Pairing Strength in Spite of the Persistence of Magnetic Excitations in the Overdoped Hubbard Model*, Phys. Rev. B **96**, 020503 (2017).

[5] 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, and P. Dai, *Uniaxial Pressure Effect on the Magnetic Ordered Moment and Transition Temperatures in $BaFe_{2-x}T_xAs_2$ (T=Co, Ni)*, Phys. Rev. B **95**, 060505 (2017).

[6] 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, and H. H. Weitering, *Itinerant Antiferromagnetism in RuO_2*, Phys. Rev. Lett. **118**, 077201 (2017).

[7] M. Altmeyer, D. Guterding, P. J. Hirschfeld, T. A. Maier, R. Valenti, and D. J. Scalapino, *Role of vertex corrections in the matrix formulation of the random phase approximation for the multiorbital Hubbard model*, Phys. Rev. B **94**, 214515 (2016).

[8] S. Maiti, T. A. Maier, T. Bhm, R. Hackl, and P. J. Hirschfeld, *Probing the Pairing Interaction and Multiple Bardasis-Schrieffer Modes Using Raman Spectroscopy*, Phys. Rev. Lett. **117**, 257001 (2016).

[9] S. Li, N. Kaushal, Y. Wang, Y. Tang, G. Alvarez, A. Nocera, T. A. Maier, E. Dagotto, and S. Johnston, *Nonlocal correlations in the orbital selective Mott phase of a one-dimensional multiorbital Hubbard model*, Phys. Rev. B **94**, 235126 (2016).

[10] F. Bao, Y. Tang, M. Summers, G. Zhang, C. Webster, V. Scarola, and T. A. Maier, *Fast and efficient stochastic optimization for analytic continuation*, Phys. Rev. B **94**, 125149 (2016).

[11] V. Mishra, D. J. Scalapino, and T. A. Maier, *$s^{\pm}$ pairing near a Lifshitz transition*, Sci. Rep. 6, 32078 (2016).

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[13] T. A. Maier, P. Staar, V. Mishra, U. Chatterjee, J.C. Campuzano, D.J Scalapino, *Pairing in a dry Fermi sea*, Nat. Comms. **7**, 11875 (2016).

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[16] A.T. Rømer, A. Kreisel, I. Eremin, M.A. Malakhov, T.A. Maier, P.J. Hirschfeld, and B.M. Anderson, *Pairing symmetry of the one-band Hubbard model in the paramagnetic weak-coupling limit: A numerical RPA study*, Phys. Rev. B. **92**, 104505 (2015).

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[18] W. Lin et al., *Role of chalcogen vapor annealing in inducing bulk superconductivity in $Fe_{1+y}Te_{1-x}Se_x$*, Phys. Rev. B. **91**, 060513(R) (2015).

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[23] P. Staar, T. A. Maier, M. S. Summers, G. Fourestey, R. Solca, and T. C. Schulthess, *Taking a quantum leap in time to solution for simulations of high-Tc superconductors*, Proceedings of Supercomputing '13, 111 (2013).

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INVITED PRESENTATIONS

1. *Computational Studies of High-Temperature Superconductors*, Lecture for Oak Ridge Institute for Continued Learning, Oak Ridge, TN, July 2017.

2. *New developments in dynamical cluster quantum Monte Carlo theory*, plenary talk at Sanibel symposium, St. Simons Island, Feb. 2017.

3. *Pairing in dry Fermi seas*, International workshop on iron-based superconductors, Munich, Germany, September 2016.

4. *Pairing in a dry Fermi sea*, Superstripes 2016 international conference, Ischia, Italy, June 2016.

5. *Glide-Plane Symmetry and Superconducting Gap Structure of Iron-Based Superconductors*, APS March meeting 2016, Baltimore, March 2016.

6. *The Dynamic Cluster Approximation and its DCA^+ extension*, Autumn School on Correlated Electrons, Forschungzentrum Jülich, Germany, September 2015.

7. *Glide Plane Symmetry and η-Pairing in a Fe-Pnictide Layer*, M2S-2015, Geneva, Switzerland, August 2015.

8. *Advanced Dynamic Cluster Calculations of High-Temperature Superconductors*, Electronic Structure Approaches and Applications to Quantum Matter, CNLS 35th Annual Conference, Santa Fe, NM, May 2015.

9. *Progress and Challenges in Cluster DMFT*, ANL Neutron Workshop, ANL, March 2015.

10. *Glide Plane Symmetry and Gap Structure in Iron-Based Superconductors*, Magnetism, Bad Metals and Superconductivity: Iron Pnictides and Beyond, KITP Program, Santa Barbara, CA, October 2014.

11. *Pairing near a nematic QCP in a 3-band CuO model*, Strong Correlations and Unconventional Superconductivity: Towards a Conceptual Framework KITP conference, KITP Santa Barbara, CA, September 2014.

12. *Dynamical cluster approximation with continuous self-energy: Superconductivity in the Hubbard model*, Simon's foundation Fall 2014 Many Electron Collaboration meeting, New York, NY, September 2014.

13. *Microscopic analysis of η-pairing in the iron-based superconductors*, International workshop on iron-based superconductors, Beijing, China, August 2014.

14. *Search for the mechanism responsible for pairing in the iron-based superconductors*, Energy Materials Nanotechnology Summer meeting, Cancun, Mexico, June 2014.

15. *Insight through computing: Understanding and predicting the physics of unconventional superconductors*, Physics colloquium, University of Florida, FL, January 2014.

16. *Spin Fluctuation Theory of Pairing in KFe_2Se_2 and Related Materials*, Workshop on Recent Developments in Fe-based High-temperature Superconductors, Riverhead, NY, September 2013.

17. *Spin Fluctuation Mediated Pairing in AFe_2Se_2 and its Consequences*, Superstripes Conference, Ischia, Italy, July 2013.

18. *Computation beyond DFT: Understanding and predicting the physics of unconventional superconductors*, Condensed matter seminar, Rensselaer Polytechnic Institute, NY, February 2013.

19. *Spin fluctuation theory of pairing in iron-based superconductors and its predictions*, Condensed Matter Seminar at University of Tennessee, Knoxville, September 2012.

20. *Review of RPA Approach for Iron-Based Superconductors*, Materials and Mechanisms of Superconductivity (M2S) conference, Washington DC, July 2012.

21. *How does the Hubbard Model guide us in the search for higher-Tc superconductors?*, Superstripes conference, Erice, Italy, July 2012.

22. *Superconductivity in heterostructures and systems with nanoscale charge inhomogeneities: Numerical studies of Hubbard models*, CECAM workshop, Lausanne, June 2012.

23. *Progress in the Computational Search for higher-T_c superconductors*, Conference on Computational Physics, Gatlinburg, Nov. 2011.

24. *How does the Hubbard Model guide us in the search for higher-Tc superconductors?*, Condensed Matter seminar, Virginia Tech, Blacksburg, VA, Oct. 2011.

25. *How does the Hubbard Model guide us in the search for higher-Tc superconductors?*, Condensed Matter seminar, University of Florida, Gainesville, Sept. 2011.

26. *Superconductivity in cuprate, organic and iron-based materials: A dynamic cluster quantum Monte Carlo perspective*, Electronic structure of novel materials conference, Tegernsee, Germany, Sept. 2011.

27. *Computational Insight into High-Temperature Superconductivity*, Annual Research Meeting of the Office of Science Graduate Fellowship Program, ORNL, July 2011.

28. *Superconductivity in Striped and Multi-Fermi-Surface Hubbard Models: From the Cuprates to the Pnictides*, Stripes 2011 Conference, Rome, Italy, July 2011.

29. *High-end Simulations of Cuprate, Organic and Iron-Based Materials: Unconventional Superconductivity from a Quantum Monte Carlo Perspective*, JICS/GRS workshop Aachen, Germany, March 2011.

30. *Unconventional superconductivity from a dynamic cluster quantum Monte Carlo perspective: Parallels and contrasts between cuprate, organic and iron-based superconductors*, Condensed matter seminar, Columbia University, New York City, February 2011.

31. *The structure of the pairing interaction in the 2D Hubbard model: How good is RPA?*, KITP miniprogram: Iron-based superconductors, Santa Barbara, CA, January 2011.

32. *Quantum Monte Carlo simulations of cuprate and organic superconductors: Parallels and Contrasts*, CIFAR Quantum Materials meeting, Whistler, CA, October 2010.

33. *Electronic inhomogeneity and superconductivity in the cuprates: Insights from Hubbard model simulations*, Psi-K conference, Berlin, Germany, September 2010.

34. *Advancing our understanding of high-temperature superconductors through extreme scale computing*, SciDAC workshop, Chattanooga, TN, July 2010.

35. *Electronic inhomogeneity and superconductivity in the cuprates: Insights from Hubbard model simulations*, Condensed Matter Seminar, Stanford, CA, June 2010.

36. *Electronic inhomogeneity and superconductivity in the cuprates: Insights from Hubbard model simulations*, Condensed Matter Seminar, Davis, CA, June 2010.

37. *Superconductivity in inhomogeneous Hubbard models*, FOR538 workshop, Munich, Germany, May 2010.

38. *Dynamic Cluster Simulations of Disorder and Inhomogeneity Effects in Cuprate Superconductors*, Fermions 2009 conference, Obergurgl, Austria, October 2009.

39. *Closing in on an Explanation for High-Temperature Superconductivity*, Fall Creek Falls Workshop, Chattanooga, TN, September 2009.

40. *Petascale Computing* and *Dynamical Mean Field Methods*, Next Generation of Quantum Simulations workshop, Moorea Island, French Polynesia, May 2009.

41. *Quantum cluster simulations of cuprate superconductors*, Correlated Electrons in Matter workshop, Park Vista Hotel, Gatlinburg, TN, April 2009.

42. *Dynamic cluster quantum Monte Carlo simulations of cuprate superconductors*, IPAM workshop on "Numerical approaches to quantum many-body systems", UCLA, Los Angeles, January 2009.

43. *Pairing in the Hubbard model of the high-Tc cuprates: Insights from dynamic cluster simulations*, Fall meeting of the Computational Materials Science Network on Predictive Capabilities for Strongly-Correlated Systems, Oak Ridge, TN, November 2008.

44. *Theory of Neutron Scattering and the superconducting gap in the Fe-pnictides*, Ringberg Symposium on properties of cuprate superconductors, Ringberg castle Rottach-Egern, Germany, November 2008.

45. *Pairing glue in the Hubbard model and a potential route to higher Tc superconductivity*, Condensed Matter Theory Seminar, UC Santa Barbara, October 2008.

46. *Neutron scattering as a probe of the Fe-pnictide superconducting gap*, Mini-workshop on new Fe-pnictide developments, UT Knoxville, May 2008.

47. *Pairing Glue in the Hubbard and t-J models: Insights from a dynamic cluster approximation study*, Sanibel Symposium, St. Simons Island, GA, February 2008.

48. *Dynamic cluster simulations of high-temperature superconductors: Scientific Impacts and Opportunities*, Workshop on Scientific Impacts and Opportunities in Computing, Maui, January 2008.

49. *Dynamic cluster quantum Monte Carlo simulations of the 2D Hubbard model: What is the cuprate pairing mechanism?*, Workshop on solving the Bogoliubov-de Gennes and Gross-Pitaevskii equations for superconductors, superfluids and BEC, Manchester, UK, September 2007.

50. *The structure of the pairing interaction in the two-dimensional Hubbard model*, Gordon Research Conference on Superconductivity, Les Diablerets, Switzerland, September 2007.

51. *The Dynamic Cluster Quantum Monte Carlo Method: Toward an Understanding of High-Temperature Superconductors*, First LLNL Workshop on Correlated Materials, Half Moon Bay, December 2006.

52. *Fermion glue in the Hubbard model: What is the cuprate pairing mechanism?*, Colloquium at Washington University, St. Louis, Nov. 1, 2006.

53. *The Dynamical Cluster Quantum Monte Carlo Method: Toward an Understanding of High-Temperature Superconductors*, International Workshop on Density Functional Theory Meets Strong Correlation, Montauk Yacht Club, Long Island, New York, Sept. 5-8, 2006.

54. *Understanding High-Temperature Superconductors with Quantum Cluster Theories*, International Conference on Materials and Mechanisms of Superconductivity and High-Temperature Superconductors (M2S-HTSC-VIII), Dresden, Germany, July 2006.

55. *A systematic quantum cluster study of superconductivity in the 2D Hubbard model*, Workshop "Quantum cluster methods for correlated materials", Sherbrooke, CA, July 2005.

56. *Beyond Dynamical Mean Field Theory: Does the 2D Hubbard model describe high-temperature superconductors?*, Condensed Matter Theory seminar, University of Sherbrooke, Sherbrooke, CA, May 2005.

57. *Does the 2D Hubbard model describe high-temperature superconductors?*, APS March meeting, Los Angeles, March 2005.

58. *Towards Full Simulations of High-Temperature superconductors*, Cray User group meeting, Knoxville, TN, May 2004.

59. *Does the 2D Hubbard model contain the right ingredients for high-T_c superconductivity?*, CMSN workshop "Predictive Capabilities for Strongly Correlated Systems", Montreal, Canada, March 2004

60. *On the nature of pairing in the cuprates*, CMSN workshop "Predictive Capabilities for Strongly Correlated Systems", University of Tennessee, Knoxville, TN, November 2003

61. *Cluster Formalism applied to Cuprates*, NSET workshop "Approaches to Collective Phenomena in Correlated-Electron Systems", Fall Creek Falls, TN, September 2003

62. *On the origin of pairing in cuprate superconductors*, Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Augsburg, September 2003

63. *Kinetic energy driven pairing*, Computational Materials Science group, Oak Ridge National Laboratory, Oak Ridge TN, October 2002.

64. *Kinetic energy driven superconductivity*, VII Training Course in the Physics of Correlated Electron Systems and High-Tc Superconductors, Vietri sul Mare (Salerno), Italy, October 2002.

65. *The role of Zinc impurities in high-temperature superconductors*, Computational Materials Science Seminar, Oak Ridge National Laboratory, Oak Ridge TN, March 2002.

66. *How Zn impurities suppress high-temperature superconductivity*, Theoretical Physics III, Cenqter for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Augsburg, Nov. 2001.

67. *How Zn impurities strongly suppress high-temperature superconductivity*, Condensed Matter Theory Group, Department of Physics, Ohio State University, Columbus, Oct. 2001.

68. *On the Effects of Zn impurities in High-T_c Superconductors*, Condensed Matter Group, Department of Physics, University of Kentucky, Lexington, Oct. 2001.

69. *The Dynamical Cluster Approximation: A Microscopic Theory for the Cuprates*, March meeting '01 of the American Physical Society, Seattle, March 2001.

70. *The Dynamical Cluster Approximation: Non-Local Correlations in the 2D Hubbard-Model*, Condensed Matter Theory Group, Department of Physics, University of Karlsruhe, July 2000.

71. *The Dynamical Cluster Approximation*, Workshop on Correlation Effects in Electronic Structure Calculations, Abdus Salam International Centre for Theoretical Physics, Trieste, June 2000.

72. *Applications and Extensions of the Dynamical Mean Field Theory*, Correlation Day on the occasion of Prof. Dr. Keiter's anniversary, Dortmund, April 2000.

73. *Antiferromagnetic Spin Correlations, Pseudogaps and Superconductivity in the Hubbard Model*, 18th General Conference of the Condensed Matter Division of the European Physical Society, Montreaux, March 2000.

74. *Dynamical mean-field theory for multi-band systems: Magnetic properties*, Mini-Workshop on Progress in the Development and Applications of the Dynamical Mean Field Theory, University of Augsburg, June 1998.