

Paul R. C. Kent

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Education and Training:

University of Cambridge, UK	Ph.D.	1999	Theoretical Physics
University of Bath, UK	B.Sc.	1996	Applied Physics

Professional Experience:

2019-present Distinguished Staff Scientist, Oak Ridge National Laboratory
2014-2019 Senior Staff Scientist, Oak Ridge National Laboratory
2009-2014 Staff Scientist, Oak Ridge National Laboratory
2005-2009 Research Scientist, Joint Institute of Computational Sciences, University of Tennessee, Knoxville, TN
2003-2005 Postdoctoral researcher, Joint Institute of Computational Sciences, University of Tennessee, Knoxville, TN
1999-2002 Postdoctoral researcher, Solid State Theory Group, National Renewable Energy Laboratory, Golden, CO
1994-5, 1996 Technical Student, Computing and Networks Division, CERN, Switzerland.

Professional Activities, Honors, Awards:

2020 ORNL Director's Award for Outstanding Individual Accomplishment in Science and Technology
2020 ORNL Research Leadership Award
2018 APS Fellowship
2010-2020 NERSC User Group Executive Committee
2011-2018 Specialist Editor, Computer Physics Communications, Elsevier
2013-2017 APS Division of Computational Physics, Member at Large
2008 IEEE/ACM Gordon Bell Prize for the first petaflop calculation. Paper: "New algorithm to enable 400+TFlop/s sustained performance in simulations of disorder effects in high-T_c superconductors"

Major Current Projects and Responsibilities:

9/2016-present, PI, "Center for Predictive Simulation of Functional Materials", funded by the DOE BES Computational Materials Sciences program, \$2.5M/year.

Matrixed staff, Center for Nanophase Materials Sciences, one of the five DOE nanoscale science research centers and user facilities.

Publications:

Author of ~186 peer-reviewed publications. $h=64$, 57987 total citations, 46 articles cited ≥ 100 times per Google Scholar, as of 15 March 2024. Statistical information and links available from [Google Scholar](https://scholar.google.com/citations?user=A-6756-2008), [ResearcherID A-6756-2008](https://orcid.org/0000-0001-5539-4017), and [ORCID 0000-0001-5539-4017](https://orcid.org/0000-0001-5539-4017).

10 representative publications:

1. “How water attacks MXene”. Tao Wu, Paul R. C. Kent, Yury Gogotsi, and De-en Jiang. [Chemistry of Materials 34 4975 \(2022\)](#).
2. “Novel boron nitride MXenes as promising energy storage materials”. Murali Gopal Muraleedharan and Paul R. C. Kent. [Nanoscale 14 9086 \(2022\)](#).
3. “QMCPACK: Advances in the development, efficiency, and application of auxiliary field and real-space variational and diffusion Quantum Monte Carlo”. P. R. C. Kent, Abdulgani Annaberdiyev, Anouar Benali, M. Chandler Bennett, Edgar Josue Landinez Borda, Peter Doak, Hongxia Hao, Kenneth D. Jordan, Jaron T. Krogel, Ilkka Kylanpaa, Joonho Lee, Ye Luo, Fionn D. Malone, Cody A. Melton, Lubos Mitas, Miguel A. Morales, Eric Neuscamman, Fernando A. Reboredo, Brenda Rubenstein, Kayahan Saritas, Shiv Upadhyay, Guangming Wang, Shuai Zhang, and Luning Zhao. [The Journal of Chemical Physics 152 174105 \(2020\)](#). Editor’s Pick.
4. “Deciphering chemical order-disorder and material properties at the single-atom level”. Y. Yang, Chien-Chun Chen, M. C. Scott, C. Ophus, R. Xu, A. Pryor Jr, L. Wu, F. Sun, W. Theis, J. Zhou, M. Eisenbach, P. R. C. Kent, R. F. Sabirianov, H. Zeng, P. Ercius, and J. Miao. [Nature 542 75 \(2017\)](#).
5. “Criteria for predicting the formation of single-phase high-entropy alloys”. C. M. Troparevsky, J. R. Morris, P. R. C. Kent, A. R. Lupini, and G. M. Stocks . [Physical Physical Review X 5 011041 \(2015\)](#).
6. Role of surface structure on Li-ion energy storage capacity of two-dimensional transition metal carbides”. Y. Xie, M. Naguib, V. N. Mochalin, M. W. Barsoum, Y. Gogotsi, X. Yu, K. Nam, X. Yang, A. I. Kolesnikov, and P. R. C. Kent. [Journal of the American Chemical Society 136 6385 \(2014\)](#).
7. “Binding and diffusion of lithium in graphite: quantum Monte Carlo benchmarks and validation of van der Waals density functional methods”. P. Ganesh, J. Kim, C. Park, M. Yoon, F. A. Reboredo, and P. R. C. Kent. [Journal of Chemical Theory and Computation 10 5318 \(2014\)](#).
8. “New algorithm to enable 400+ TFlop/s sustained performance in simulations of disorder effects in high-Tc superconductors”. G. Alvarez, M. S. Summers, D. E. Maxwell, M. Eisenbach, J. S. Meredith, J. M. Larkin, J. Levesque, T. A. Maier, P. R. C. Kent, E. F. D’Azevedo, and T. C. Schulthess. Proceedings of the 2008 ACM/IEEE conference on Supercomputing (2008). Gordon Bell Prize winner.
9. “GEANT 4 - a simulation toolkit”. S. Agostinelli et al. (GEANT 4 Collaboration). [Nuclear Instruments and Methods in Physics Research A 506 250 \(2003\)](#). [>35K citations and cited by the Higgs boson papers].
10. “Theory of electronic structure evolution in GaAsN and GaPN alloys”. P. R. C. Kent and Alex Zunger. [Physical Review B 64 115208 \(2001\)](#).

Advisory Committees:

- 2020-present External Advisory Committee, T-Rex European Center of Excellence, <https://exdci.eu/collaboration/coe>. Prof. Claudia Filippi, University of Twente, PI.
- 2018-present External Advisory Committee, M2QM Energy Frontier Research Center, <https://efrc.ufl.edu>. Prof. Xiaoguang Zhang, University of Florida, PI.

Graduate and Postdoctoral Advisors:

- Thomas C. Schulthess (CSCS, Swiss Supercomputer Center)
Mark Jarrell (Louisiana State University)
Alex Zunger (University of Colorado)
Richard J. Needs (Cambridge University, UK)