

# Paul R. C. Kent

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## Education

Cambridge University, United Kingdom	Theoretical Physics	Ph.D, 1999
Bath University, United Kingdom	Applied Physics	BSc, First class, 1996

## Research Interests

Research is focused on predicting and explaining the properties of materials using atomistic computer simulation. Methods are actively developed for greater accuracy and efficiency, and in particular tuned for the largest scale supercomputers. Methods include quantum Monte Carlo, density functional theory, quantum chemistry, and reactive classical molecular dynamics (ReaxFF, AIREBO). Recent projects include nanoscale catalysis, nanostructured thermoelectrics, the dynamics of the water-oxide interface, nanophase stability reversals in nanoparticles, electrolytes for Li-ion batteries, supercapacitor materials, and the development of several new quantum Monte Carlo algorithms.

## Professional Experience

2009-p	Research Staff, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory
2005-2009	Research Scientist, Joint Institute of Computational Science, University of Tennessee
2003-2005	Post doc, Joint Institute of Computational Science, University of Tennessee
1999-2002	Post doc, National Renewable Energy Laboratory

## Professional and Synergistic Activities

2010	DOE Computational Science Graduate Fellowship selection committee
2009	Program Committee SciDAC 2009 conference
2006-p	Developer CNMS Materials Science Endstation. Optimized plane wave density functional codes, e.g. VASP, for leadership computing platforms
1994-5, 1996	GEANT 4 developer, <a href="http://geant4.org">http://geant4.org</a> , High Energy Physics detector simulation tool
1992-p	Member: Institute of Physics (1992+), Materials Research Society (1999+), American Physical Society (1998+)

## Honors and Awards

2009	ORNL Significant Event Award, for contribution to the Gordon Bell Prize in Superconductivity Simulation
2008	Gordon Bell Prize. ACM/IEEE Conference on Supercomputing, for the first petaflop calculation.

**Selected Peer-Reviewed Publications** (Author of 65 articles in refereed journals and books, 3 articles with over 100 citations, see <http://www.ornl.gov/~pk7/publications.html> )

- “*Anomalous Lattice Dynamics near Ferroelectric Instability in PbTe*”. Y. Zhang, X. Ke, P. R. C. Kent, C. Chen, and J. Yang. Accepted in Physical Review Letters (2011).
- “*Formation, characterization and dynamics of onion like carbon structures from nanodiamonds using reactive force-fields for electrical energy storage*”. P. Ganesh, P. R. C. Kent, and V. Mochalin. Accepted in Journal of Applied Physics (2011).
- “*Nanodopant-induced band modulation in AgPbmSbTe<sub>2+m</sub>-type thermoelectrics*”. Y. Zhang, X. Ke, C. Chen, J. Yang, and P. R. C. Kent. Physical Review Letters 106 206601 (2011).
- “*Accurate static and dynamic properties of liquid electrolytes for Li-ion batteries from ab initio molecular dynamics*”. P. Ganesh, D. Jiang, P. R. C. Kent. Journal of Physical Chemistry B 115 3085 (2011).
- “*Simple impurity embedded in a spherical jellium: Approximations of density functional theory compared to quantum Monte Carlo benchmarks*”. M. Bajdich, P. R. C. Kent, J. Kim, F. A. Reboredo. Physical Review B 84 075131 (2011).

- “Phonon softening and metallization of a narrow-gap semiconductor by thermal disorder”. O. Delaire, K. Marty, M. B. Stone, P. R. C. Kent, M. S. Lucas, D. L. Abernathy, D. Mandrus, B. C. Sales. *Proceedings of the National Academy of Sciences* 108 4725 (2011).
- “Faster Proton Transfer Dynamics of Water on SnO<sub>2</sub> Compared to TiO<sub>2</sub>”. N. Kumar, P. R. C. Kent, A. V. Bandura, J. D. Kubicki, D. J. Wesolowski, D. R. Cole and J. O. Sofo. *Journal of Chemical Physics* 134 044706 (2011).
- “A fast and efficient algorithm for Slater determinant updates in Quantum Monte Carlo simulations”. Phani K. V. V. Nukala and P. R. C. Kent. *J. Chem. Phys.* 130 204105 (2009).
- “Hydrogen bonds and vibrations of water on (110) rutile”. N. Kumar, S. Neogi, P. R. C. Kent, A. V. Bandura, J. D. Kubicki, D. J. Wesolowski, D. Cole, J. O. Sofo. Accepted in *Journal of Physical Chemistry C* 113 (2009).
- “The origin of nanoscale phase stability reversals in titanium oxide polymorphs”. D. R. Hummer, J. D. Kubicki, P. R. C. Kent, J. E. Post, P. J. Heaney. *Journal of Physical Chemistry C* 113 4240 (2009).
- “Self-healing diffusion quantum Monte Carlo algorithms: direct reduction of the fermion sign error in electronic structure calculations”. F. A. Reboredo, R. Q. Hood, and P. R. C. Kent. *Physical Review B* 79 195117 (2009).
- “New algorithm to enable 400+ TFlop/s sustained performance in simulations of disorder effects in high-T<sub>c</sub> 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).
- “Computational Challenges of Large-Scale Long-Time First-Principles Molecular Dynamics”. P. R. C. Kent. *Journal of Physics: Conference Series* 125 012058 (2008).
- “Quantum Monte Carlo algorithms for electronic structure at the petascale; the endstation project”. Kenneth P. Esler, Jeongnim Kim, David M. Ceperley, Wirawan Purwanto, Eric J. Walter, Henry Krakauer, Shiwei Zhang, P. R. C. Kent, Richard G. Hennig, Cyrus Umrigar, Michal Bajdich, Jindrich Kolorenc, Lubos Mitas, Ashok Srinivasan. *Journal of Physics: Conference Series* 125 012057 (2008).
- “Charge-order fluctuations in one-dimensional silicides”. Changgan Zeng, P. R. C. Kent, Tae-Hwan Kim, An-Ping Li, and Hanno H. Weitering. *Nature Materials* 7 539 (2008).
- “Neutral and charged excitations in carbon fullerenes from first-principles many-body theories”. Murilo L. Tiago, P.R.C. Kent, Randolph Q. Hood, and Fernando A. Reboredo. *Journal of Chemical Physics* 129 084311 (2008).
- “Combined density functional and dynamical cluster quantum Monte Carlo calculations of the three-band Hubbard model for hole-doped cuprate superconductors”. P. R. C. Kent, T. Saha-Dasgupta, O. Jepsen, O. K. Andersen, A. Macridin, T. A. Maier, M. Jarrell and T. C. Schulthess. *Physical Review B* 78 035132 (2008).
- “Electronic structure of xDNA”. Miguel Fuentes-Cabrera, Xiongce Zhao, P. R. C. Kent, and Bobby G. Sumpter. *Journal of Physical Chemistry B* 111 9057 (2007).
- “Epitaxial stabilization of ferromagnetism in the nanophase of FeGe”. Changgan Zeng, P. R. C. Kent, M. Eisenbach, G. M. Stocks, Maria Torija, Jian Shen, and Hanno H. Weitering. *Physical Review Letters* 96 127201 (2006).
- “A systematic study of superconductivity in the 2D Hubbard model”. T. A. Maier, M. Jarrell, T. C. Schulthess, P. R. C. Kent, J. B. White. *Physical Review Letters* 95 237001 (2005).
- “Quantum Monte Carlo Study of the Optical and Diffusive Properties of the Vacancy Defect in Diamond”. Randolph Q. Hood, P. R. C. Kent, R. J. Needs, and P. R. Briddon. *Physical Review Letters* 91 076403 (2003).
- “GEANT 4 - a simulation toolkit”. S. Agostinelli et al. (GEANT 4 Collaboration). *Nuclear Instruments and Methods in Physics Research A* 506 250 (2003).
- “Pseudopotential theory of dilute III-V nitrides”. P. R. C. Kent, L. Bellaiche, and Alex Zunger. *Semiconductor Science and Technology* 17 851 (2002).
- “Theory of electronic structure evolution in GaAsN and GaPN alloys”. P. R. C. Kent and Alex Zunger. *Physical Review B* 64 115208 (2001).
- “Carrier localization and the origin of luminescence in cubic InGaN alloys”. P. R. C. Kent and Alex Zunger. *Applied Physics Letters* 79 1977 (2001).
- “Evolution of III-V Nitride Alloy Electronic Structure: The Localized to Delocalized Transition”. P. R. C. Kent and Alex Zunger. *Physical Review Letters* 86 2613 (2001).
- “Carbon clusters near the crossover to fullerene stability”. P. R. C. Kent, M. D. Towler, R. J. Needs, and G. Rajagopal. *Physical Review B* 62 15394 (2000).
- “Development and performance of a mixed OpenMP/MPI quantum Monte Carlo code”. Lorna Smith and Paul Kent. *Concurrency: Practice and Experience* 12 1121 (2000).
- “Monte Carlo energy and variance-minimization techniques for optimizing many-body wave functions”. P. R. C. Kent, R. J. Needs, and G. Rajagopal. *Physical Review B* 59 12344 (1999).

**Graduate and Postdoctoral Advisors:** Prof. Richard J. Needs, Cavendish Laboratory, University of Cambridge. Dr. Alex Zunger, National Renewal Energy Laboratory. Prof. Mark Jarrell, Louisiana State University. Thomas C. Schulthess, Director Swiss Supercomputing Center.

