

Paul R. C. Kent

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Nanomaterials Theory Institute
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Education

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

Professional Experience

2009-present	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, http://geant4.org , High Energy Physics detector simulation tool
1992-present	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.

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.

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.