# **Peter Doak**

# **Scientific Software Engineer**

Computational Chemistry and Nanomaterials, Oak Ridge National Laboratory, Oak Ridge, TN 37830

**Web**: http://www.ornl.gov/~epd **Voice**: 865-407-3995 **Email**: doakpw@ornl.gov

# Professional Preparation

***Graduate****:* PhD, Physical Chemistry, University of California, Berkeley 2014.

***Undergraduate****:* BA, Modern Culture and Media, Brown University 1996.

# Appointments

***Current Position:*** Scientific Software Engineer, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37830, Dec 2017 – present.

***Previous Position:*** Postdoctoral Researcher, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37830, Dec 2014 – Dec 2017.

# Recent Publications and Open Source Scientific Code

1. Giovanni Balduzzi; Arghya Chatterjee; Ying Wai Li; Peter W. Doak; Urs Haehner; Ed F. D'Azevedo; Thomas A. Maier; Thomas Schultess "Accelerating DCA++ (Dynamical Cluster Approximation) Scientific Application on the Summit Supercomputer," 2019 28th International Conference on Parallel Architectures and Compilation Techniques (PACT), Seattle, WA, USA, 2019, pp. 433-444, doi: 10.1109/PACT.2019.00041.
2. Source code repository for DCA++, https://github.com/CompFUSE/DCA
3. Paul Kent; Abdulgani Annaberdiyev; Anouar Benali; M. Bennett; Edgar Josue; Landinez Borda; Peter Doak; Kenneth Jordan; Jaron Krogel; Ilkka Kylanpaa; Joonho Lee; Ye Luo; Fionn Malone; Cody Melton; Lubos Mitas; Miguel Morales; Eric Neuscamman; Fernando Reboredo; Brenda Rubenstein; Kayahan Saritas; Shiv Upadhyay; Hongxia Hao; Guangming Wang; Shuai Zhang; Luning Zha. “QMCPACK: Advances in the development, efficiency, and application of auxiliary field and real-space variational and diffusion quantum Monte Carlo” The Journal of Chemical Physics May 2020 Vol. 152 Issue 17 Pages 17410. <https://doi.org/10.1063/5.0004860>
4. Source Code Repository for QMCPACK, https://github.com/QMCPACK/qmcpack
5. Jared L. Wilmoth, Peter W. Doak, Andrea Timm, Michelle Halsted, John D. Anderson, Marta Ginovart, Clara Prats, Xavier Portell, Scott T. Retterer, Miguel Fuentes-Cabrera “A Microfluidics and Agent-Based Modeling Framework for Investigating Spatial Organization in Bacterial Colonies: The Case of Pseudomonas Aeruginosa and H1-Type VI Secretion Interactions.” Front. Microbiol., 06 February 2018 | https://doi.org/10.3389/fmicb.2018.00033

# Research Interests and Expertise

# Building tools that allow more extensive investigation of molecules on interfaces and study of dynamic materials. Using hybrid CPU/GPU methods in C++, CUDA, OPENMPI, OPENMP. Focused on abinitio based modeling especially of systems not captured by conventional methods with a special interest in interfaces. Developing high speed massively parallel directed energy surface scanning for both dimer interactions and material deformation modes. Also developing a monte carlo code that load parameters directly from abinitio outputs for exploration of interface structures.