Peter W. Doak

Senior Scientific Software Engineer
Computational Chemsitry and Nanomaterials Group
Advanced Computing Methods for Physical Sciences Section
Computational Sciences and Engineering Division
Computing and Computational Sciences Directorate
Oak Ridge National Laboratory
P. O. Box 2008,
Bldg. 8610 Rm. P-298
Oak Ridge, TN 37831-6494

web: staff webpage
email: doakpw@ornl.gov

Appointments

2022 - Present	Senior Scientific Software Engineer, Oak Ridge National Laboratory.
2017 - 2022	Scientific Software Engineer, Oak Ridge National Laboratory.
2014 - 2017	Postdoctoral Researcher, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory.

Education

2014	Physical Chemistry, University of California, Berkeley	Ph.D.
1996	Modern Culture and Media, Brown University	B.A.

Publications

P. Doak, G. Balduzzi, P. Laurell, E. Dagotto, and T. A. Maier, "Spin-singlet topological superconductivity in the attractive rashba-hubbard model", Physical Review B **107**, 10.1103/physrevb.107.224501 (2023).

Y. W. Li, P. W. Doak, G. Balduzzi, W. Elwasif, E. F. D'Azevedo, and T. A. Maier, "Machine-learning accelerated studies of materials with high performance and edge computing", in *Communications in computer and information science* (Springer International Publishing, 2022), pp. 190–205.

Y. Luo, P. Doak, and P. Kent, "A high-performance design for hierarchical parallelism in the qmcpack monte carlo code", in 2022 ieee/acm international workshop on hierarchical parallelism for exascale computing (hipar) (Nov. 2022).

N. Sivadas, P. Doak, and P. Ganesh, "Anharmonic stabilization of ferrielectricity in $CuInP_2Se_6$", Physical Review Research **4**, 10.1103/physrevresearch.4.013094 (2022).

P. R. C. Kent, A. Annaberdiyev, A. Benali, M. C. Bennett, E. J. Landinez Borda, P. Doak, H. Hao, K. D. Jordan, J. T. Krogel, I. Kylänpää, J. Lee, Y. Luo, F. D. Malone, C. A. Melton, L. Mitas, M. A. Morales, E. Neuscamman, F. A. Reboredo, B. Rubenstein, K. Saritas, S. Upadhyay, G. Wang, S. Zhang, and L. Zhao, "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 **152**, 10.1063/5.0004860 (2020).

S. Jeon, M. Kim, P. W. Doak, H. A. Atwater, and H. Kim, "Probing surface chemistry at an atomic level: decomposition of 1-propanethiol on GaP(001) (2×4) investigated by STM, XPS, and DFT", The Journal of Physical Chemistry C **123**, 2964–2972 (2019).

Updated: Tuesday 19th March, 2024

J. L. Wilmoth, P. W. Doak, A. Timm, M. Halsted, J. D. Anderson, M. Ginovart, C. Prats, X. Portell, S. T. Retterer, and M. 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", Frontiers in Microbiology **9**, 10.3389/fmicb.2018.00033 (2018).

P. Doak, "Covalent functionalization of gap(110) surfaces via a staudinger-type reaction with perfluorophenyl azide", Journal of Physical Chemistry C, 10.1021/acs.jpcc.6b10691 (2016).

S. Jeon, P. W. Doak, B. G. Sumpter, P. Ganesh, and P. Maksymovych, "Thermodynamic control of two-dimensional molecular ionic nanostructures on metal surfaces.", ACS nano **10**, 7821–9 (2016).

Y. Li, P. Zolotavin, P. Doak, L. Kronik, J. B. Neaton, and D. Natelson, "Interplay of bias-driven charging and the vibrational stark effect in molecular junctions", Nano Letters **16**, 1104–1109 (2016).

D. Cedeno, A. Krawicz, P. Doak, M. Yu, J. B. Neaton, and G. F. Moore, "Using molecular design to control the performance of hydrogen-producing polymer-brush-modified photocathodes", Journal of Physical Chemistry Letters **5**, 3222–3226 (2014).

Y. Li, P. Doak, L. Kronik, J. B. Neaton, and D. Natelson, "Voltage tuning of vibrational mode energies in single-molecule junctions", Proceedings of the National Academy of Sciences of the United States of America **111**, 1282–1287 (2014).

M. M. Ugeda, M. Yu, A. J. Bradley, P. Doak, W. J. Liu, G. F. Moore, I. D. Sharp, T. D. Tilley, J. B. Neaton, and M. F. Crommie, "Adsorption and stability of pi-bonded ethylene on gap(110)", Journal of Physical Chemistry C **117**, 26091–26096 (2013).

M. Yu, P. Doak, I. Tamblyn, and J. B. Neaton, "Theory of covalent adsorbate frontier orbital energies on functionalized light-absorbing semiconductor surfaces", Journal of Physical Chemistry Letters **4**, 1701–1706 (2013).

S. Sharifzadeh, I. Tamblyn, P. Doak, P. T. Darancet, and J. B. Neaton, "Quantitative molecular orbital energies within a g(0)w(0) approximation", European Physical Journal B **85** (2012).

J. A. Malen, P. Doak, K. Baheti, T. D. Tilley, A. Majumdar, and R. A. Segalman, "The nature of transport variations in molecular heterojunction electronics", Nano Letters **9**, 3406–3412 (2009).

J. A. Malen, P. Doak, K. Baheti, T. D. Tilley, R. A. Segalman, and A. Majumdar, "Identifying the length dependence of orbital alignment and contact coupling in molecular heterojunctions", Nano Letters **9**, 1164–1169 (2009).

K. Baheti, J. A. Malen, P. Doak, P. Reddy, S.-Y. Jang, T. D. Tilley, A. Majumdar, and R. A. Segalman, "Probing the chemistry of molecular heterojunctions using thermoelectricity", Nano Letters **8**, 715–719 (2008).

G. Dukovic, M. Balaz, P. Doak, N. D. Berova, M. Zheng, R. S. McLean, and L. E. Brus, "Racemic single-walled carbon nanotubes exhibit circular dichroism when wrapped with dna", Journal of the American Chemical Society **128**, 9004–9005 (2006).

Research Interests

Scientific HPC Application Architecture; Correlated and Interfacial Electronic Structure; Quantum Monte Carlo Methods; Many Body Theory

Major Projects

- Maintainer and lead developer of the DCA++ code.

- Maintainer and lead developer of the QMCPACK code.

Professional Memberships

IEEE • APS