

Curriculum Vitae

Kevin P. Driver

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Career Summary

Ph.D. in Physics with a research background in large-scale simulations in the areas of high energy density physics and condensed matter physics. Significant experience in the application of first-principles simulations, including quantum molecular dynamics (QMD), quantum Monte Carlo (QMC), and path integral Monte Carlo (PIMC). Co-author of 15 scientific publications, a similar number of grant proposals, and 30 conference presentations.

Research Positions **University of California, Berkeley**

2011-Present

- Postdoctoral Research Associate
- Grant Title: *Path Integral Monte Carlo Simulations of Dense Plasmas with Heavier Elements* (DE-SC0010517, Office of Fusion Science)
- PI: Prof. Burkhard Militzer
Contributed to the development and application of PIMC for computing equations of state of heavier elements.

Education

2011

The Ohio State University

- Ph.D., Physics (Computational Condensed Matter)
- Thesis Title: *Establishing Quantum Monte Carlo and Hybrid Density Functional Theory as Benchmarking Tools for Complex Solids*
- Advisor: Prof. John Wilkins

2006

M.S., Physics

2003

University of Louisville

- B.S., Physics, *Suma Cum Laude*
- Honors Thesis: *Tight-binding Molecular Dynamics Simulations of Nanocrystalline Diamond and Graphite*

Publications (Peer-Reviewed)

1. Y. Lin, A. Floris, L. Shulenburger, **K. P. Driver**, and R. E. Cohen, *Earth's D" layer is indeed consistent with the silicate perovskite to post perovskite transition*, submitted to Science Advances (2016)

2. S. X. Hu, B. Militzer, L. A. Collins, **K. P. Driver**, and J. D. Kress, *First-principles prediction of the softening of the silicon shock Hugoniot curve* submitted to Phys. Rev. B (under review, 2016)
3. **K. P. Driver** and B. Militzer, *First-principles equation of state calculations of warm dense nitrogen*, Phys. Rev. B 91, 064101 (2016).
4. **K. P. Driver**, F. Soubiran, Shuai Zhang, and B. Militzer, *First-principles equation of state and electronic properties of warm dense oxygen*, J. Chem. Phys. 143, 164507 (2015).
5. B. Militzer and **K. P. Driver**, *Development of Path Integral Monte Carlo Simulations with Localized Nodal Surfaces for Second-Row Elements*, Phys. Rev. Lett. 115, 176403 (2015)
6. **K. P. Driver** and B. Militzer, *First-principles simulations and shock Hugoniot calculations of warm dense neon*, Phys. Rev. B, 04510 (2015)
7. Y. Lin, R. E. Cohen, S. Stackhouse, **K. P. Driver**, B. Militzer, L. Schulenburg, and J. Kim, *Equations of state and stability of MgSiO₃ perovskite and post-perovskite phases from quantum Monte Carlo simulations*, Phys. Rev. B, 90, 184103 (2014)
8. L. X. Benedict, **K. P. Driver**, S. Hamel, B. Militzer, T. Qi, A. A. Correa, A. Saul, and E. Schwegler, *Multiphase equation of state for carbon addressing high pressures and temperatures*, Phys. Rev. B, 89, 224109 (2014)
9. S. Zhang, H. F. Wilson, **K. P. Driver**, B. Militzer, *H₂O and other hydrogen-oxygen compounds at giant-planet core pressures*, Phys. Rev. B 87, 024112 (2013)
10. **K. P. Driver** and Burkhard Militzer, *All-electron path integral Monte Carlo simulations of warm dense matter: Application to water and carbon plasmas*, Phys. Rev. Lett., 108, 115502 (2012)
11. **K. P. Driver**, R. E. Cohen, Zhingang Wu, R. Militzer, R. Lopez Rios, M. D. Towler, R. J. Needs, and J. W. Wilkins, *Quantum Monte Carlo computations of phase stability, equations of state, and elasticity of high-pressure silica*, Proc. Natl. Acad. Sci. USA, 107, 9519-9524 (2010)
12. R. G. Hennig, A. Wadehra, **K. P. Driver**, W. D. Parker, C. J. Umrigar, and J. W. Wilkins, *Phase transformation in Si from semiconducting diamond to metallic beta-Sn phase in QMC and DFT under hydrostatic and anisotropic stress*, Phys. Rev. B, 82, 014101 (2010).
13. M. Floyd, Y. Zhang, **K. P. Driver**, Jeff Drucker, P.A. Crozier, D. J. Smith, *Nanometer-scale composition variations in Ge/Si(100) islands*, Appl. Phys. Lett. 82, 1473 (2003).

14. Y. Zhang, M. Floyd, **K. P. Driver**, Jeff Drucker, P.A. Crozier, D. J. Smith, *Evolution of Ge/Si(100) island morphology at high temperature*, Appl. Phys. Lett. 80, 3623 (2002).
15. P. J. Ouseph, **K. P. Driver**, J. Conklin, *Polarization of Light By Reflection and the Brewster Angle*, Am. J. Phys. 69, 1166 (2001).

Successful Proposals Co-authored

- Funded Research Proposals:

1. DOE Office of Science, 2015 (\$690,450)
2. DOE Office of Science, 2012 (\$250,000)
3. DOE-BES-DMS, 2008 (\$750,000)

- Funded Computational Resource Proposals:

1. OLCF INCITE 2014, 100 million CPU hours
2. NERSC 2008-2015, 1-3million CPU hours per year
3. NCAR CISL 2011-2015, 1-4 million CPU hours per year
4. OSC 2006-2010 1-4 million CPU hours per year

Invited Talks

1. K. P. Driver and B. Militzer, *Path Integral Monte Carlo Simulations of Warm Dense Matter and Planetary Interiors*, SFPUP, Zhangjiajie, China, 2014.
2. K. P. Driver, S. Zhang, B. Militzer, and R. E. Cohen, *Post-DFT Methods for Earth Materials: Quantum Monte Carlo Simulations of (Mg,Fe)O*, AGU, San Francisco, CA, 2013.
3. Kevin P. Driver, *Predictive materials simulations: No longer the weak link in computational materials design*, Ohio State University, 2010.

Contributed Talks

1. K. P. Driver *et al.*, *Path Integral Monte Carlo Simulations of Warm Dense PLasmas with mid-Z Elements*, APS-DPP Meeting, San Jose, CA, 2016.
2. K. P. Driver *et al.*, *First-Principles Equations of State and Shock Hugoniot of First- and Second-Row Plasmas*, APS March Meeting, Baltimore, MD, 2016.

3. K. P. Driver, F. Soubiran, S. Zhang, and B. Militzer, *First-Principles Equation of State and Electronic Structure of Oxygen, Neon, and Silicon Plasmas* ICHED, San Diego, CA, 2015.
4. K. P. Driver *et al.*, *Quantum Monte Carlo Simulations of a Single Iron Impurity in MgO*, APS March Meeting, Denver, CO, 2014.
5. K. P. Driver and B. Militzer, *Path Integral Monte Carlo Study of Warm Dense Matter: Second-row elements*, APS March Meeting, Baltimore, MD, 2013.
6. K. P. Driver and B. Militzer, *All-electron Path Integral Monte Carlo Simulations of Warm Dense Matter: Application to Water and Carbon Plasmas*, APS March Meeting, Boston, MA, 2012.
7. Kevin P. Driver *et al.* *Quantum Monte Carlo Equations of State of alpha- and beta-Magnesium Silicate* APS March Meeting, Pittsburgh, PA, 2009.
8. Kevin P. Driver *et al.* *Quantum Monte Carlo Study of the Elastic Instability of Stishovite Under Pressure* APS March Meeting, New Orleans, LA, 2008.
9. Kevin P. Driver, *Pushing the Envelope of Accuracy and Cost in High-Pressure Electronic Theory: Application to elasticity of silica*, Laboratory Seminar, Carnegie Institution of Washington, Geophysical Laboratory, Washington, D.C; August, 2007.
10. Kevin P. Driver *et al.* *QMC and DFT Functional Performance for Silica*, American Physical Society March Meeting, Denver, CO, 2007.
11. Kevin P. Driver *et al.* *Silicon-interstitials-based Benchmarking of DFT Exchange-correlation Potentials*, American Physical Society March Meeting, Baltimore, MD, 2006.
12. Kevin P. Driver *et al.* *Diffusion Monte Carlo Formation Energies of Silicon Self-Interstitial Defects*, American Physical Society March meeting, Los Angeles, CA, 2005.
13. Kevin P. Driver *et al.* *The Morphological Evolution and Composition of Epitaxially Self-Assembled Ge/Si(100) Quantum Dots*, APS March Meeting, Indianapolis, IN, 2002.

Posters

1. K. P. Driver, F. Soubiran, S. Zhang, and B. Militzer, *First-Principles Simulations of Warm Dense Matter*, Gordon Conference, Holderness, NH, USA, 2016.
2. K. P. Driver, F. Soubiran, S. Zhang, and B. Militzer, *Comparison of Electronic Properties and Equations of State of First-Row Plasmas*, High Energy Density Laboratory Astrophysics, Menlo Park, CA, USA, 2016.

3. K. P. Driver, F. Soubiran, S. Zhang, and B. Militzer, *First-Principles Equations of State Calculations of First- and Second-Row Plasmas*, NIF User Meeting, Livermore, CA, 2016.
4. K. P. Driver, F. Soubiran, S. Zhang, and B. Militzer, *First-Principles Equations of State Calculations of First- and Second-Row Plasmas* AGU, San Francisco, CA, 2015.
5. K. P. Driver and B. Militzer *First-Principles Simulations and Shock-Hugoniot Calculations of Warm Dense Neon*, AGU, San Francisco, 2014.
6. K. P. Driver and B. Militzer, *All-electron Path Integral Monte Carlo Simulations of Warm Dense Matter: Application to Water and Carbon Plasmas*, AGU, San Francisco, 2012.
7. Kevin P. Driver *et al.* *Quantum Monte Carlo Study of the Elastic Instability of Stishovite Under Pressure*, American Geophysical Union Fall Meeting, San Francisco, CA, December, 2011.
8. Kevin P. Driver *et al.* *Quantum Monte Carlo Study of the Elastic Instability of Stishovite Under Pressure*, Electronic Structure Workshop, UIUC, June, 2008.
9. Kevin P. Driver *et al.* *Hybrid Density Functional Performance for Silica*, Quantum Monte Carlo Summer School, University of Illinois, Urbana-Champaign, IL, July, 2007.
10. Kevin P. Driver *et al.* *Quantum Monte Carlo Study of the Elastic Instability of Stishovite Under Pressure*, American Geophysical Union Fall Meeting, San Francisco, CA, December, 2007.
11. Kevin P. Driver *et al.* *Hybrid Density Functional Performance for Silica*, Electronic Structure Workshop, North Carolina State university, Raleigh, NC, June, 2007.
12. Kevin P. Driver *et al.* *Simulations of Silica Phases Beyond the Generalized-Gradient Approximation*, American Geophysical Union Fall Meeting, San Francisco, CA, December, 2006.
13. Kevin P. Driver *et al.* *Quantum Mechanical Predictions of Defect Properties for Realistic Device Simulations*, Electronic Structure Workshop, The Ohio State University, Columbus, OH, June, 2006.
14. Kevin P. Driver *et al.* *Quantum Mechanical Predictions of Defect Properties for Realistic Device Simulations*, Ohio Nanotechnology Summit, Columbus, OH, April, 2006.
15. Kevin P. Driver *et al.* *Diffusion Monte Carlo Formation Energies of Silicon Self-Interstitial Defects*, Electronic Structure Workshop, Cornell university, Ithica, NY, June, 2005.

16. Kevin P. Driver *et al.* *Formation Energies of Small Interstitial Clusters: DMC vs. DFT*, Quantum Monte Carlo Workshop, Banff, Canada, January, 2005.

Awards Received

- 2007 AGU, Outstanding Student Paper Award
- 2007,2008 Winner of OSU-Physics Graduate Student Poster Competition
- 2003-2005 Fowler Fellowship, Ohio State University, Physics.

Professional Organizations

- 2006-Present Member, American Geophysical Union.
- 1999-Present Member, American Physical Society.

Schools and Workshops Attended

- 2012 UIUC Computational Physics Summer School on PIMC (lecturer)
- 2007 University of Illinois-UC, Summer School on Computational Materials Science
- 2005 Cornell University, Summer School on Density Functional Theory
- 2005 University of Illinois-UC, Summer School on Electronic Structure Methods

Technical Skills

- *Computational*: Linux tools, Mathematica, Octave, Maple, L^AT_EX, git/svn, make, bash, massively parallelized HPC
- *Mathematical Expertise*: Linear Algebra, probability and statistics, stochastic processes, non-linear optimization, Monte Carlo
- *Languages*: C, C++, Python, Fortran, Bash
- *C++ Libraries*: HDF5, LAPACK, BLAS, MKL, MPI, OpenMP
- *Python Libraries*: NumPy, SciPy, SymPy, Pyplot, Pandas, Matplotlib

Academic Service

- Reviewer for Phys. Rev. Lett., Phys. Rev. B, J. Chem Phys., J. Comp. Phys., Scientific Advances, DOE/NSF proposals, and MDPI (open-access journal).

References

Internal to LLNL:

1. Dr. Marius Millot
email: millot1@llnl.gov
2. Dr. Richard Kraus
email: kraus4@llnl.gov
3. Dr. Lorin Benedict
email: benedict5@llnl.gov

External:

1. Prof. Burkhard Militzer (Postdoc advisor 2011-present)
University of California, Berkeley
email: militzer@berkeley.edu
2. Dr. Ronald E. Cohen (Collaborator)
Carnegie Institution for Science
email: rcohen@carnegiescience.edu
3. Prof. John W. Wilkins (M.S. and Ph.D. advisor 2004-2011)
The Ohio State University
email: wilkins@mps.ohio-state.edu