Charles C. Peterson, Ph.D.

High-Performance Computing R&D Scientist

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Interdisciplinary researcher, collaborator, and information technology professional with over ten years of experience in scientific computing and computational research applications across STEM and non-STEM areas. My focus is in applying advanced High-Performance Computing (HPC) capabilities to enhance research throughput that involves closely collaborating with a diverse research community. My interests are using data modeling (Artificial Intelligence and Big Data techniques) and molecular modeling to describe Rare Earth Element systems. Using HPC and other advanced scientific computing techniques is essential to expand research by developing computational protocols to study heavy element chemistry with national security and other applications.

Education

Doctor of Philosophy in Physical Chemistry, 12/2015
University of North Texas, Denton, TX
Dissertation: Accurate Energetics across the Periodic Table via Quantum Chemistry

Bachelor of Science in Chemistry, 05/2009
University of North Texas, Denton, TX
Major: Chemistry
Minor: Computer Science

Professional Experience

Senior HPC System Administrator 12/2020 – Present
Office of Advance Research Computing
University of California, Los Angeles
Responsibilities include the operation of UCLA's HPC resources and consultation services to a board range of UCLA researchers. This is a senior programmer/analyst position that involve installing and maintain hardware and software to ensuring scientific application are running at maximum efficiency.

Research Scientist II 11/2019 – 12/2020
North Texas Scientific Computing
University of North Texas (UNT), Denton, TX

Provides consultation services for UNT researchers across all disciplines pursued on-campus using advance scientific computing resources. Explores and evaluates grant opportunities for HPC related projects. Assesses new and emerging computing to advance enabling HPC technologies for UNT's research computing. Provides research collaboration services and performs research in artificial intelligence and machine learning applications in STEM and non-STEM areas. Mentors and instructs graduate students on applying HPC resources to their masters and doctoral research.

Cross-Functional IT Support Analyst, 02/2018 - 11/2019
Research IT Services
University of North Texas, Denton, TX
Enhanced scientific computing resources at UNT, including supporting advance data storage and computational technologies. Optimized software and libraries for best performance for material science and data analytics applications. Conducted community training and outreach programs that included creating material for interactive workshops and tutorials.

IT Manager I – High Performance Computing, 04/2015 - 02/2018
Academic Computing & User Services
University of North Texas, Denton, TX
Maintained HPC resources and allocations for UNT researchers and courses. Provided end-user HPC support and software development.

Graduate Research Assistant, 05/2008 - 12/2015
Center for Advanced Scientific Computing and Modeling (CASCaM)
University of North Texas, Denton, TX
Developed new composite strategies for computational quantum chemistry for greater understanding and accurate predictions for advancements of not only basis science, but also in applications needed for the growth and health of the U.S. economy. Advanced theoretical techniques for simulating the structural, thermochemical, and spectroscopic properties of chemical compounds. Studies of energetics range from silicon modules and clusters, noble gases and transition metal bonds, and small lanthanide systems.

Graduate Research Assistant, 01/2012 - 04/2015
System administrator for HPC resources
University of North Texas, Denton, TX
Academic Computing & User Services - University Information Technology

Graduate Research Assistant, 08/2009 - 05/2012
Computational Chemistry Instructional Laboratory (CCIL)
University of North Texas, Denton, TX
Lab Assistant - Maintained the laboratory and providing computational chemistry support.

Awards and Recognitions

"Extra Mile" Award – University of North Texas (2018)
Tuition Reduction Benefit Award - University of North Texas (2015)
Graduate Research Assistant Scholarship - University of North Texas (2009)
Dallas/Fort Worth American Chemical Society Award (2009)
J. L. Carrico Award - Department of Chemistry, University of North Texas (2009)
American Chemical Society Analytical Chemistry Award (2008)
Undergraduate Dean's List - University of North Texas (2005, 2006, 2008)

Professional Activities

Publication and Editorial Service

Reviewer for PEARC21 conference, 2021

Editor, American Chemical Society Book Series **"Computational Science Applications in Nuclear and Radiochemistry"**, 2020

HPC allocation management for *University of North Texas* HPC allocations, 2015 - 2022

Reviewer for XSEDE EMPOWER Program, 2020

Professional Organizations

Senior Scientific Fellow, 06/2017 – Present
Institute for Nuclear Security, Howard H. Baker Jr. Center for Public Policy
University of Tennessee, Knoxville, TN
High-Performance Computing applications in national and nuclear security.

Member of ÚNeTe – Latinx Faculty/Staff Alliance at *University of North Texas,* 2020

Member of American Chemical Society
Division of Nuclear Chemistry & Technology 2015 - Present
Division of History 2015 - 2016
Division of Physical Chemistry 2015 - 2016

Member of Association for Computing Machinery SIGHPC 2020 – Present

XSEDE Campus Champion, 06/2016 – 12/2020

Provides access and application support to researchers and students in NSF eXtreme Scale Engineering Discovery Environment (XSEDE) computational resources.

Committee and Organizational Activities

Member, Diversity, Equity, and Inclusion Action Committee (DEIAC), Nuclear Engineering, *University of Tennessee*, 2020 - Present

Social Media Manager for UNT Research IT Services, 2018 - 2020

Chair, American Chemical Society Annual Meeting, Nuclear Chemistry and Technology Division (ACS NUCL), Session "**Data Science & Artificial Intelligence Applications in Nuclear and Radiochemistry**", 05/2021, 05/2022, and 08/2022, 08/2023

Chair, American Chemical Society Annual Meeting, Nuclear Chemistry and Technology Division (ACS NUCL), Session "**Computational Methods for Lanthanides & Actinides: Theory & Applications**", 08/2020, 05/2020, 08/2019, 05/2019, and 08/2018

Presider, American Chemical Society Annual Meeting, Nuclear Chemistry and Technology Division (ACS NUCL), Session "**Computational Methods for Lanthanides & Actinides: Theory & Applications**" 05/2020, 08/2019, 08/2018, and 05/2018

Presider, American Chemical Society Annual Meeting, Division of Physical Chemistry (ACS PHYS), Session "**Thermodynamics, reactivity, and spectroscopy of the heavy elements**" 05/2014

Professional Training

QMCPack User Workshop, Oak Ridge National Laboratory, TN, 05/2019
Workshop for current users and developers. Provided training in added features and planned improvements for the electronic structure code, QMCPACK (scientific software), which specializes in quantum Monte Carlo techniques

OpenFabrics Alliance Workshop, Austin, TX, 03/2017
Workshop focused on the current and emerging needs of high-performance network community. This workshop discussed the emerging technologies of OpenFabrics and future needs and challenges in computing over high speed networks.

DDN EXAScaler Technical Training, Colorado Spring, CO, 02/2016
Training course on setting up and maintaining high performance parallel file systems, managing large data storage and Lustre design for Big Data projects.

XSEDE/PRACE EU-US HPC Summer School, Dublin, Ireland, 06/2012
Summer school for challenges of High-Performance Computing in computational sciences. Interactive training in current programming skills and software libraries.

Publications

Edward F. Valeev, Robert J. Harrison, **Charles C. Peterson**, Deborah A. Penchoff, "Direct determination of optimal real-space orbitals for correlated electronic structure of molecules", J. Chem. Theory Comput, 2023.

Deborah A. Penchoff, **Charles C. Peterson**, Eleigha M. Wrancher, George Bosilca, Robert J. Harrison, Edward F. Valeev, Paul D. Benny, "Evaluations of Molecular Modeling and Machine Learning for Predictive Capabilities in Binding of Lanthanum and Actinium with Carboxylic Acids", JRNC, 331 (12), 2022.

Edward F. Valeev, Robert J. Harrison, **Charles C. Peterson**, Deborah A. Penchoff, "Direct determination of optimal real-space orbitals for correlated electronic structure of molecules", arXiv:2207.10841, 2022.

Joseph F. DeJesusa, Ryan W. F. Kerr, Deborah A. Penchoff, Xian B. Carrolla, **Charles C. Peterson**, Polly L. Arnold and David M. Jenkins. "Actinide tetra-N-heterocyclic carbene sandwiches". Chem. Sci., 2021.

Deborah A. Penchoff, **Charles C. Peterson**, Eleigha M. Wrancher, George K. Schweitzer, Robert J. Harrison, Rose A. Boll, Paul D. Benny, Howard L. Hall. "Evaluating Complexation of Lanthanum and Actinium for Applications in Radiochemical Separations". American Chemical Society Book series "Computational Science for Lanthanides and Actinides", 2020. Invited chapter.

Charles C. Peterson, Jack Burn, Deborah A. Penchoff. "Artificial Intelligence in Nuclear and Radiochemistry" – American Chemical Society Book Series "Computational Science for Lanthanides and Actinides", 2021. Invited chapter.

Charles C. Peterson, Deborah A. Penchoff, John D. Auxier II, Howard L. Hall, "Establishing Cost-Effective Computational Models for the Prediction of Lanthanoid Binding in $[Ln(NO_3)]^{2+}$ (with Ln = La to Lu)", ACS Omega, 2019, 4, 1, 1375-1385.

Deborah A. Penchoff, **Charles C. Peterson**, Jon P. Camden, James Bradshaw, John D. Auxier II, George K. Schweitzer, David M. Jenkins, Robert J. Harrison, Howard L. Hall, "Structural Analysis of the Complexation of Uranyl, Neptunyl, Plutonyl, and Americyl with Cyclic Imide Dioximes", ACS Omega, 2018, 3, 10, 13984-13993.

Deborah A. Penchoff, **Charles C. Peterson**, Mark S. Quint, John D. Auxier II, George K. Schweitzer, David M. Jenkins, Robert J. Harrison, Howard L. Hall. "Structural Characteristics, Populations Analysis, and Binding Energies of $[An(NO_3)]^{2+}$, [with An = Ac – Lr]", ACS Omega, 2018, 3, 10, 14127-14143.

Charles Peterson, Deborah A. Penchoff, and Angela K. Wilson, "Prediction of thermochemical properties across the periodic table: A review of correlation consistent Composite Approach (ccCA) strategies and applications" *Annual Reports in Computational Chemistry*, Vol. 12, 2016.

Charles Peterson, Deborah A. Penchoff, and Angela K. Wilson, "*Ab initio* approaches for the determination of heavy element energetics: Ionization energies of trivalent lanthanides (Ln = La-Eu)" *J. Chem. Phys*., 2015, 143, 19, 194109.

Cong Liu, **Charles Peterson**, and Angela K. Wilson, "C-O Bond Cleavage of Dimethyl Ether by Transition Metal Ions: A Systematic Study on Catalytic Properties of Metals and Performance of DFT Functionals" *J. Phys. Chem. A*, 2013, 117, 5140.

Gbenga A. Oyedepo, **Charles Peterson**, George Schoendorff, and Angela K. Wilson, "Spectroscopic properties of Ar_x-Zn and Ar_x-Ag^+ (x=1,2) van der Waals complexes" *J. Chem. Phys.*, 2013, 138, 104116.

Gbenga A. Oyedepo, **Charles Peterson**, and Angela K. Wilson, "Accurate predictions of the energetics of silicon compounds using the multireference correlation consistent composite approach" *J. Chem. Phys.,* 2011, 135, 094103.

Presentations

Charles C. Peterson, Deborah A. Penchoff "REACKT: Advancing Separations of Lanthanides and Actinides" ACS National Meeting and Expo, Division of Nuclear Chemistry and Technology, Fall 2024.

Charles C. Peterson, Deborah A. Penchoff "Advanced Computational Strategies for Lanthanide and Actinide Systems" ACS National Meeting and Expo, Division of Nuclear Chemistry and Technology, Fall 2023.

Charles C. Peterson "Big Data on HPC", Workshop Series, UCLA, 06/29/2023.

Charles C. Peterson, "Hoffman2 Happy Hour: Using RStudio", Workshop Series, UCLA, 09/28/2022.

Charles C. Peterson, "Hoffman2 Happy Hour: Anaconda", Workshop Series, UCLA, 09/21/2022.

Charles C. Peterson, "Building Containers for HPC", Workshop Series, UCLA, 07/06/2022.

Charles C. Peterson, "Using Containers on HPC Resources", Workshop Series, UCLA, 04/20/2022.

Charles C. Peterson, "Singularity on Hoffman2: Using containers on HPC resources" Workshop Series, UCLA, 04/29/2021.

Charles C. Peterson, D. A. Penchoff, "Understanding Binding Selectivity of Lanthanide and Actinide Compounds by Computational Protocols" International Workshop on Theory Frontiers in Actinide Sciences: Chemistry and Materials, Santa Fe, NM, 02/2 – 5/2020.

Charles C. Peterson, D. A. Penchoff, "Understanding Binding Selectivity of Lanthanides and Actinides by Computational Protocols" 64th Annual Radiobioassy & Radiochemical Measurements Conference, Santa Fe, NM, 08/28 – 30/2019.

Charles C. Peterson "Machine Learning Techniques with High Performance Computing" Invited Webinar, Institute for Nuclear Security, University of Tennessee, Knoxville TN, 08/05/2019.

Charles C. Peterson, D. A. Penchoff, "Computational protocol for binding selectivity of lanthanide and actinide systems" Division of Nuclear Chemistry and Technology, Computational Methods for Lanthanide & Actinide Chemistry, 258th American Chemical Society National Meeting & Exposition, San Diego CA, 08/ 2019.

Charles C. Peterson, D. A. Penchoff, H. L. Hall, R. J. Harrison, "Understanding selectivity of lanthanide and actinide compounds by computational techniques" Division of Nuclear Chemistry and Technology, Computational Methods for Lanthanide & Actinide Chemistry, 257th American Chemical Society National Meeting & Exposition, Orlando FL, 05/2019.

Charles C. Peterson, D. A. Penchoff, H. L. Hall, R. J. Harrison, "Utilizing computational protocols for binding selectivity of lanthanide and actinide compounds", Division of Nuclear Chemistry and Technology, Computational Methods for Lanthanides & Actinides: Theory & Application, 256th American Chemical Society National Meeting & Exposition, Boston MA, 08/2018.

Charles C. Peterson, "Understanding structural and thermochemical properties of actinide-containing compounds", Division of Nuclear Chemistry and Technology, Computational Methods for Lanthanides & Actinides: Theory & Application Session, 255th American Chemical Society National Meeting & Exposition, New Orleans LA, 05/2018.

Charles Peterson, Deborah A. Penchoff, Robert J. Harrison, "Investigation of the Selectivity of Cyclic Amidoxime Ligands to Uranyl by Theoretical Techniques", 62nd Conference on Radiobioassay & Radiochemical Measurements, Honolulu, Hawai'i, 02/2017.

Charles Peterson, Deborah Penchoff, Angela Wilson" Composite Approaches for accurate predictions of lanthanide and actinide chemistry" Division of Computers in Chemistry, Quantum Mechanics Session, 252nd American Chemical Society National Meeting & Exposition, Philadelphia PA, 08/2016.

Charles Peterson, Deborah Penchoff, Angela Wilson, "Composite Approach Towards Accurate Predictions of Lanthanide and Actinide Thermochemistry" Division of Computers in Chemistry, Quantum Mechanics Session, 251st American Chemical Society National Meeting & Exposition, San Diego CA, 05/2016.

Charles Peterson, Angela Wilson, "*Ab initio* Approaches for Accurate Predictions of Lanthanide Thermochemistry", Division of Physical Chemistry, Physical Chemistry Poster Session 249th American Chemical Society National Meeting & Exposition, Denver CO, 05/2015.

Charles Peterson, Angela K. Wilson, *"Ab initio* Approaches for the Predictions of Energetic Properties of Lanthanides", Division of Physical Chemistry, Thermodynamics, Reactivity, and Spectroscopy of the Heavy Elements Fundamental Advances in Theory and Computation Session, 247th American Chemical Society National Meeting & Exposition, Dallas TX, 05/2014.

Charles Peterson, Angela K. Wilson, "C-O Bond Activation of Dimethyl Ether by Transition Metal Ions", 24th Austin Symposium on Molecular Structure and Dynamics at Dallas, 05/2014.

Charles Peterson, Angela K. Wilson *"*Designing Advance *Ab Initio* Composite Methods for Scalable Computing" *XSEDE/PRACE* EU-US High Performance Computing Summer School, 06/2012, Dublin, Ireland

Charles Peterson, Angela K. Wilson, "Accurate Predictions of Energetic Properties using the Multi-Reference correlation consistent Composite Approach (MR-ccCA)", 22nd Austin Symposium on Molecular Structure and Dynamics, 05/2012.

Charles Peterson, Angela K. Wilson, "MR-ccCA Predictions of the Energetics of Silicon-containing Compounds", Physical Division, 44thAmerican Chemical Society Meeting in Miniature, Tarleton State University, 04/2011.

Charles Peterson, Angela K. Wilson, "MR-ccCA Predictions of the Energetics of Silicon-containing Compounds", Poster Session, Southwest Theoretical Chemistry Conference, University of North Texas, 10/2010.

Charles Peterson, Angela K. Wilson, "Application of the Multi-Reference correlation consistent Composite Approach (MR-ccCA)", Physical Division, 43rd American Chemical Society Meeting in Miniature, University of Texas at Dallas, 04/2010.