WILLIAM HUHN, PH. D.

Duke University Energy Initiative ◇ Durham, NC 27708
701-866-6125 ◇ william.paul.huhn@gmail.com
www.williamphuhn.com ◇ www.linkedin.com/in/williamhuhn

EDUCATION

Ph. D., Physics *May 2014*
Department of Physics, Carnegie Mellon University, Pittsburgh, PA
· Advisor: Prof. Michael Widom
· Dissertation: "Thermodynamics from First Principles: Prediction of Phase Diagrams and Materials Properties Using Density Functional Theory"

M. S., Physics *May 2010*
Department of Physics, Carnegie Mellon University, Pittsburgh, PA

B. S., Physics and Mathematics *May 2008*
North Dakota State University, Fargo, ND
· Minor in Computer Science

TECHNICAL SKILLS

Computing Skills	High performance computing, GPU acceleration, parallel programming, data analysis, large scale simulations, Linux administration
Programming Languages	Fortran 2003, Python, C/C++, Bash
Libraries & APIs	MPI, BLAS, (Sca)LAPACK, CUDA, cuBLAS, NumPy, matplotlib
Software & Tools	git, GitLab CI, CMake, GNU Make, LaTeX

RESEARCH EXPERIENCE

Postdoctoral Associate *July 2014 - Present*
Department of Mechanical Engineering and Materials Science, Duke University (PI: Prof. Volker Blum)

· Developer for FHI-aims, a massively-parallel scientific computation package for modeling quantum mechanics at the atomic level
  – Achieved 3x-4x overall GPU speedups, as measured on 103 calculations across three HPC platforms
  – Enabled simulations on 1000+ HPC nodes using vectorized domain decomposition and parallelized linear algebra
  – Maintained CMake build system and GitLab CI test suite to ensure portability across HPC resources
  – Top developer (out of 70) in number of git commits over last four years
· Lead postdoctoral developer for the ELectronic Structure Infrastructure (ELSI), an open source library for high performance computing which unites algorithms solving the Kohn-Sham eigenvalue equation
  – Led team of 20 US and European researchers to release May 2017 version
· Organized two international scientific software development conferences
· Administrator of a local Linux development cluster containing 18 nodes with 348 cores and three GPUs

Research Assistant *August 2010 - June 2014*
Physics Department, Carnegie Mellon University (Advisor: Dr. Michael Widom)

· Predicted new order-disorder phase transitions using Monte Carlo simulations derived from cluster expansion models
· Modeled corrosion resistance of membranes using free energy models fitted to datasets of calculations
· Calculated theoretical trends in elastic properties for early-late transition metal alloys

LEADERSHIP EXPERIENCE

Co-Organizer, Solving or Circumventing Eigenvalue Problems in Electronic Structure Theory *August 2018*
Co-Organizer, Electronic Structure Theory with Numeric Atom-Centered Basis Functions *July 2018*
Co-Organizer, ELectronic Structure Infrastructure (ELSI) Connector Meeting 2017 *August 2017*
Lead Tutor, Hands-On Workshop Density-Functional Theory and Beyond *August 2017*
ELSI Representative, Electronic Structure Library Coding Workshop: Drivers *July 2017*
Session Chair, APS March Meeting 2017 *March 2017*
Team Leader, 2016 Oak Ridge National Laboratory GPU Hackathon *October 2016*
ELSI Representative, Electronic Structure Library Coding Workshop: Solvers *June 2016*
Lead Tutor, Hands-On Workshop Density-Functional Theory and Beyond *July 2015*

PROFESSIONAL SERVICE

Mentor to Graduate Students (Tong Zhu, Tiago Botari, Chi Liu, Wen-Zhe Yu) *August 2014 - Present*
Council Member, Duke University Postdoctoral Association (DUPA) *December 2014 - Present*
Professional Development Chair, DUPA *November 2017 - Present*
Panelist, Choosing a Postdoc Position: What to Know Before You Go *April 2018*
Social Chair, DUPA *May 2015 - February 2016*
Physics Representative, CMU MCS Graduate Student Advisory Committee *June 2011 - May 2014*
Physics Representative, CMU Graduate Student Association *August 2011 - May 2014*
Participant, Fall 2013 Legislative Action Days Sponsored by NAGPS *September 2013*

FELLOWSHIPS AND AWARDS

Fellowship to Promote Scientific Cooperation Between Countries ($15k) *July 2014 - December 2014*
· Research fellowship awarded by Fritz Haber Institute of the Max Planck Society (Berlin, Germany)
George E. and Majorie S. Pake Fellowship ($8k) *August 2010 - December 2010*
· Endowed research fellowship awarded by CMU Physics Department
NSF Research Experience for Undergraduates Recipient *June 2006 - August 2006*
· Awarded by NSF and Rice Quantum Institute (Rice University, Houston, TX)
Arizona State University Barrett Honors College Student *August 2003 - May 2005*
· Awarded by ASU to academically outstanding undergraduates from across the nation
New American University Scholar - President's Award ($10k) *August 2003 - May 2005*
· Awarded by ASU to top students from Arizona high schools

SELECTED CONFERENCE PRESENTATIONS (OUT OF 20)

"GPU-Accelerated Real Space Electronic Structure Theory on HPC Resources", GPU Technology Conference (GTC) Europe; Munich, Germany, October 2018

"Unified Access to Kohn-Sham DFT Solvers for Different Scales and HPC: The ELSI Project", APS March Meeting 2018; Los Angeles, LA, March 2018

"Proposal for a Performance and Scaling Benchmark Set for Electronic Structure Calculations", ELectronic Structure Infrastructure (ELSI) Connector Meeting 2017; Durham, NC, August 2017

"Benchmarking Relativistic Effects in Materials", Electronic Structure Theory with Numeric Atom-Centered Basis Functions; Munich, Germany, July 2016

"Prediction of A2 to B2 Phase Transition in the High Entropy Alloy Mo-Nb-Ta-W", APS March Meeting 2014; Denver, CO, March 2014

"First Principles Prediction of a New Low Temperature Phase in Boron Carbide", Density Functional Theory and Beyond: Computational Materials Science for Real Materials; Trieste, Italy, August 2013

PUBLICATIONS

W. P. Huhn, B. Lange, V. Yu, V. Blum, S. Lee, M. Yoon, "GPGPU Acceleration of All-Electron Electronic Structure Theory Using Localized Numeric Atom-Centered Basis Functions" (in preparation, expected: *Comput. Phys. Commun.*, 2018)

C. Liu, **W. Huhn**, K.-Z. Du, Á. Vázquez-Mayagoitia, D. Dirkes, W. You, Y. Kanai, D. B. Mitzi, V. Blum, "Tunable Semiconductors: Control over Carrier States and Excitations in Layered Hybrid Organic-Inorganic Perovskites" (*Phys. Rev. Lett.*, 2018)

G. Wessler, T. Zhu, J.-P. Sun, A. Harrell, **W. Huhn**, V. Blum, D. Mitzi, "Band Gap Tailoring and Structure-Composition Relationship Within the Alloyed Semiconductor $Cu_2BaGe_{1-x}Sn_xSe_4$" (*Chem. Mater.*, 2018)

V. W.-Z. Yu, F. Corsetti, A. García, **W. P. Huhn**, M. Jacquelin, W. Jia, B. Lange, L. Lin, J. Lu, W. Mi, A. Seifitokaldani, Á. Vázquez-Mayagoitia, C. Yang, H. Yang, V. Blum, "ELSI: A Unified Software Interface for Kohn-Sham Electronic Structure Solvers" (*Comput. Phys. Commun.*, 2018)

T. Zhu, **W. P. Huhn**, G. C. Wessler, D. Shin, B. Saparov, D. B. Mitzi, V. Blum, "I_2-II-IV-VI_4 (I = Cu, Ag; II = Sr, Ba; IV = Ge, Sn; VI = S, Se): Chalcogenides for Thin Film Photovoltaics" (*Chem. Mater.*, 2017)

W. P. Huhn and V. Blum, "One-Hundred-Three Compound Band-Structure Benchmark of Post-Self-Consistent Spin-Orbit Coupling Treatments in Density Functional Theory" (*Phys. Rev. Mater.*, 2017)

S. K. Wallace, K. L. Svane, **W. P. Huhn**, T. Zhu, D. B. Mitzi, V. Blum, A. Walsh, "Candidate Photoferroic Absorber Materials for Thin-Film Solar Cells from Naturally Occurring Minerals: Enargite, Stephanite, and Bournonite" (*Sustain. Energy Fuels*, 2017)

T. Botari, **W. P. Huhn**, V. W.-H. Lau, B. V. Lotsch, V. Blum, "Thermodynamic Equilibria in Carbon Nitride Photocatalyst Materials and Conditions for the Existence of Graphitic Carbon Nitride g-C_3N_4" (*Chem. Mater.*, 2017)

S. R. Jensen, S. Saha, J. A. Flores-Livas, **W. Huhn**, V. Blum, S. Goedecker, L. Frediani, "The Elephant in the Room of Density Functional Theory Calculations" (*J. Phys. Chem. Lett.*, 2017)

D. Shin, B. Saparov, T. Zhu, **W. P. Huhn**, V. Blum, D. B. Mitzi, "$BaCu_2Sn(S,Se)_4$: Earth-Abundant Chalcogenides for Thin-Film Photovoltaics" (*Chem. Mater.*, 2016)

T. Theis, G. X. Ortiz Jr., A. W. J. Logan, K. E. Claytor, Y. Feng, **W. P. Huhn**, V. Blum, S. J. Malcolmson, E .Y. Chekmenev, Q. Wang, W. S. Warren, "Direct and Cost-efficient Hyperpolarization of Long-Lived Nuclear Spin States on Universal $^{15}N_2$-Diazirine Molecular Tags" (*Sci. Adv.*, 2016)

S. Yao, **W. P. Huhn**, M. Widom, "Phase Transitions of Boron Carbide: Pair Interaction Model of High Carbon Limit" (*Solid State Sci.*, 2015)

W. P. Huhn, M. Widom, M. C. Gao, "First Principles Modeling of the Temperature Dependent Ternary Phase Diagram for the Cu-Pd-S system" (*Comput. Mat. Sci.*, 2014)

W. P. Huhn, M. Widom, A. M. Cheung, G. J. Shiflet, S. J. Poon, J. Lewandowski, "First-Principles Calculation of Elastic Moduli of Early-Late Transition Metal Alloys" (*Phys. Rev. B*, 2014)

M. Widom, **W. P. Huhn**, S. Maiti, W. Steurer, "Hybrid Monte Carlo/Molecular Dynamics Simulation of a Refractory Metal High Entropy Alloy" (*Metall. Mater. Trans.*, 2014)

W. P. Huhn and M. Widom, "Prediction of A2 to B2 Phase Transition in the High-Entropy Alloy Mo-Nb-Ta-W" (*J. Metals*, 2013)

W. P. Huhn and M. Widom, "A Free Energy Model of Boron Carbide" (*J. Stat. Phys.*, 2013)

M. Widom and **W. P. Huhn**, "Prediction of Orientational Phase Transition in Boron Carbide" (*Solid State Sci.*, 2012)