William Huhn
Postdoctoral Associate

Duke University
Department of Mechanical Engineering and Materials Science
144 Hudson Hall
Durham, NC 27708, USA

Tel.: (701) 866-6125
E-mail: william.paul.huhn@gmail.com
Web: www.williamphuhn.com
LinkedIn: www.linkedin.com/in/williamhuhn
ORCID: orcid.org/0000-0002-8815-4594

RESEARCH INTERESTS

Electronic structure theory on high performance computing resources: scientific software development, new computer architectures, scalability of simulations (system size and parallel execution); benchmarking the accuracy of implementations of electronic structure theory; relativistic corrections to electronic structure theory; inorganic and organic-inorganic materials for energy conversion and storage

EDUCATION

Carnegie Mellon University, Pittsburgh, PA
Ph. D., Physics (May 2014)
Thesis: *Thermodynamics from First Principles: Prediction of Phase Diagrams and Materials Properties Using Density Functional Theory*
Doctoral advisor: Prof. Michael Widom

Carnegie Mellon University, Pittsburgh, PA
M. S., Physics (May 2010)

North Dakota State University, Fargo, ND
B. S., Physics and Mathematics (May 2008)

PROFESSIONAL EXPERIENCE

Postdoctoral Associate (July 2014 - present)
Duke University, Durham, NC
Department of Mechanical Engineering and Materials Science
Postdoctoral advisor: Prof. Volker Blum

HONORS & AWARDS

- *Fellowship to Promote Scientific Cooperation Between Countries*, Fritz Haber Institute of the Max Planck Society (July 2014 - December 2014)
- *George E. and Majorie S. Pake Fellowship*, Carnegie Mellon University (August 2010 - December 2010)
- *Research Experience for Undergraduates Recipient*, National Science Foundation (June 2006 - August 2006)
- *Barrett Honors College Student*, Arizona State University (August 2003 - May 2005)

- *New American University Scholar - President's Award*, Arizona State University (August 2003 - May 2005)

PUBLICATIONS (Underlined authors: Co-mentored students and postdocs)

A. Peer-Reviewed Journal Publications

J 1. Chi Liu, **William Huhn**, Ke-Zhao Du, Álvaro Vázquez-Mayagoitia, David Dirkes, Wei You, Yosuke Kanai, David B. Mitzi, Volker Blum, "Tunable Semiconductors: Control Over Carrier States and Excitations in Layered Hybrid Organic-Inorganic Perovskites," *Physical Review Letters*, accepted. Preprint: arXiv:1803.07230 [cond-mat.mtrl-sci]

J 2. Garrett C. Wessler, Tong Zhu, Jon-Paul Sun, Alexis Harrell, **William P. Huhn**, Volker Blum, David B. Mitzi, "Band Gap Tailoring and Structure-Composition Relationship Within the Alloyed Semiconductor $Cu_2BaGe_{1-x}Sn_xSe_4$," *Chemistry of Materials*, Vol. 30, No. 18, 6566-6574 (2018). DOI: 10.1021/acs.chemmater.8b03380 .

J 3. Victor Wen-zhe Yu, Fabiano Corsetti, Alberto García, **William P. Huhn**, Mathias Jacquelin, Weile Jia, Björn Lange, Lin Lin, Jianfeng Lu, Wenhui Mi, Ali Seifitokaldani, Álvaro Vázquez-Mayagoitia, Chao Yang, Haizhao Yang, Volker Blum, "ELSI: A Unified Software Interface for Kohn-Sham Electronic Structure Solvers," *Computer Physics Communications*, Vol. 222, Supplement C, 267-285 (2018), DOI: 10.1016/j.cpc.2017.09.007 . Preprint: arXiV:1705.11191 [physics.comp-ph]

J 4. Tong Zhu, **William P. Huhn**, Garrett C. Wessler, Donghyeop Shin, Bayrammurad Saparov, David B. Mitzi, Volker Blum, "I_2-II-IV-VI_4 (I = Cu, Ag; II = Sr, Ba; IV = Ge, Sn; VI = S, Se): Chalcogenides for Thin Film Photovoltaics," *Chemistry of Materials*, Vol. 29, No. 18, 7868-7879 (2017). DOI: 10.1021/acs.chemmater.7b02638 .

J 5. **William P. Huhn** and Volker Blum, "One-Hundred-Three Compound Band Structure Benchmark of Post-Self-Consistent Spin-Orbit Coupling Treatments in Density Functional Theory," *Physical Review Materials*, Vol. 1, No. 3, 033803 (2017). DOI: 10.1103/PhysRevMaterials.1.033803 . Preprint: arXiv:1705.01804 [cond-mat.mtrl-sci]

J 6. Suzanne K. Wallace, Katrine L. Svane, **William P. Huhn**, Tong Zhu, David B. Mitzi, Volker Blum, Aron Walsh, "Candidate Photoferroic Absorber Materials for Thin-Film Solar Cells from Naturally Occurring Minerals: Enargite, Stephanite, and Bournonite," *Sustainable Energy & Fuels*, Vol. 1, No. 6, 1339-1350 (2017). DOI: 10.1039/C7SE00277G .

J 7. Tiago Botari, **William Paul Huhn**, Vincent Wing-hei Lau, Bettina V. Lotsch, Volker Blum, "Thermodynamic Equilibria in Carbon Nitride Photocatalyst Materials and Conditions for the Existence of Graphitic Carbon Nitride g-C_3N_4," *Chemistry of Materials*, Vol. 29, No. 10, 4445-4453 (2017). DOI: 10.1021/acs.chemmater.7b00965 .

J 8. Stig Rune Jensen, Santanu Saha, José A. Flores-Livas, **William Huhn**, Volker Blum, Stefan Goedecker, Luca Frediani, "The Elephant in the Room of Density Functional Theory Calculations," *Journal of Physical Chemistry Letters*, Vol. 8, No. 7, 1449-1457 (2017). DOI: 10.1021/acs.jpclett.7b00255 . Preprint: arXiv:1702.00957 [physics.comp-ph]

J 9. Donghyeop Shin, Bayrammurad Saparov, Tong Zhu, **William P. Huhn**, Volker Blum, David B. Mitzi, "$BaCu_2Sn(S,Se)_4$ - Earth-Abundant Chalcogenides for Thin-Film Photovoltaics, " *Chemistry of Materials*, Vol. 28, No. 13, 4771-4780 (2016). DOI: 10.1021/acs.chemmater.6b01832 .

J 10. Thomas Theis, Gerardo X. Ortiz, Jr, Angus W. J. Logan, Kevin E. Claytor, Yesu Feng, **William P. Huhn**, Volker Blum, Steven J. Malcolmson, Eduard Y. Chekhmenev, Qiu Wang, Warren S. Warren,

"Direct and Cost-efficient Hyperpolarization of Long-lived Nuclear Spin States on Universal $^{15}N_2$-Diazirine Molecular Tags," *Science Advances* Vol. 2, No. 3, e1501483 (2016). DOI: 10.1126/sciadv.1501438 .

J 11. Sanxi Yao, **W. P. Huhn**, M. Widom, "Phase Transitions of Boron Carbide: Pair Interaction Model of High Carbon Limit," *Solid State Sciences*, Vol. 47, 21-26 (2015). DOI: 10.1016/j.solidstatesciences.2014.12.016 . Preprint: arXiv:1410.2946 [cond-mat.mtrl-sci]

J 12. **William Paul Huhn**, "Thermodynamics from First Principles: Prediction of Phase Diagrams and Materials Properties Using Density Functional Theory," Doctoral Thesis (2014). Download: repository.cmu.edu/dissertations/369 .

J 13. **William Paul Huhn**, Michael Widom, Michael C. Gao, "First Principles Modeling of the Temperature Dependent Ternary Phase Diagram for the Cu-Pd-S System," *Computational Material Science*, Vol. 92, 377-386 (2014). DOI: 10.1016/j.commatsci.2014.05.065 . Preprint: arXiv:1303.3536 [cond-mat.mtrl-sci]

J 14. **William Paul Huhn**, Michael Widom, Andrew M. Cheung, Gary J. Shiflet, S. Joseph Poon, John Lewandowski, "First-Principles Calculation of Elastic Moduli of Early-Late Transition Metal Alloys," *Physical Review B*, Vol. 89, 104103 (2014). DOI: 10.1103/PhysRevB.89.104103 . Preprint: arXiv:1310.6709 [cond-mat.mtrl-sci]

J 15. Michael Widom, **W. P. Huhn**, S. Maiti, W. Steurer, "Hybrid Monte Carlo/Molecular Dynamics Simulation of a Refractory Metal High Entropy Alloy," *Metallurgical and Materials Transactions A*, Vol. 45A, 196-200 (2014). DOI: 10.1007/s11661-013-2000-8 . Preprint: arXiv:1304.7800 [cond-mat.mtrl-sci]

J 16. **William Paul Huhn** and Michael Widom, "Prediction of A2 to B2 Phase Transition in the High-Entropy Alloy Mo-Nb-Ta-W," *Journal of Metals*, Vol. 65, No. 12, 1772-1779 (2013). DOI: 10.1007/s11837-013-0772-3 . Preprint: arXiv:1306.5043 [cond-mat.mtrl-sci]

J 17. **W. P. Huhn** and M. Widom, "A Free Energy Model of Boron Carbide," *Journal of Statistical Physics*, Vol. 150, 432-441 (2013). DOI: 10.1007/s10955-012-0642-3 . Preprint: arXiv:1208.2708 [cond-mat.mtrl-sci]

J 18. M. Widom and **W. P. Huhn**, "Prediction of Orientational Phase Transition in Boron Carbide," *Solid State Sciences*, Vol. 14, 1648 - 1652 (2012). DOI: 10.1016/j.solidstatesciences.2012.05.010 . Preprint: arXiv:1111.1737 [cond-mat.mtrl-sci]

Journal Articles In Preparation

J 19. **William P. Huhn**, Björn Lange, Victor W.-z. Yu, Seyong Lee, Mina Yoon and Volker Blum, "GPGPU Acceleration of All-Electron Electronic Structure Theory Using Localized Numeric Atom-Centered Basis Functions," target: *Computer Physics Communications*.

J 20. Raul Laasner, **William P. Huhn**, Johannes Collel, Thomas Theis, Warren Warren, Victor W.-z. Yu and Volker Blum, "Molecular NMR Shieldings, J-Couplings, and Magnetizabilities from Numeric Atom-Centered Orbital Based Density-Functional Theory." Preprint: arXiv:1805.12225 [physics.comp-ph]

B. Technical Reports

B 1. V. Blum, **W. P. Huhn**, C. Liu, D. B. Mitzi, Y. Kanai, V. W.-z. Yu, T. Rose, N. Marom, F. Curtis, À. Vázquez-Mayagoitia, "Electronic Structure-Based Discovery of Hybrid Photovoltaic Materials on Next-Generation HPC Platforms," Technical Report for the ALCF Theta Early Science Program (2018).

C. Major Scientific Computer Codes

C 1. "FHI-aims," URL: aims.fhi-berlin.mpg.de . Computer code for electronic structure theory based computational molecular and materials science. Top developer (by number of git commits) since 2014. Over 100 participating developers to date, over 100 licensing groups. Stable release versions participated in: March 2016, December 2017.

C 2. "ELSI - ELectronic Structure Infrastructure," URL: www.elsi-interchange.org . Open-source software library infrastructure for scalable solutions or circumvention of the effective single-particle eigenvalue problem in electronic structure theory. Lead postdoctoral developer (since 2016). Stable release versions participated in: May 2017, May 2018.

D. Published Datasets

D 1. **W. P. Huhn** and V. Blum, "103 Compound Band Structure Benchmark Set, With and Without Spin-Orbit Coupling (WIEN2k, DFT, PBE, Benchmark Settings)," (2017).
DOI: 10.17172/NOMAD/2017.04.27-1 .

D 2. **W. P. Huhn** and V. Blum, "103 Compound Band Structure Benchmark Set, With and Without Spin-Orbit Coupling (FHI-aims, DFT, PBE, Benchmark Settings)," (2017).
DOI: 10.17172/NOMAD/2017.04.27-2 .

D 3. **W. P. Huhn** and V. Blum, "103 Compound Band Structure Benchmark Set, With and Without Spin-Orbit Coupling (FHI-aims, DFT, HSE06 and PBE, Tight Production Settings)," (2017).
DOI: 10.17172/NOMAD/2017.04.27-3 .

Datasets In Preparation

D 4. **W. P. Huhn**, R. Laasner, V. W-z. Yu, V. Blum, "A Performance and Scaling Benchmark Set for Electronic Structure Calculations," in preparation (2018). Current version at git.elsi-interchange.org/elsi-devel/PerformanceBenchmark .

PRESENTATIONS

P 1. *Invited*, "GPU-Accelerated Real Space Electronic Structure Theory on HPC Resources," GPU Technology Conference (GTC) Europe 2018, Munich, Germany, October 2018.

P 2. *Co-organized*, "GPU-Accelerated Real Space Electronic Structure Theory on HPC Resources," MolSSI Workshop / ELSI Conference: Solving or Circumventing Eigenvalue Problems in Electronic Structure Theory, Richmond, VA, August 2018.

P 3. *Co-organized*, "GPU-Accelerated Real Space Electronic Structure Theory on HPC Resources," Electronic Structure Theory with Numeric Atom-Centered Basis Functions, Munich, Germany, July 2018.

P 4. *Poster*, "GPGPU-Accelerated Large-Scale Electronic Structure Theory with a First-Principles All-Electron Code," 255th ACS National Meeting & Exposition, New Orleans, LA, March 2018.

P 5. "Unified Access to Kohn-Sham DFT Solvers for Different Scales and HPC: The ELSI Project," APS March Meeting 2018, Los Angeles, LA, March 2018.

P 6. *Co-organized*, "Proposal for a Performance and Scaling Benchmark Set for Electronic Structure Calculations," ELectronic Structure Infrastructure (ELSI) Connector Meeting 2017, Durham, NC, August 2017.

P 7. "GPU-Accelerated Large-Scale Electronic Structure Theory on Titan with a First-Principles All-Electron Code," APS March Meeting 2017, New Orleans, LA, March 2017.

P 8. *Invited*, "Benchmarking Relativistic Effects in Materials," Electronic Structure Theory with Numeric Atom-Centered Basis Functions, Munich, Germany, July 2016.

P 9. *Invited*, "Benchmarking Relativistic Effects in Materials," Frontiers of Multi-scale Modeling in Materials, Energy & Catalysis, Monte Isola, Italy, June 2016.

P 10. "First Principles for Energy Materials," 2016 Energy Research Collaboration Workshop, Durham, NC, May 2016.

P 11. "Benchmarking Post-SCF Treatments of Spin-Orbit Coupling in Electronic Structure Theory," APS March Meeting 2016, Baltimore, MD, March 2016.

P 12. "The Marriage of Hybrid Functionals and Spin-Orbit Coupling: A Generalized Kohn-Sham Band Structure Benchmark for 3D Solids and 2D Materials," 2015 Materials Research Society Fall Meeting and Exhibit, Boston, MA, November 2015.

P 13. "Kohn-Sham Band Structure Benchmark Including Spin-Orbit Coupling for 2D and 3D Solids," APS March Meeting 2015, San Antonio, TX, March 2015.

P 14. *Doctoral Defense*, "Phase Transitions from First Principles: Boron Carbide and the High-Entropy Alloy Mo-Nb-Ta-W," Carnegie Mellon University, Pittsburgh, PA, April 2014.

P 15. "Prediction of A2 to B2 Phase Transition in the High Entropy Alloy Mo-Nb-Ta-W," APS March Meeting 2014, Denver, CO, March 2014.

P 16. *Poster*, "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.

P 17. "First Principles Calculation of Elastic Properties of Early-Late Transition Metal Alloys," APS March Meeting 2013, Baltimore, MD, March 2013.

P 18. "First Principles Modeling of the Temperature Dependent Ternary Phase Diagram, Activities, and Sulfidization Thresholds for the Cu-Pd-S System," Materials Science & Technology 2012 Conference and Exhibition, Pittsburgh, PA, October 2012.

P 19. "First Principles Modeling of the Temperature Dependent Ternary Phase Diagram for the Cu-Pd-S System," APS March Meeting 2012, Boston, MA, February 2012.

P 20. "Hydrogen Binding Sites in Nickel-Based Amorphous Metals," APS March Meeting 2011, Dallas, TX, March 2011.

CO-MENTORED STUDENTS AND POSTDOCTORAL FELLOWS

The following is a list of students and postdoctoral fellows for whom I provided guidance and input as part of my role as a senior member of a research group, which is reflected in various co-authored publications.

Postdoctoral Fellows

- Rundong Zhao (March 2018 - present), Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC.
- Svenja Janke (May 2017 - present), Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC.
- Wenhui Mi (August 2016 - July 2017), Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC.

- Raul Laasner (December 2015 - present), Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC.

Doctoral Students

- Wen-zhe (Victor) Yu (August 2015 - present), Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC, graduation anticipated in August 2020.
- Chi (Garnett) Liu (April 2015 - present), Department of Chemistry, Duke University, Durham, NC, graduation anticipated in August 2019.
- Tong (Eric) Zhu (August 2014 - present), Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC, graduation anticipated in August 2019.
- Sanxi Yao (August 2013 - June 2014), Department of Physics, Carnegie Mellon University, Pittsburgh, PA, graduated May 2017.
- Qin Gao (August 2011 - June 2014), Department of Physics, Carnegie Mellon University, Pittsburgh, PA, graduated May 2016.

Undergraduate Students

- Wolfgang Seiya (September 2015 - May 2016), Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC, graduated May 2016.
- Xiaochen Du (September 2017 - present), Department of Chemistry, Duke University, Durham, NC, graduation anticipated in May 2021.

Visiting Students

- Xinyi Li (September 2017 - August 2018), Ph. D. Visiting Student, Fritz Haber Institute, Berlin, Germany.
- Simon Erker (August 2017 - October 2017), Ph. D. Visiting Student, Technical University of Graz, Austria.
- Suzanne Wallace (March 2016, September 2016 - November 2016), Ph. D. Visiting Student, University of Bath, UK.
- Georg Michelitsch (March 2016 - April 2016), Ph. D. Visiting Student, Technical University of Munich, Germany.
- Markus Sinstein (March 2016 - April 2016), Ph. D. Visiting Student, Technical University of Munich, Germany.
- Tiago Botari (September 2014 - September 2015), Ph. D. Visiting Student, State University of Campinas (UNICAMP), Brazil.

PROFESSIONAL MEMBERSHIPS

- American Physical Society (APS)
- American Chemical Society (ACS)

William Huhn
Postdoctoral Associate
Duke University
Department of Mechanical Engineering and Materials Science

PROFESSIONAL ACTIVITIES

Co-Organized International Conferences and Workshops

- MolSSI Workshop / ELSI Conference: Solving or Circumventing Eigenvalue Problems in Electronic Structure Theory, Richmond, VA, August 15-17, 2018 (with Volker Blum (Duke University), Lin Lin (University of California Berkeley), Jianfeng Lu (Duke University), Álvaro Vázquez-Mayagoitia, (Argonne National Laboratory), Chao Yang (Lawrence Berkeley National Laboratory), funding: MolSSI (NSF) and NSF).
- Electronic Structure Theory with Numeric Atom-Centered Basis Functions – FHI-aims Users' and Developers' Workshop 2018, Technical University of Munich, Germany, July 9-11 2018 (with Volker Blum (Duke University), Harald Oberhofer (TU Munich), Mariana Rossi (FHI Berlin), Xinguo Ren (USTC Hefei), funding: psi-k.org).
- ELectronic Structure Infrastructure (ELSI) Connector Meeting 2017, Duke University, Durham, NC, August 16, 2017 (with Volker Blum (Duke University), Lin Lin (University of California Berkeley), Jianfeng Lu (Duke University), funding: NSF).

Workshop Participation

- Lead Tutor for "The Basics of Electronic Structure Theory (Periodic Systems)," Hands-On Workshop Density-Functional Theory and Beyond: Accuracy, Efficiency and Reproducibility in Computational Materials Science, Humboldt University, Berlin, Germany, July 31 - August 11, 2017.
- ELSI Representative, Electronic Structure Library Coding Workshop: Drivers, International Centre for Theoretical Physics, Trieste, Italy, July 10 - 21, 2017.
- Team Leader, 2016 Oak Ridge National Laboratory GPU Hackathon, Knoxville, TN, October 17 - 21, 2016.
- ELSI Representative, Electronic Structure Library Coding Workshop: Solvers, University of Zaragoza, Spain, June 6 - 17, 2016.
- Lead Tutor for "Periodic Systems," Hands-On Workshop Density-Functional Theory and Beyond: First-Principles Simulations of Molecules and Materials, Fritz Haber Institute, Berlin, Germany, July 13 - 25, 2015.

Society Service

- Session Chair for "First-Principles Modeling of Excited-State Phenomena II: Computational Advances," American Physical Society March Meeting 2017, New Orleans, LA, March 2017.
- Sorter, American Physical Society March Meeting 2017 Sorter's Meeting, College Park, MD, December 2016.
- Sorter, American Physical Society March Meeting 2016 Sorter's Meeting, College Park, MD, December 2015.

UNIVERSITY ACTIVITIES

University Committees

- Council Member, Duke University Postdoctoral Association (December 2014 - present).
- Professional Development Chair, Duke University Postdoctoral Association (November 2017 - present).

- Social Chair, Duke University Postdoctoral Association (May 2015 - February 2016).
- Physics Representative, Mellon College of Sciences Graduate Student Advisory Committee (June 2011 - May 2014).
- Physics Representative, Carnegie Mellon University Graduate Student Association (August 2011 - May 2014).

Community Outreach

- Panelist, Choosing a Postdoc Position: What to Know Before You Go, Duke University, Durham, NC, April 2018.
- Participant, Fall 2013 Legislative Action Days, National Association of Graduate-Professional Students, Washington, D. C., September 2013.