SAMUEL S. WELBORN

Curriculum Vitae

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Google Scholar

EDUCATION & TRAINING

National Energy Research Scientific Computing Center (NERSC)

• NERSC Science Acceleration Program (NESAP) Postdoctoral Fellow

2022-Present

• Supervisors: Dr. Deborah J. Bard, Dr. Shane Canon

SLAC National Accelerator Laboratory

• DOE-SCGSR Fellow

2021 - 2022

• Advisor: Dr. Johanna Nelson Weker

University of Pennsylvania

• PhD in Materials Science and Engineering

2022

- Thesis: 'X-ray Scattering Investigations into Nanoporous Gold's Kinetic Behavior During Dealloying and Coarsening for Applications in 3D Energy Storage'
- Advisor: Prof. Eric Detsi

Virginia Polytechnic Institute and State University

• B.S. Chemical Engineering, summa cum laude

2016

• B.A. Chemistry, summa cum laude

2016

POSTDOCTORAL RESEARCH EXPERIENCE

Data Science Engagement Group (DSEG), NERSC

NESAP for Data Postdoctoral Fellow

Nov 2022-Present

- Streaming from the National Center for Electron Microscopy (NCEM) to NERSC
 - Identified file I/O bottleneck on the 4D Camera detector, which generates data at 480 Gbit/s.
 - Implemented ZeroMQ-based messaging to stream data over 100 GbE directly to Perlmutter compute nodes, boosting raw throughput by 5-14x.
 - Enhanced *Distiller*, NCEM's React (TypeScript) web portal, to enable non-HPC experts to initiate and control streaming services at NERSC through the Superfacility API.
 - Two manuscripts accepted on this work: (1) ISC 2024 (preprint) and (2) Microscopy and Microanalysis.
 - Demonstrated the workflow live at SC23 at the DOE Booth (Computing Sciences photo).
 - Developed a proof-of-concept for an interactive, containerized operator pipeline that replicates the above workflow.
- Streaming from the Advanced Light Source (ALS) to NERSC
 - Gathered requirements from tomography and ptychography beamlines at ALS.
 - Developed prototype for real-time tomography data reconstruction that sustains at least 3x the current beamline throughput requirement.
 - Collaborating with the ALS Computing Group to integrate streaming into real data acquisition systems.

- NERSC-centered Activities
 - Instructed and mentored new users of NERSC's Kubernetes cluster, Spin, in multiple training events.
 - Ensured NCEM's continued operations through a Perlmutter scheduled maintenance by piloting the Perlmutter On Demand (POD) service. This effort served as a major proof-ofconcept for POD.
 - Active member of the Streaming Working Group, meeting bi-weekly to discuss streaming efforts with colleagues at NERSC and ESNet.
- Professional Development
 - Accepted to and participated in the two-week Argonne Training Program on Extreme-Scale Computing (ATPESC) in 2023.

TECHNICAL SKILLS

- Expertise: data streaming and real-time data processing, full-stack development, user interface development (TomoPyUI, Distiller), synchrotron X-ray techniques (microscopy, tomography, spectroscopy, diffraction, scattering)
- Programming languages: Python, C++, TypeScript, MATLAB
- Technologies used: ZeroMQ, NATS, git, pvaPy, CMake, vcpkg, pydantic, MessagePack, React, Redux, FastAPI, PostgreSQL, Alembic, Kubernetes, Helm, Docker, podman, GitHub Actions, slurm, Spin (NERSC Kubernetes cluster), Dask, ipywidgets, Superfacility API
- **Professional skills:** Public speaking (14 national and international scientific conference talks, 3 invited talks, panelist at ISC 2024 workshop), federal grant writing for scientific funding

GRADUATE RESEARCH EXPERIENCE

Nelson Weker Group: SLAC National Accelerator Laboratory 2021–2022 Fellowship: Office of Science Graduate Student Research Fellowship (DOE-SCGSR, \$39,000)

- X-ray absorption studies on the impact of curvature on charge storage behavior in 3D aperiodic nanoporous battery electrodes
 - Developed atomic layer deposition recipe for coating multicomponent cathode ($LiMn_2O_4$) on aperiodic 3D nanoporous scaffolds
 - Operated multiple X-ray beamlines at the Stanford Synchrotron Radiation Lightsource (SSRL) to study novel energy storage materials
 - Developed software to align and reconstruct X-ray nanotomography data: TomoPyUI

Detsi Group: University of Pennsylvania

2016-2022

Fellowship: Vagelos Institute for Energy Science and Technology Fellowship (VIEST, \$58,000)

- X-ray scattering studies on the kinetic behavior of aperiodic nanoporous materials in real time during electrochemical and thermal processing
 - Studied morphological evolution of nanoporous gold during synthesis and thermal coarsening using small- and wide-angle X-ray scattering
 - Developed a suite of MATLAB and Mathematica programs to model and post-process the corresponding X-ray scattering and electrochemical data

- Development of three-dimensional tricontinuous bulk conductor-insulator-conductor nanocomposites for high-rate electrical energy storage
 - Developed clean room fabrication protocol to make 3D nanoporous metal scaffolds and grow dissimilar layers inside their void space to create bulk conductor-insulator-conductor nanocomposites
 - Characterized the 3D nanocomposites using electrochemical characterization techniques including cyclic voltammetry and electrochemical impedance spectroscopy

PUBLICATIONS

Preprints

[1] Welborn, S. S., Enders, B., Harris, C., Ercius, P., Bard, D. J., Accelerating Time-to-Science by Streaming Detector Data Directly into Perlmutter Compute Nodes. Accepted. ISC24: Third Combined Workshop on Interactive and Urgent High-Performance Computing. 2024. arXiv: 2403.14352 [cs.NI].

Journal Articles

Summary: 6 first author, 12 co-author, 400+ citations (Google Scholar)

- [1] Welborn, S. S., Harris, C., Ribet, S. M., Varnavides, G., Ophus, C., Enders, B., Ercius, P., "Streaming Large-Scale Electron Microscopy Data to a Supercomputing Facility". In: *Microscopy and Microanalysis* (2024). DOI: 10.1093/mam/ozae109.
- [2] Welborn, S. S., Preefer, M. B., Nelson Weker, J., "TomoPyUI: a user-friendly tool for rapid tomography alignment and reconstruction". In: *Journal of Synchrotron Radiation* 31.4 (2024), pp. 979–986. DOI: 10.1107/S1600577524003989.
- [3] Li, M., Qiu, T., Welborn, S. S., Foucher, A. C., Fu, J., Lesel, B. K., Wang, Z., Wang, L., Stach, E. A., Rappe, A. M., "Understanding the fast kinetics and mechanism of sodium storage in antimony using ab initio grand canonical Monte Carlo simulation and operando X-ray scattering". In: *Journal of Materials Chemistry A* 12.6 (2024), pp. 3671–3681. DOI: 10.1021/acs.chemmater.7b04124.
- [4] Lee, T., Fu, J., Wang, L., Liu, J., **Welborn, S. S.**, Weker, J. N., Detsi, E., "Isolating intermediate Mg11Cu6Al12 phase in ternary Mg-Cu-Al alloy by electrolytic dealloying". In: Scripta Materialia 222 (2023), p. 115039. DOI: 10.1016/j.scriptamat.2022.115039.
- [5] Corsi, J. S., Fu, J., Wang, L., Welborn, S. S., Wang, Z., Detsi, E., "Sacrificial Silver Recovery during Nanoporous Gold Formation by Electrolytic Dealloying of Gold-Silver Alloy". In: *Journal of The Electrochemical Society* 169.6 (2022), p. 063501. DOI: 10.1149/1945-7111/ ac6344.
- [6] Fu, J., Welborn, S. S., Detsi, E., "Dealloyed air-and water-sensitive nanoporous metals and metalloids for emerging energy applications". In: ACS Applied Energy Materials 5.6 (2022), pp. 6516–6544. DOI: 10.1021/acsaem.2c00405.
- [7] Ng, A. K., **Welborn, S. S.**, Detsi, E., "Time-dependent power law function for the post-dealloying chemical coarsening of nanoporous gold derived using small-angle X-ray scattering". In: *Scripta Materialia* 206 (2022), p. 114215. DOI: 10.1016/j.scriptamat.2021.114215.

- [8] Preefer, M. B., Tanim, T. R., Welborn, S. S., Agyeman-Budu, D. N., Dunlop, A. R., Trask, S. E., Dufek, E. J., Jansen, A. N., Nelson Weker, J., "The Evolution of LiNio. 5Mno. 3Coo. 2O2 Particle Damage from Fast Charging in Optimized, Full Li-Ion Cells". In: The Journal of Physical Chemistry C 126.50 (2022), pp. 21196–21204. DOI: 10.1021/acs.jpcc.2c06977.
- [9] Welborn, S. S., Simafranca, A., Wang, Z., Wei, H., Detsi, E., "Chelation-mediated synthesis of nanoporous gold at near-neutral pH and room temperature by free corrosion dealloying of gold-copper alloy driven by oxygen reduction". In: Scripta Materialia 200 (2021), p. 113901. DOI: 10.1016/j.scriptamat.2021.113901.
- [10] Welborn, S. S., Corsi, J. S., Wang, L., Lee, A., Fu, J., Detsi, E., "Effects of side reactions on the kinetics of nanoporous gold formation revealed by real-time X-ray scattering during electrolytic dealloying". In: *Journal of Materials Chemistry A* 9.35 (2021), pp. 19994–20005. DOI: 10.1039/D1TA04822H.
- [11] Welborn, S. S., Van Der Meer, S., Corsi, J. S., De Hosson, J. T. M., Detsi, E., "Using X-ray scattering to elucidate the microstructural instability of 3D bicontinuous nanoporous metal scaffolds for use in an aperiodic 3D tricontinuous conductor—insulator—conductor nanocapacitor". In: ACS Applied Materials & Interfaces 13.10 (2021), pp. 11721–11731. DOI: 10.1021/acsami.0c16869.
- [12] Corsi, J. S., **Welborn, S. S.**, Stach, E. A., Detsi, E., "Insights into the degradation mechanism of nanoporous alloy-type Li-ion battery anodes". In: *ACS Energy Letters* 6.5 (2021), pp. 1749–1756. DOI: 10.1021/acsenergylett.1c00324.
- [13] Fu, J., Corsi, J. S., **Welborn, S. S.**, Basile, V., Wang, L., Ng, A. K., Detsi, E., "Ecofriendly synthesis of nanoporous magnesium by air-free electrolytic dealloying with recovery of sacrificial elements for energy conversion and storage applications". In: *ACS Sustainable Chemistry & Engineering* 9.7 (2021), pp. 2762–2769. DOI: 10.1021/acssuschemeng.0c08157.
- [14] Maguire, S. M., Bilchak, C. R., Corsi, J. S., Welborn, S. S., Tsaggaris, T., Ford, J., Detsi, E., Fakhraai, Z., Composto, R. J., "Effect of nanoscale confinement on polymer-infiltrated scaffold metal composites". In: ACS Applied Materials & Interfaces 13.37 (2021), pp. 44893–44903. DOI: 10.1021/acsami.1c12491.
- [15] Welborn, S. S., Detsi, E., "Small-angle X-ray scattering of nanoporous materials". In: Nanoscale Horizons 5.1 (2020), pp. 12–24. DOI: 10.1039/C9NH00347A.
- [16] Mooraj, S., Welborn, S. S., Jiang, S., Peng, S., Fu, J., Baker, S., Duoss, E. B., Zhu, C., Detsi, E., Chen, W., "Three-dimensional hierarchical nanoporous copper via direct ink writing and dealloying". In: Scripta Materialia 177 (2020), pp. 146–150. DOI: 10.1016/j.scriptamat. 2019.10.013.
- [17] Wang, L., **Welborn, S. S.**, Kumar, H., Li, M., Wang, Z., Shenoy, V. B., Detsi, E., "High-Rate and Long Cycle-Life Alloy-Type Magnesium-Ion Battery Anode Enabled Through (De) magnesiation-Induced Near-Room-Temperature Solid-Liquid Phase Transformation". In: *Advanced Energy Materials* 9.45 (2019), p. 1902086. DOI: 10.1002/aenm.201902086.
- [18] Yaghoobnejad Asl, H., Fu, J., Kumar, H., **Welborn, S. S.**, Shenoy, V. B., Detsi, E., "In situ dealloying of bulk Mg2Sn in Mg-ion half cell as an effective route to nanostructured Sn for high performance Mg-ion battery anodes". In: *Chemistry of Materials* 30.5 (2018), pp. 1815–1824. DOI: 10.1021/acs.chemmater.7b04124.

CONFERENCES AND SEMINARS

$\mathrm{Date}(\mathrm{s})$	Location	Conference/Seminar	Contribution
Nov 17–22, 2024	Atlanta, GA	SC24: Streaming Birds of a Feather	Oral
May 12–16, 2024	Hamburg, Germany	ISC High Performance 2024	Oral & Panelist
Oct 22–24, 2024	Berkeley, CA	NERSC 50th Anniversary User Group Meeting	Poster
Feb 21–22, 2024	Berkeley, CA	NERSC Data Day	Oral
Nov 12–17, 2023	Denver, CO	SC23: DOE Booth	Live Demo
Sep 11–15, 2023	Busan, South Korea	20th International Microscopy Congress	Oral & Poster
Jun 6, 2022	(Virtual)	APS Scientific Computation Seminar Series	Invited Oral
Oct 12, 2021	(Virtual)	Nanoporous Metals by Alloy Corrosion Symposium	Invited Oral
Oct 10–14, 2021	Orlando, FL (Virtual)	ECS Fall Meeting	Oral
Apr 15, 2021	Philadelphia, PA (Virtual)	Penn MSE Departmental Seminar	Invited Oral
Oct 4–9, 2020	Honolulu, HI (Virtual)	ECS PRiME 2020	Oral
Jun 12, 2020	Philadelphia, PA (Virtual)	Dual-source and Environmental X-ray Scattering Facility Seminar	Oral
May 21, 2020	Philadelphia, PA (Virtual)	Philadelphia Regional ECS Graduate Student Seminar Series	Oral
Dec 1–6, 2019	Boston, MA	MRS 2019	Oral
Aug 22–23, 2019	Dearborn, MI	MetFoam 2019	Oral
Aug 19–22, 2019	Los Angeles, CA	AAAFM 2019	Oral
Mar 10–14, 2019	San Antonio, TX	TMS 2019	Oral
Feb 24–28, 2019	Philadelphia, PA	ISNM 2019	Oral & Poster
Nov 25–30, 2018	Boston, MA	MRS 2018	Oral
Jun 24–29, 2018	Hong Kong	NANO 2018	Poster

AWARDS AND DISTINCTIONS

 Graduate 2021 DOE Office of Science SCGSR Fellow (Full Stipend, 1 year) 2020 NNCI Plenty of Beauty at the Bottom image contest 2019 VIEST Graduate Student Fellow (Full Tuition + Stipend, 1 year) TMS MetFoam 2019 Registration Award 	\$39,000 \$1,000 \$58,000 \$370	
Undergraduate		
• 2016 HyperCube Scholar Award, Virginia Tech Chemistry Department		
• 2016 Phi Kappa Phi Graduate Fellowship		
• 2016 Inducted into Phi Kappa Phi and Phi Beta Kappa Honor Societies		
• 2015 Accepted into study abroad program at Ruhr-Universität Bochum		
• 2015 Recipient of Julius P. Bilisoly Scholarship, Virginia Tech Chemistry	\$1,700	
• 2015 Recipient of Gerhard H. Beyer Chemical Engineering Scholarship	\$2,000	
• 2014 Recipient of Steven Reese, R.H. Bogle Chemical Engineering Scholarships	\$2,700	
• 2014 Recipient of Chemistry Summer Research Scholarship		
• 2014 Academic Excellence Award — Chemistry Department at Virginia Tech		

MENTORING & OUTREACH

Mentoring

- Spring-Summer 2020: Mentored a VIPER undergraduate and master's student on a simulation project during the COVID lockdown
- Fall 2019: Mentored two students before and during Materials Research Society (MRS) 2019 & Exhibit in collaboration with NSF's Partnerships for Research and Education in Materials (PREM) program
- Fall 2019: Mentored a master's student and two undergraduate Materials Science and Engineering (MSE) students
- Spring 2019: Mentored an MSE undergraduate student
- Summer 2018–2019: Mentored VIPER undergraduate students

Outreach

- Fall 2019: Developed and conducted electrochemistry demos at NanoDay@Penn
- Summer 2019: Demonstrated electrochemical energy storage systems for the annual Middle School Science Outreach Program at Penn supported by the NSF-MRSEC program.
- 2019–2022: Helped recruit new PhD students at Materials Science and Engineering open houses
- 2019–2021: Served as The Electrochemical Society Student Chapter Secretary
- Fall 2019: Co-founded The Electrochemical Society UPenn student chapter
- 2017–2018: Served as the President of the MSE Materials Graduate Organization (MatGO)
- 2015–2016: Co-Produced Rock the Blocks Music and Arts Festival
- 2012–2016: Served in leadership roles in The Environmental Coalition at Virginia Tech