

STACEY J. SMITH

Associate Professor of Chemistry
Department of Chemistry & Biochemistry, Brigham Young University, Provo, UT, 84602
Office: C308 BNSN Phone: (801) 422-2090 Laboratory: C330 BNSN
Email: stacey.smith@byu.edu

PROFESSIONAL APPOINTMENTS

2019- present *Associate Professor, Department of Chemistry, Brigham Young University,
X-ray Diffraction Facility Director*

2013- 2019 *Assistant Professor, Department of Chemistry, Brigham Young University,
X-ray Diffraction Facility Director*

EDUCATION

2012- 2013 *Postdoctoral research, X-ray Crystallography, Massachusetts Institute of Technology (MIT)*

2007- 2012 *Ph.D., Physical Chemistry, Brigham Young University*

2003-2007 *B.S., Chemistry, Summa Cum Laude, Brigham Young University*

AWARDS & RECOGNITIONS

Faculty Awards

2022 Roland K. Robins Department Service Teaching Award,
Department of Chemistry & Biochemistry, BYU

2020 Early Career Teaching Award,
Brigham Young University

Awards Received by Students Mentored

2022 Peter Mpaata. Etter Student Lecturer Award, ACA Annual Meeting, Portland, OR

2022 Peter Mpaata. ACA Student Travel Grant award winner. ACA Annual Meeting, Portland, OR

2019 Gabriel Valdivia-Berroeta. ACA Student Travel Grant award winner, ACA Annual Meeting,
Covington, KY

2017 Ying Zhang. Etter Student Lecturer Award, ACA Annual Meeting, New Orleans, LA

2017 Ying Zhang. ACA Student Travel Grant award winner, ACA Annual Meeting, New Orleans, LA

TEACHING EXPERIENCE

Instructor: Chem 105: General College Chemistry (4.0 credit hours) – 20 classes (166 sections)

Course Content: Atomic and molecular structure, periodic properties of the elements, bonding, intermolecular interactions, reaction stoichiometry, chemical thermodynamics, gas properties.

Semesters taught:

- Fall 2023 (2 classes) – 19 sections, 422 students*
- Winter 2023 (2 classes) – 15 sections, 340 students*
- Winter 2022 (2 classes) – 14 sections, 323 students*
- Winter 2021 (2 classes) – 12 sections, 336 students*
- Fall 2018 (2 classes) – 18 sections, 452 students*
- Spring 2018 (1 class) – 5 sections, 94 students*
- Winter 2018 (2 classes) – 20 sections, 490 students*
- Winter 2017 (2 classes) – 20 sections, 495 students*
- Fall 2015 (2 classes) – 19 sections, 440 students*
- Summer 2015 (1 class) – 6 sections, 120 students*
- Winter 2014 (2 classes) – 18 sections, 439 students*

Instructor: Chem 575: X-ray Diffraction Theory & Practice (3.0 credit hours) – 6 classes

Formerly Chem 596R: Intro to X-ray Diffraction Theory & Practice prior to 2022

Course Content: Lecture & lab components. Lecture teaches fundamental concepts involved in X-ray diffraction & crystallography. Lab teaches students to use the X-ray diffraction (XRD) equipment at BYU to characterize the atomic structure of solid, crystalline materials using both single crystal (SC-XRD) and powder (P-XRD) diffraction techniques.

Semesters taught: Winter 2024 (1 class) – 4 sections/lab periods, 11 students (plus 1 auditing)
Fall 2022 (1 class) – 3 sections/lab periods, 9 students (including 1 auditing)
Fall 2021 (1 class) – 4 sections/lab periods, 11 students
Fall 2020 (1 class) – 4 sections/lab periods, 11 students (including 1 auditing)
Winter 2019 (1 class) – 6 sections/lab periods, 11 students (including 1 auditing)
Fall 2016 (1 class) – 6 sections/lab periods, 12 students (including 1 auditing)

Co-Instructor: Chem 518: Advanced Inorganic Laboratory – 12 classes (evaluated as co-instructor for the last 3)

Involvement: ~40 hrs/semester involving one 3-hr training session on XRD principles, two 3-hr lab sessions involving P-XRD experiments & analyses, 5-11 SC-XRD experiments (3-5 hrs/experiment) meeting individually with students/groups to mount, solve, and refine single crystal structures, and assistance with student/group independent projects.

Semesters taught: Fall 2023 (XRD training, P-XRD, SC-XRD for 8 groups)
Winter 2023 (XRD training, P-XRD, SC-XRD for 5 groups, 2 ind. projects)
Fall 2022 (XRD training, P-XRD, SC-XRD for 8 groups, 3 independent projects)
Winter 2022 (XRD training, P-XRD, SC-XRD for 7 groups)
Winter 2021 (XRD training, P-XRD, SC-XRD for 8 groups)
Winter 2020 (XRD training, P-XRD, SC-XRD for 10 groups)
Winter 2019 (XRD training, P-XRD, SC-XRD for 5 groups)
Winter 2018 (XRD training, P-XRD, SC-XRD for 11 groups)
Winter 2017 (XRD training, P-XRD, SC-XRD for 8 groups)
Winter 2016 (XRD training, P-XRD, SC-XRD for 10 groups)
Winter 2015 (XRD training, P-XRD, SC-XRD for 10 groups)
Winter 2014 (XRD training, P-XRD)

Guest Lecturer: WS 370: Women in Science – 6 classes

Involvement: 1-2 lectures (1.5hr each) on women in crystallography

Semesters taught: Fall 2023 (2 crystallography lectures + lab tour)
Fall 2022 (2 crystallography lectures + lab tour)
Fall 2021 (1 crystallography lecture + lab tour)
Fall 2017 (2 crystallography lectures + lab tour)
Fall 2015 (1 crystallography lecture + lab tour)
Winter 2014 (1 chemistry & 1 crystallography lecture)

Guest Lecturer: Chem 455/555 – 4 classes

Involvement: One 1-hr lecture and 1-2 lab demonstrations (1.5 hr/each)

Semesters taught: Fall 2023 (1 crystallography lecture)
Fall 2022 (1 crystallography lectures + 2 lab demonstrations)
Fall 2021 (1 crystallography lecture)
Fall 2020 (1 crystallography lectures + 1 lab demonstration)

Guest Lecturer: UVU Structural Biology course – 2 classes

Involvement: One 3-4-hr lab demonstration with lecture

Semesters taught: Fall 2022
Fall 2021

Instructor: Chem 594R: General Seminar (0.5 credit hours) – 2 classes

Chem 495: Senior Seminar (1.0 credit hours) – 2 classes

Course Content: >10, 1-hour seminars given by visiting scientists. Students write summaries of 2-3 papers published by a speaker of their choice. Chem 495 has an additional requirement to compile portfolios for graduation.

Semesters taught: Fall 2014, 95 students in 594R, 8 students in 495
Fall 2013, 98 students in 594R, 11 students in 495

RESEARCH EXPERIENCE

- 2013-Present* **BYU X-ray Diffraction Specialist & Facility Director**
Single crystal X-ray diffraction (SC-XRD) analyses of organic and inorganic small molecule compounds (<100 atoms/molecule). Collaborative projects, student mentoring, lab management, instrument maintenance, data management
Polycrystalline X-ray diffraction (P-XRD) analyses of powders, thin films, machined parts, and other materials. Collaborative projects, student mentoring, lab management, instrument maintenance, data management
- 2012- 2013* *Postdoctoral studies, MIT, Cambridge, MA*
Advisor: Dr. Peter Mueller (MIT SC-XRD lab director)
With additional training from Dr. Scott Speakman (MIT P-XRD lab director)
SC-XRD and P-XRD analyses of organic and inorganic small molecule compounds. X-ray reflectivity (XRR) studies of semiconductor thin films.
- 2007- 2012* *Graduate studies, Brigham Young University, Provo, UT*
Advisors: Dr. Branton J. Campbell, Dr. Julie Boerio-Goates, Dr. Brian F. Woodfield
X-ray-PDF, Rietveld, EXAFS, Solid-state NMR, BET, and TEM analyses of Al₂O₃ catalyst supports and La-doped supports to determine Al₂O₃ phase progression, nanoparticle morphology, agglomerate porosity, and La dopant location vs. synthetic temperature. Symmetry-mode analyses of the Al₂O₃ phase diagram & select phase transitions to determine the mechanism by which the La dopant stabilizes transitional Al₂O₃ phases to higher temperatures
P-XRD, TG/DTA-MS, FTIR analysis of the reaction mechanism for a novel synthetic method for making metal oxide nanoparticles.
- June 2009* *National School of Neutron and X-ray Scattering (NXS 2009)*
2-week training on synchrotron X-ray and neutron scattering techniques at Oakridge and Argonne National Laboratories sponsored by DOE. 60 students/yr competitively selected to participate.
- 2004-2007* *Undergraduate Research Assistant, Brigham Young University, Provo, UT*
Advisors: Dr. Brian F. Woodfield, Dr. Julie Boerio-Goates
Adiabatic/semi-adiabatic calorimetric studies of hexagonal ice, akaganeite (β-FeOOH), and adsorbed water and related low-T Schottky anomaly on nano/bulkTiO₂.
- Summer 2003* *Research Assistant, Arkansas State University, Jonesboro, AR*
Advisor: Dr. Roger Buchanon
Surgically implanted electrodes in live rats in preparation for a study on the effects of nicotine addiction on electrical signals in the brain

PRESENTATIONS

Colors indicate BYU undergraduate student (red), BYU graduate student (green), and BYU faculty coauthors

1. Ho, S.-H.; Valdivia-Berroeta, G.; Rader, C.; Green, N. K.; Ludlow, D. J.; Petersen, P.; Chartrand, C.; Barlow, C.; Smith, S. J.; Michaelis, D. J.; Johnson, J. A. "How to Identify Nonlinear Optical Crystals for THz Generation." *American Crystallographic Association (ACA) Annual Meeting*, Baltimore, Maryland, July 9, 2023. (Oral)
2. Torrie, J.; Adams, J.; Smith, S.; Rappleye, D. "Novel Chloride Volatility Scheme for Reprocessing Advanced Reactor Used Nuclear Fuel." *Actinide Separations Conference*, Idaho Falls, Idaho, May 18, 2023. (Oral)
3. Mpaata, P.; Bonsrah, D.; Camp, A.; Miller C.; Ballard, K.; Johnson, Z.; Angelie, L.; Smith, S. J.; Andrus, M. B., "Novel chiral aryltetraline lactone core and furo[3,4-c] pyranone structure for the synthesis of bioactive

- lignins and furopyranones.” *Pan African Conference on Crystallography (PCCr3)*, Bomas of Kenya, Nairobi-Kenya, January 18, **2023**. (Oral)
4. **Smith, S. J.; Harrison, R. G.**, “Counterion Quandary.” *American Crystallographic Association (ACA) Annual Meeting*, Portland, Oregon, July 31, **2022**. (Oral)
 5. **Mpaata, P.; Bonsrah, D.; Camp, A.; Miller C.; Ballard, K.; Johnson, Z.; Angelie, L.; Smith, S. J.; Andrus, M. B.**, “Novel chiral aryltetraline lactone core and furo[3,4-c] pyranone structure for the synthesis of bioactive lignins and furopyranones.” *American Crystallographic Association (ACA) Annual Meeting*, Portland, Oregon, August 2, **2022**. (Oral)
 6. **Mpaata, P.; Bonsrah, D.; Camp, A.; Miller C.; Ballard, K.; Johnson, Z.; Angelie, L.; Smith, S. J.; Andrus, M. B.**, “Development of asymmetric intramolecular styryl\hetero Diels-Alder protocol for the total synthesis of lignans and furopyranone containing natural products.” *American Chemical Society (ACS) National Meeting*, San Diego, California, **2022**.
 7. Fuller, S.; Martinez, E.; Larson, A. J. S.; Petersen, K. M.; Smith, S. J.; Michaelis, D. J. In “Palladium N-H N-heterocyclic carbene complexes and their reactivity in Suzuki-Miyaura reactions of aryl chlorides.” *American Chemical Society (ACS) National Meeting*, San Diego, California, **2022**.
 8. **Johnson, J. A.; Smith, S. J.; Michaelis, D. J.; Ho, S.-H.; Valdivia-Berroeta, G.; Rader, C.; Green, N. K.; Ludlow, D. J.; Petersen, P.; Chartrand, C.; Barlow, C.**; “A New Screening Methodology for THz Generation Crystals.” *Laser Science 2022*, Rochester, New York, October, **2022**. (Oral)
 9. **Johnson, J. A.; Smith, S. J.; Michaelis, D. J.; Ho, S.-H.; Valdivia-Berroeta, G.; Zaccardi, Z.; Pettit, S. K. F.; Palmer, B. W.; Lutz, M. J.; Rader, C.; Hunter, B. P.; Green, N. K.; Barlow, C.; Wayment, C. Z.; Harmon, D. J.; Petersen, P.** “Data Mining for Terahertz Generation Crystals.” *47th International Conference on Infrared, Millimeter and Terahertz Waves (IRMMW-THz)*, Delft, Netherlands, August, **2022**. (Oral)
 10. **Smith, S. J.; Ho, S.-H.; Baral, R.**, Workshop on Powder Diffraction: It doesn’t always have to be a single crystal.” *2021 USA Bruker Users Meeting*, Virtual, October 18-19, **2021**. (Oral, Invited Presentation)
 11. **Smith, S. J.; Valdivia, G.** “Misbehaving twins: How messy is too messy?” *American Crystallographic Association (ACA) Annual Meeting*, Cincinnati, Ohio, July 23, **2019**. (Oral, Invited Presentation)
 12. **Valdivia-Berroeta, G. A.; Wayment, A. X.; Kenney, K. C.; Jackson, E. W.; Tangen, I. C.; Bahr, C. B.; Smith, S. J.; Michaelis, D. J.; Johnson, J. A.** “Designing molecular terahertz generation crystals: optimal packing could be just one carbon away.” *American Crystallographic Association (ACA) Annual Meeting*, Cincinnati, Ohio, July 22, **2019**. (Oral)
 13. **Woodfield, B. F.; Smith, S. J.; Zhang, Y.**, The determination of the local structure and phase evolution of unique boehmite-derived mesoporous aluminas. In *NATO Advanced Research Workshop: Security Through Science*, Odessa, Ukraine, October, **2019**. (Oral)
 14. **Harris, L.; Colton, J. S.; Smith, S. J.; Campbell, B. J.**, The Crystal Structure of Zn_3As_2 . In *Four Corners Section Meeting American Physical Society*, Embry-Riddle Aeronautical University, Prescott, AZ, October, **2019**. (Oral)
 15. **Weir, E. S.; Valdivia, G.; Kenney, K.; Wayment, A.; Smith, S. J.; Johnson, J.; Michaelis, D. J.** “Centrosymmetric versus non-centrosymmetric crystals for terahertz generation: Just one carbon away” 257th American Chemical Society (ACS) National Meeting, Orlando, Florida, March 31 – April 4, **2019**; pp PHYS-0601 (Oral)
 16. **Smith, S. J.; Calvin, J. J.; Woodfield, B. F.** “The Missing Link: First Successful Structural Analysis of 2-ethylimidazole, a ZIF linker.” *American Crystallographic Association (ACA) Annual Meeting*, Toronto, Canada, July 24, **2018**. (Oral)
 17. **Heki, L.; Valdivia-Berroeta, G.; McMurray, E.; Smith, S.; Michaelis, D.; Johnson, J.** “Organic crystals for THz generation.” 255th American Chemical Society (ACS) National Meeting, New Orleans, Louisiana, March 18-22, **2018**. pp CHED-1702.

18. Ying, Z.; Smith, S. J.; Woodfield, B. F.; Ess, D. H. "Investigating the Local Structure and Phase Evolution of Mesoporous Gamma Alumina Using Pair Distribution Function (PDF) Analysis." *American Crystallographic Association (ACA) Annual Meeting*, New Orleans, Louisiana, May 27, **2017**. (Oral)
19. Smith, S. J. "Using the Tools at Hand to Study Whatever Comes My Way." *American Crystallographic Association (ACA) Annual Meeting*, Denver, Colorado, July 23, **2016**. (Oral)
20. Smith, S. J. "The Vast Capabilities of X-ray Diffraction & Scattering in Material Analysis." *Pittcon Conference & Expo 2015*, New Orleans, Louisiana, March 12, **2015**. (Oral, Invited Presentation)
21. Smith, S. J.; Ruf, M. "X-ray Crystallography: It doesn't always have to be a single crystal." *Bruker-AXS International Webinar Presentation*, October 7, **2014**. (Oral, Invited Presentation)
22. Smith, S. J.; Mueller, P., Comparing single crystal and powder XRD instruments for routine quantitative powder analyses. *American Crystallographic Association (ACA) Annual Meeting*, Honolulu, Hawaii, July 24, **2013**. (Oral)
23. Smith, S. J.; Amin, S.; Woodfield, B. F.; Boerio-Goates, J.; Campbell, B. J. "Phase Progression of Al₂O₃ nanoparticles determined via XRD and ²⁷Al MAS NMR analyses." *Bruker/MIT Symposium*, February, **2013**. (Poster)
24. Smith, S. J.; Huang, B.; Bartholomew, C. H.; Woodfield, B. F.; Boerio-Goates, J.; Campbell, B. J. "The role of a La dopant in inhibiting the gamma to alpha Al₂O₃ phase transition." *American Crystallographic Association (ACA) Annual Meeting*, Boston, Massachusetts, August 1, **2012**. (Oral)
25. Smith, S. J.; Huang, B.; Cook, K.; Olsen, R. E.; Bartholomew, C. H.; Woodfield, B. F.; Boerio-Goates, J.; Campbell, B. J. "Revised mechanism of La stabilization for La-doped alumina catalyst supports." *242nd American Chemical Society (ACS) National Meeting*, Denver, Colorado, August 30, **2011**. (Oral)
26. Smith, S. J.; Campbell, B. J. "Symmetry-mode analysis of the alumina phase diagram." *International Union of Crystallography (IUCr) XXII Congress and General Assembly*, Madrid, Spain, August 22-30, **2011**. (Poster)
27. Smith, S. J.; Huang, B.; Cook, K.; Olsen, R. E. B., C. H.; Woodfield, B. F.; Boerio-Goates, J.; Campbell, B. J. "Revised mechanism of La stabilization for La-doped Al₂O₃ catalyst supports." *Spring Research Conference*, BYU, Provo, Utah, March 19, **2011**. (Oral)
28. Smith, S. J.; Campbell, B. J.; Huang, B.; Bartholomew, C. H.; Woodfield, B. F.; Boerio-Goates, J.; Page, K.; Kim, H.; Chapman, K. "Phase progression of alumina nanoparticle catalyst supports as a function of synthetic temperature." *American Crystallographic Association (ACA) Annual Meeting* Chicago, Illinois, July 24-29, **2010**. (Oral)
29. Smith, S. J.; Olsen, R. E.; Cook, K.; Huang, B.; Bartholomew, C. H.; Woodfield, B. F.; Boerio-Goates, J.; Campbell, B. J. "Novel synthesis of metal oxide-nanoparticle catalysts and catalyst supports and their structural characterization via combined PDF/EXAFS analysis." *Pacificchem 2010*, Honolulu, Hawaii, December 15-20, **2010**. (Poster)
30. Smith, S. J.; Olsen, R. E.; Cook, K.; Huang, B.; Bartholomew, C. H.; Woodfield, B. F.; Boerio-Goates, J.; Campbell, B. J. "Revised mechanism of La stabilization for La-doped alumina catalyst supports." *2010 American Institute of Chemical Engineers (AIChE) Annual Meeting*, Salt Lake City, Utah, November 7-12, **2010**. (Poster)
31. Smith, S. J.; Campbell, B. J.; Bartholomew, C. H.; Woodfield, B. F.; Boerio-Goates, J.; Astle, L. "Structural characterization of alumina nanoparticle supports using TEM, XAFS, Rietveld, and PDF techniques." *239th American Chemical Society (ACS) National Meeting*, San Francisco, California, March 21-25, **2010**. (Oral)
32. Smith, S. J.; Campbell, B. J.; Bartholomew, C. H.; Woodfield, B. F.; Boerio-Goates, J. "Structural characterization of alumina nanoparticle catalyst supports." *Spring Research Conference*, BYU, Provo, Utah, March 20, **2010**. (Oral)

33. Smith, S. J.; Olsen, R. E.; Liu, Q.; Liu, S.; Woodfield, B. F.; Boerio-Goates, J. "Mechanism behind a novel green, two-step, general method for synthesizing metal and metal oxide nanoparticles." *North American Solid State Chemistry Conference (NASSC)*, Columbus, Ohio, March 17-20, **2009**. (Poster)
34. Smith, S. J.; Liu, Q.; Boerio-Goates, J.; Woodfield, B. F. "The Mechanism behind a Novel Two-Step Solid-State Method for Synthesizing Metal Oxide Nanoparticles." *Joint 63rd Northwest and 21st Rocky Mountain Regional Meeting of the American Chemical Society (ACS)*, Park City, Utah, June 15–18, **2008**. (Oral)
35. Smith, S. J.; Liu, Q.; Boerio-Goates, J.; Woodfield, B. F. "How does it work? The mechanism behind a novel two-step solid-state synthesis method for making metal oxide nanoparticles." *Spring Research Conference*, BYU, Provo, Utah, March 15, **2008**. (Oral)
36. Smith, S. J.; Boerio-Goates, J.; Woodfield, B. F. "Using models of TiO₂ to study unusual surface phenomena." *1st Annual Utah Conference for Undergraduate Research (UCUR)*, Salt Lake City, Utah, **2007**. (Poster)

PUBLICATIONS

Colors indicate *BYU undergraduate student (red)*, *BYU graduate student (green)*, and *BYU faculty coauthors*

1. D. J. Ludlow, B. W. H. Palmer, N. K. Green, S.-H. E. Ho, C. Z. Wayment, B. M. Kelleher, C. D. Barlow, O. N. Rollans, B. P. Hunter, C. Rader, M. J. Lutz, T. Manwaring, S. J. Smith, D. J. Michaelis, J. A. Johnson, Intense THz Generation with New Organic NLO Crystal NMBA. *Adv. Optical Mater.* **2024**, 2302402. <https://doi.org/10.1002/adom.202302402>
2. Mpaata, Peter; Miller, Chandler; Bonsrah, Dickson; Camp, Alexander; Ballard, Karson; Angelie, Liahona; Kirkland, Justin; Joy, Jyothish; Hirschi, William; Smith, Stacey; Ess, Daniel; Andrus, Merritt. Intramolecular Heteroatom and Styryl Diels-Alder Reactions, Asymmetric Cycloadditions of Chiral 3-Phenylallyl Maleic Esters. *J. Org. Chem.* **2024**, Submitted. *Tier 1 Journal*
3. Schill, A. L.; Martinez, E. E.; Larson, A. J. S.; Richardson, E. L.; Parkman, J. A.; Forson, K.; Pettit, S. K. F.; Smith, S. J.; Michaelis, D. J., Synthesis and Reactivity of Monometallic and Bimetallic 2-Phosphinoimidazole Complexes of Platinum. *Organometallics* **2024**, Accepted for publication. <https://doi.org/10.1021/acs.organomet.3c00508> *Tier 1 Journal*
4. Aztatzi-Mendoza, M. A.; Ortega-Villarreal, A. S.; Lopez, I.; Espinosa Roa, A.; Lopez-Cortina, S.; Bernal, W.; Maldonado, J. L.; Valdivia-Berroeta, G. A.; Smith, S. J.; Christensen, K. A.; Michaelis, D. J. Hernandez-Fernandez, E. Synthesis, characterization, optical properties, and solvatochromism of highly fluorescent benzotriazolyl vinyl aniline based D- π -A fluorophores. *J. Photochem. Photobiol., A.* **2024**, 449, 115400. <https://doi.org/10.1016/j.jphotochem.2023.115400> *Tier 1 Journal*
5. Roy, R.; Bandi, S.; Li, X.; Schooff, B.; Kuttler, R.; Aichele, M.; Montgomery, S.; Tuttle, J.; Wendt, J. O. L.; Smith, S. J.; Iverson, B.; Fry, A. Synergistic reduction of SO₂ emissions while co-firing biomass with coal in pilot scale (1.5 MW_{th}) and full scale (471 MW_e) combustors. *Fuel.* **2024**, 358, 130191. <https://doi.org/10.1016/j.fuel.2023.130191> *Tier 1 Journal*
6. Forson, K.; Owens, R.; Parkman, J.; Bohman, B.; Wayment, C.; McKnight, C.; Davis, R.; Stillwell, L.; Kini-Lopes, K.; Cole, R.; Marchenko, A.; Smith, S. J.; Michaelis, D. Allene Trifluoroacetoxylation with a 2-Phosphinoimidazole-Derived Bimetallic Rh(II) Catalyst. *ACS Catal.* **2023**, 13(19) 12458-12463. <https://doi.org/10.1021/acscatal.3c02994> *Tier 1 Journal*
7. Hassan, E.; Mostafa, M.; Smith, S. J.; Harrison, R. G.; Youssef, M. Structural variety of Co²⁺, Ni²⁺, Pd²⁺, and Pt⁴⁺ complexes of a hydrazone based on Girard's T: synthesis, spectroscopic, molecular docking simulation on CTX-M-14 β -lactamase, and theoretical (DFT) studies. *Appl. Organomet. Chem.* **2023**, DOI: [10.1002/aoc.7220](https://doi.org/10.1002/aoc.7220). *Tier 2 Journal*
8. Alnasar, H. F.; Smith, S. J.; Sparks, T. D. Structural investigations of the Bi_{1-*x*}Sb_{*x*}Te_{3-*y*}Se_{*y*} topological insulator. *J. Solid State Chem.* **2023**, 320, 123868. <https://doi.org/10.1016/j.jssc.2023.123868> *Tier 1 Journal*
9. Valdivia-Berroeta, G. A.; Zaccardi, Z. B.; Pettit, S. K. F.; Ho, S.-H.; Palmer, B. W.; Lutz, M. J.; Rader, C.; Hunter, B. P.; Green, N. K.; Barlow, C.; Wayment, C. Z.; Ludlow, D. J.; Petersen, P.; Smith, S. J.; Michaelis, D.

- J.; Johnson, J. A., Data Mining for Terahertz Generation Crystals. *Adv. Mater. (Weinheim, Ger.)* **2022**, *34* (16), 2107900. <https://doi.org/10.1002/adma.202107900> *Tier 1 Journal*
10. Rader, C.; Zaccardi, Z. B.; Ho, S.-H. E.; Harrell, K. G.; Petersen, P. K.; Nielson, M. F.; Stephan, H.; Green, N. K.; Ludlow, D. J. H.; Lutz, M. J.; Smith, S. J.; Michaelis, D. J.; Johnson, J. A., A New Standard in High-Field Terahertz Generation: the Organic Nonlinear Optical Crystal PNPA. *ACS Photonics* **2022**, *9* (11), 3720-3726. <https://doi.org/10.1021/acsp Photonics.2c01336> *Tier 1 Journal*
 11. Palmer, B. W. H.; Rader, C.; Ho, E. S.-H.; Zaccardi, Z. B.; Ludlow, D. J.; Green, N. K.; Lutz, M. J.; Alejandro, A.; Nielson, M. F.; Valdivia-Berroeta, G. A.; Chartrand, C. C.; Holland, K. M.; Smith, S. J.; Johnson, J. A.; Michaelis, D. J., Large Crystal Growth and THz Generation Properties of 2-Amino-5-Nitrotoluene (MNA). *ACS Appl. Electron. Mater.* **2022**, *4* (9), 4316-4321. <https://doi.org/10.1021/acsaelm.2c00592> *Tier 1 Journal*
 12. Forson, K. G.; Bohman, B. O.; Wayment, C. Z.; Owens, R. N.; McKnight, C. E.; Davis, R. C.; Stillwell, L. R.; Smith, S. J.; Michaelis, D. J., Medium and Large N-Heterocycle Formation via Allene Hydroamination with a Bimetallic Rh(II) Catalyst. *J. Am. Chem. Soc.* **2022**, *144* (1), 63-68. <https://doi.org/10.1021/jacs.1c10534> *Tier 1 Journal*
 13. Ence, C. C.; Martinez, E. E.; Himes, S. R.; Nazari, S. H.; Moreno, M. R.; Matu, M. F.; Larsen, S. G.; Gassaway, K. J.; Valdivia-Berroeta, G. A.; Smith, S. J.; Ess, D. H.; Michaelis, D. J., Experiment and Theory of Bimetallic Pd-Catalyzed α -Arylation and Annulation for Naphthalene Synthesis. *ACS Catal.* **2021**, *11* (16), 10394-10404. <https://doi.org/10.1021/acscatal.1c02731> *Tier 1 Journal*
 14. Martinez, E. E.; Larson, A. J. S.; Fuller, S. K.; Petersen, K. M.; Smith, S. J.; Michaelis, D. J., 2-Phosphinoimidazole Ligands: N-H NHC or P-N Coordination Complexes in Palladium-Catalyzed Suzuki-Miyaura Reactions of Aryl Chlorides. *Organometallics* **2021**, *40* (11), 1560-1564. <https://doi.org/10.1021/acs.organomet.1c00165> *Tier 1 Journal*
 15. Hernandez-Fernandez, E.; Ortega-Villarreal, A. S.; Garcia-Lopez, M. C.; Chan-Navarro, R.; Garrard, S.; Valdivia-Berroeta, G. A.; Smith, S. J.; Christensen, K. A.; Michaelis, D. J., Synthesis and characterization of benzotriazolyl acrylonitrile analogs-based donor-acceptor molecules: Optical properties, in vitro cytotoxicity, and cellular imaging. *Dyes Pigm.* **2021**, *189*, 109251. <https://doi.org/10.1016/j.dyepig.2021.109251> *Tier 1 Journal*
 16. Valdivia-Berroeta, G. A.; Kenney, K. C.; Jackson, E. W.; Zaccardi, Z.; Tangen, I. C.; Bahr, C. B.; Ho, S.-H.; Rader, C.; Smith, S. J.; Michaelis, D. J.; Johnson, J. A., Terahertz generation of two methoxy stilbazolium crystals: MBST and MBSC. *Opt. Mater. (Amsterdam, Neth.)* **2021**, *117*, 111119. <https://doi.org/10.1016/j.optmat.2021.111119> *Tier 1 Journal*
 17. Valdivia-Berroeta, G. A.; Kenney, K. C.; Jackson, E. W.; Bloxham, J. C.; Wayment, A. X.; Brock, D. J.; Smith, S. J.; Johnson, J. A.; Michaelis, D. J., 6MNEP: a molecular cation with large hyperpolarizability and promise for nonlinear optical applications. *J. Mater. Chem. C* **2020**, *8* (32), 11079-11087. <https://doi.org/10.1039/D0TC01829E> *Tier 1 Journal*
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PATENTS

Woodfield, B. F.; Smith, S.; Selck, D.; Bartholomew, C. H.; Ma, X.; Xu, F.; Olsen, R. E.; Astle, L. Single reaction synthesis of texturized catalysts. US 9,079,164 B2. Filed March 26, 2012, Issued July 14, 2015.

PROPOSALS

NSF Major Research Instrumentation Proposal (MRI), "MRI: Acquisition of a multipurpose X-ray diffractometer for materials research" PIs: Smith, S. J.; Stowers, K. J.; Johnson, J.; Frandsen, B.; Fullwood, D. Submitted Nov. 2023. Under Review.

NSF Major Research Instrumentation Proposal (MRI), "MRI: Acquisition of a dual wavelength X-ray diffractometer for structural chemistry research and education" PIs: Smith, S. J.; Michaelis, D. J.; Johnson, J.; Harrison, R. G.; Price, J. Submitted Jan. 2019. Not funded.

NSF Major Research Instrumentation Proposal (MRI), "MRI: Acquisition of a dual wavelength X-ray diffractometer for structural chemistry research and education" PIs: Smith, S. J.; Michaelis, D. J.; Johnson, J.; Harrison, R. G.; Price, J. Submitted Jan. 2018. Recommended for funding but not funded.

NSF Major Research Instrumentation Proposal (MRI), “Acquisition of an X-ray diffractometer for thin film and materials research” PIs: Smith, S. J.; Linfood, M. R.; Hawkins, A. R.; Chesnel, K.; Turley, R. S. Submitted Jan 2014. Not funded.

NSF Major Research Instrumentation Proposal (MRI-R2), “Acquisition of a powder X-ray diffractometer for chemistry research,” PIs: Woodfield, B. F.; Boerio-Goates, J.; Harrison, R. G.; Campbell, B. J. (Smith, S. J. wrote the initial draft as a graduate student.) Submitted 2009. Funds (\$200,000) were received in 2010 and used to purchase the P-XRD instrument currently used by the BYU Chemistry Dept.

Proposals for beamtime at the Advanced Photon Source (APS) at Argonne National Laboratory:

1. Structural analysis of Zn_3As_2 (GUP-65614). PIs: Stacey Smith, Lydia Harris, John Colton. Awarded beamtime 8/2019.
2. Configuration of Manganese and Iron Mixed Oxide Spinel (APS proposal 52754). PIs: Megan Asplund and Stacey Smith. Awarded beamtime 2/2017.
3. Configuration of Cobalt and Iron Mixed Oxide Spinel (APS proposal 52755). PIs: Megan Asplund and Stacey Smith. Awarded beamtime 2/2017.
4. Determining the local structure and phase evolution of mesoporous gamma alumina using PDF analysis (GUP-48523), PIs: Ying Zhang and Stacey Smith. Awarded beamtime 6/2016.
5. PDF analysis of Fischer-Tropsch catalyst reduction and reaction processes (GUP22776). PIs: Kari Cook and Stacey Smith. Awarded beamtime 10/2010.
6. Determining the local structure and phase evolution of Al_2O_3 catalyst supports using PDF/Rietveld analysis (GUP20741). PI: Stacey Smith. Awarded beamtime 03/2010.
7. Determining the location and local structure of dopants within catalysts/catalyst supports using XAFS (GUP20737). PI: Stacey Smith. Awarded beamtime 03/2010.

AFFILIATIONS

2007- present American Chemical Society (ACS)

2010- present American Crystallographic Association (ACA): The Structural Science Society

2011- present International Union of Crystallographers (IUCr)

CITIZENSHIP

BYU Department of Chemistry & Biochemistry citizenship roles:

2015 – present *Chair of the Professional Faculty Area*

2021 – present *Chair of the Major Instruments Committee*

2022 *Member of the Faculty Search Committee, spring/summer 2022*

2013 – 2022 *Member of the Undergraduate Student Advisement Committee*

2019 – 2021 *Member of the Major Instruments Committee*

2013 – 2019 *Chair of the XRD committee*

2015 – 2016 *Member of an ad-hoc committee that unified dept. graduate student standards*

2013 – 2014 *Member of the graduate student recruiting committee*

BYU community citizenship roles:

2018 – present *National Chemistry Week Magic Show presentations:*

2018, 2020, 2021, 2022, 2023

2014- present *Judge for the BYU Student Research Conference (SRC):*

2014, 2015, 2016, 2018, 2019, 2020, 2021, 2022

2015 *BYU Women's Career Conversations Panel Member, February 6, 2015*

2013 *Co-organizer of “STEM Out,” a free day of science fun and hands-on activities for 220 middle-school aged girls held at BYU on November 9, 2013*

Professional citizenship roles outside BYU:

2021 *Invited Workshop on Powder Diffraction at the 2021 USA Bruker Users Meeting, Oct 19, 2021*

<https://brukerusersmeeting.chem.wisc.edu/> Gave a 2-hour workshop on how to use single crystal XRD instruments to collect excellent powder XRD data and then perform Rietveld Refinement

- using TOPAS. >80 crystallographers from across the world participated. The video recording is available at <https://vimeo.com/showcase/9075925> for those who attended the meeting
- 2016 *NSF MRI 2016 grant reviewer, DMR X-ray panel*
- 2015 *Invited talk on XRD at the 2015 Pittcon Conference & Expo in New Orleans, LA*
- 2014 *Invited International Webinar for Bruker-AXS on October 7, 2014*
 Gave 30 minutes of a 50 minute webinar on how & when to use single crystal XRD instruments to collect powder XRD data. Crystallographers from 8 countries and 15 states participated.

Leadership positions in the American Crystallographic Association (ACA) as elected by peers
 (<https://www.amercrystalassn.org/>). *SIG = Scientific Interest Group*

- 2023-2027 *ACA Meeting Committee Member (Conference Organizer)*
 One of four individuals elected for a 4-year term to oversee and organize all scientific aspects of the annual ACA Meeting including organizing the scientific program, recruiting keynote speakers, onboarding & coordinating with session chairs and workshop organizers, coordinating & attending all SIG meetings, speaking in the opening & closing ceremonies, & fielding all questions about the conference. Most visible leadership position in the ACA other than President.
- 2023-2024 *ACA Nominating Committee Member*
 One of three individuals appointed by the ACA President & Vice President to nominate and secure at least two candidates to run for all elected positions (except SIG officers) in the ACA including President, Secretary, Treasurer, Meeting Committee, Education Committee, Communications Committee.
- 2021-2022 *Secretary of the Small Molecule SIG (Scientific Interest Group)*
 Helped edit the 2021 Service Crystallography Special Interest Group Salary and Work Environment Survey (111 participants)
- 2016-2017 *Chair-elect (2016) and Chair (2017) of the Small Molecule SIG*
- 2014-2015 *Chair-elect (2014) and Chair (2015) of the General Interest Group SIG*
- 2014-2015 *Secretary of the Service Crystallography SIG*
 Helped organize, disseminate, and analyze the 2016 Service Crystallography Special Interest Group Salary and Work Environment Survey (164 participants)

Conference sessions organized and chaired at the ACA Annual Meetings:

- 2022 *2 half-day sessions at the ACA Meeting in Portland, OR, July 29-Aug 2, 2022*
 Session 4.1.5 Cool Structures I: Important Science from X-ray & Electron diffraction
 Session 4.2.3 Cool Structures II: Important Science from Small Molecule Crystallography
- 2019 *2 half-day sessions at the ACA Meeting in Cincinnati, OH, July 20-24, 2019*
 Session 4.1.3 Cool Structures: Important Science from Small Molecule Crystallography
 Session 4.2.3 Cool Structures: Important Science from Small Molecule Crystallography
- 2016 *2 half-day sessions at the ACA Meeting in Denver, CO, July 22-26, 2016*
 Session 01.05.01 General Interest I: Active learning techniques involving crystallography
 Session 01.05.01 General Interest II: Macromolecular topics of broad interest
- 2015 *3 half-day sessions at the ACA Annual Meeting in Philadelphia, PA, July 26-31, 2015*
 Session 2.1.3 General Interest I: Developments in instrument & software technology
 Session 4.1.2 General Interest II: Macromolecular topics of broad interest
 Session 4.2.1 General Interest III: Useful tools in crystallographic analyses

Peer reviewer for the following journals:

Applied Catalysis B, ACS Catalysis, Inorganic Chemistry, Acta Crystallographica Section C, Journal of Chemical Crystallography, Thermochemica Acta, Journal of Chemical Thermodynamics

Outreach efforts:

- 2022 *Wasatch Elementary Guest Science Teacher (February 2022 – April 2022)*
 Taught 8 lessons (45-60 minutes each, once per week) using hands-on labs/activities to teach basic science principles to a small group of advanced 1st grade students at Wasatch Elementary
- 2021- present *XRD Lab tours for elementary or high school students.* In 15-20 minutes, I introduce students to diffraction and demonstrate how XRD helps us “see” the molecules in sugar crystals.

- 2021: ACS virtual tour via zoom
 2023: BYU Biochem Camp students (4 groups), Manilla High School students (3 groups)
- 2021 *BYU preschool magic show, "What is Chemistry?" 1 hr, Dec 6, 2021*
- 2020 *Created "Sticking with chemistry," a pre-recorded Magic Show for National Chemistry Week for local schools. I wrote, performed, recorded, & edited the presentation for internet distribution during the 2020 pandemic. Prof. Rebecca Sansom compiled the clips and posted it to her YouTube channel: <https://www.youtube.com/watch?v=9qxHVp4FnMM> 1.5K views.*
- 2019 *Judge in the Science category for the Deseret News/KSL Sterling Scholar program, Feb. 2019*
- 2008-present *Volunteer Judge for the Senior Division Chemistry & Biochemistry section of the Central Utah STEM Fair: 2008, 2009, 2011, 2012, 2014, 2016, 2018, 2022*
- 2018 *Judge in the Science category for the Deseret News/KSL Sterling Scholar program, Feb. 27, 2018*
- 2015 *ACA representative presenting the 3rd place award in the US National IYCr Crystal Growing Competition to Mrs. Esplin's 2nd grade class in Tremonton, UT.*
 Presented a \$250 check to the 3rd place winner of the crystal growing competition sponsored by the ACA in honor of 2014 being the International Year of Crystallography (IYCr). To enliven it, I made an over-sized (fake) check, certificates, and did a small magic show explaining basic chemistry & crystallography concepts.
- 2013 *Invited speaker at the 22nd Utah Debate Teacher-Student Annual Conference, Nov. 22, 2013*
 Gave two 25 minute presentations titled "The Chemistry of Plastic: What is it? Why do we use it? And How long does it last?" for several hundred students between 4th-9th grade
- 2013 *Provo Mentoring Magic Show, Nov. 1, 2013*
 Gave a 1 hour presentation & chemistry magic show for 6th grade students in the Provo Mentoring Program, encouraging them to attend college (and study chemistry)

OTHER AWARDS & RECOGNITIONS

Academic Recognitions as a Student

- 2012 Finalist for the Student Award in the Utah Women Tech Awards
- 2011 3rd place paper/presentation, Industrial & Engineering Chemistry (I&EC) Graduate Student Award Symposium, ACS National Conference, Denver, CO
- 2011 BYU Outstanding Chemistry/Biochemistry Graduate Student
- 2010 Etter Student Lecturer Award, American Crystallographic Association (ACA) Annual Meeting, Chicago, IL
- 2009-2010 BYU Roland K. Robins Graduate Research Fellowship for outstanding scholarship
- 2009 Neutron & X-ray Scattering School (NXS) student presentation award
- 2008, 2010 BYU Spring Research Conference session winner
- 2007-2008 BYU Nicholes/Maw Award for outstanding first-year graduate students
- 2007 Garth L. Lee award for outstanding Teaching Assistants
- 2003-2007 BYU outstanding freshman (2003-2004), physical chemistry student (2005-2006), and senior (2006-2007) in chemistry

Scholarships/Grants as a Student

- 2011 USNCCr/NSF Travel Fellowship for the XXII IUCr Congress in Madrid, Spain
- 2011 International Union of Crystallography (IUCr) student bursary
- 2011 Conference supplement from the I&EC Division for the ACS Conference in Denver, CO
- 2010 ACA Conference student travel grant
- 2010(2), 2011 BYU graduate student Research Presentation Awards (RPA) for conference travel
- 2009 DOE sponsorship for the National School of Neutron and X-ray Scattering
- 2008-2009 BYU Mentored Research Grant
- 2006 BYU Department of Chemistry Summer Undergraduate Research Award (stipend)

2003-2007 National Merit Scholarship
2003 SAMMY scholarship (Scholar Athlete Milk Mustache of the Year), sponsored by 'Got Milk?'
and USA Today