

SOPHIA E. HAYES

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Professional Positions

- 2021- Vice Dean of Graduate Education, Arts & Sciences
- 2015- Professor of Chemistry, and by courtesy, Institute of Materials Science & Engineering, Washington University
- 2008-2015 Associate Professor of Chemistry, Washington Univ.
- 2001-2008 Assistant Professor of Chemistry, Washington Univ.
- 2001 Alexander von Humboldt Postdoctoral Fellow, Department of Physics, Technical University of Dortmund, Germany. Subject: optically-detected NMR studies of semiconductor quantum wells. Advisor: Prof. Dieter Suter
- 1998-2000 Directorate Postdoctoral Fellow, Lawrence Livermore National Laboratory, Livermore, CA and Dept. of Chemical Engineering, University of California, Berkeley, CA. Subject: development of optically-pumped NMR instrumentation and studies of passivation of nanoclusters. Advisors: Dr. Glenn Fox (LLNL) Prof. Jeffrey A. Reimer (UC Berkeley)
- 1993-1998 Graduate Research and Teaching Assistant, Department of Chemistry, Univ. of California, Santa Barbara, CA. Subject: Solid-state NMR of lithium intercalated graphitic anodes. Advisors: Prof. Hellmut Eckert and Dr. William R. Even
- 1993 Summer Intern, Sandia National Laboratories, Livermore, CA. Subject: materials synthesis of polymer-derived high-surface area carbon foams. Advisor: Dr. William R. Even
- 1990-1993 Associate, Hagler, Bailly, Inc. San Francisco, CA (*management consulting firm specializing in energy efficiency, environmental assessments, energy generation, and technology transfer*)

Education

- 2013 Executive Education Program, Olin Business School, Washington University
- 1999 Ph.D., Chemistry, University of California, Santa Barbara with Prof. Hellmut Eckert and Dr. William R. Even (Sandia Nat'l Labs). Thesis title: *Lithium intercalation of amorphous carbons: a solid state NMR study of structure and electronic properties*
- 1990 B.S., Chemistry, University of California, Berkeley

Awards and Honors (Selected)

- Fellow of the American Association for the Advancement of Science – 2022
- American Physical Society, "5 σ Physicist" Award, 2020 (for professional service to the community)
- TEDx Speaker - "Science the Heck Out of Climate Change" – 2019
- DOE Office of Science, Team Science Award, 2017, Hayes- and Sholl-groups from DOE EFRC Center for Understanding and Control of Acid Gas-induced Evolution of Materials for Energy
- St. Louis Award, American Chemical Society, 2015
- Regitze R. Vold Memorial Prize, Alpine Solid-State NMR Conference (organized under the Groupement Ampere and Int'l Society of Magnetic Resonance, ISMAR), 2009
- ACS Progress/Dreyfus Lectureship, 2008
- Alfred P. Sloan Research Fellow, 2007-2009
- Washington Univ. Graduate Student Senate Special Recognition for Excellence in Mentoring, 2004
- NSF Early Career Development (CAREER) Award, 2003
- Alexander von Humboldt Research Fellow, Dept. of Physics, Univ. of Dortmund, Germany, 2001

Chemistry and Materials Science Directorate Award, Lawrence Livermore National Lab, 1999
Directorate Postdoctoral Fellow, Lawrence Livermore National Laboratory, 1998-2000

Leadership Highlights (selected)

Vice Dean of Graduate Education, School of Arts & Sciences, 2021 – present. Tasked with developing a new role to innovate and guide graduate education among the approximately 30 graduate degree-granting departments and programs in Arts & Sciences.

Co-Chair, Chemistry Steering Committee, WU, 2021 – present (an executive committee to advise the Chair on a multi-year strategic plan to restructure and set new directions in the department)

Arts & Sciences, WU Strategic Planning Group, 2021 – present (an executive committee for strategic planning with the dean, college-wide)

WU (university-wide) Faculty Committee for Tech Transfer, 2020 – present (an executive committee to act as liaison between the Office of Technology Management and the Faculty)

Executive Committee (and former Chair), Rocky Mountain NMR Conference (RMC) 2022—organization and leadership of a 200 to 300-person international conference

Chair and Organizer, Experimental NMR Conference (ENC), 2021—organization and leadership of an 820-person international conference, the premier meeting for NMR

Chair and leader of the American Chemical Society (ACS) St. Louis section, (succession 3-year term) 2019-2022—provide leadership and new initiatives for a group of ~1400-1500 chemical scientists in the region. During my tenure, we launched diversity initiatives for awareness of issues surrounding equity and inclusion, implemented a trial student travel grant at 4 PhD-granting universities, and assisted the community during the COVID-19 pandemic with chemical expertise and led efforts for PPE donation drives.

Helium policy leadership – 2015 - present –advocate and advisor for U.S. policy concerning the helium supply and U.S. Strategic Helium Reserve, in particular for researchers and science and technology, via the American Physical Society and American Chemical Society.

Executive Committee, NSF Center for Chemical Innovation “Center for Sustainable Materials Chemistry” 2012 – 2019 (set research directions for a \$4M/year center, develop education and training programs including innovation, and lead diversity, equity, and inclusion activities)

Chair-Elect/Vice Chair, Gordon Research Conference, Magnetic Resonance, 2011

Co-creator of the Blue Skies Group (via WashU’s Institute for School Partnership) – a reading and discussion group for K-12 educators, to address topics surrounding energy and the environment (<https://schoolpartnership.wustl.edu/event/blue-skies-discussion-group/>)

Co-chair and creator of the “Washington U. Frontiers in Technology & Science” conference: a grass-roots faculty-driven conference highlighting emerging research projects from young faculty, facilitating connections between departments and schools in STEM fields.

Research Interests

Optically-pumped NMR: Development and application of optically-pumped (OPNMR) and optically-detected (ODNMR) NMR of bulk semiconductors and quantum wells to gain insight into the interplay between photo-generation of conduction electrons, electron spin polarization, and resulting nuclear spin polarization. Surface and interface structures, as well as characterization of defects in the materials and spin diffusion processes that can polarize distant spins are being studied. These research foci have particular relevance to solar energy materials and LED applications.

Computation of NMR tensors and spectra prediction: Creation of an NMR library of spin-1/2 and quadrupolar tensors through The Materials Project, computing NMR tensors from crystal structures of dominantly inorganic compounds. Density functional theory calculations of NMR tensors in CASTEP and VASP.

NMR crystallography: using the tensor catalogue, we work on refinements of atomic coordinates for materials where the NMR and X-ray diffraction lead to slightly different predictions of structure. NMR can be used to refine atomic coordinates, especially for species such H-atoms.

Carbon capture & sequestration: NMR characterization of CO₂ (and CH₄) chemisorption and physisorption in materials tailored for greenhouse gas removal. Some studies are by *in situ* high-pressure high-temperature CO₂ NMR studies of gas, liquid, and supercritical CO₂ in the presence of geological (porous) rock samples and in materials designed for the capture of CO₂ or other gaseous materials (such as methane, and acid gases including SO_x, NO_x).

Solid-state NMR studies on quadrupolar systems: diverse nuclei studied, including many Group III inorganic molecular clusters that are deposited as thin metal oxide films used as dielectrics in semiconductor devices. The focus has been predominantly ²⁷Al, ⁶⁹Ga, ⁷¹Ga, ⁵¹V measurements and modeling of the quadrupolar lineshapes.

Topochemistry: solid-state single crystal-to-single crystal photo-cycloaddition reactions can be monitored via solid-state NMR, given our unique hardware for incorporating laser irradiation at the sample space. NMR was able to determine reaction kinetics of cinnamic acid to truxillic acid conversions, and examine additional derivatives.

Publications (* indicates corresponding authors)

76. West, Michael E.; Willmering, Matthew M.; Ma, Zayd, L.; *Hayes, Sophia E. "Long lived coherences exhibited for ¹¹³Cd-¹²⁵Te spin pairs in CdTe using optically-pumped NMR" in preparation for Phys. Rev. Lett.
75. Cui Jinlei; Prisk, Timothy R.; Olmsted, David L.; Su, Vicky; Asta Mark; *Hayes, Sophia E. "Resolving the Chemical Formula of Nesquehonite: Complementary NMR Crystallography, DFT Computation, and Neutron Diffraction" **2022** *Angew. Chemie*. submitted.
74. Henkelis, Susan E.; Judge, Patrick T.; Hayes, Sophia E.; Nenoff, Tina M. "Preferential SO_x Adsorption in Mg-MOF-74 from a Humid Acid Gas Stream" *ACS Appl. Mater. Interface*. **2021**, *13*, 7278-7284. DOI: 10.1021/acsami.0c21298.
73. Lee, Zachary R.; Quinn, La'Darious J.; Jones, Christopher W.; Hayes, Sophia E.; and *Dixon, David A. "Predicting the Mechanism and Products of CO₂ Capture by Amines in the Presence of H₂O" *J. Phys. Chem. A* **2021**, *125*, 9802-9818. DOI: 10.1021/acs.jpca.1c05950
72. Chen, Chia-Hsin; Sesti, Erika; Lee, Jason J.; Mentink-Vigier, Frederic; Sievers, Carsten; Jones, Christopher W.; *Hayes, Sophia E. "NMR reveals two bicarbonate environments in SBA-15-solid-amine CO₂ sorbents" *J. Phys. Chem. C* **2021** *125*, 16759–16765. DOI: 10.1021/acs.jpcc.1c04145

71. Cendejas, A.J.; Sun, H.; Hayes, Sophia E.; Kortshagen, U.; *Thimsen, E. "Predicting plasma conditions necessary for synthesis of γ -Al₂O₃ nanocrystals" *Nanoscale* **2021**, *13*, 11387-11395. DOI: 10.1039/D1NR02488D
70. Sun, He; Hammann, Blake, A.; Brady, Alexander B.; Singh, Gurpreet; House, Lisa M.; Takeuchi, Esther S.; Takeuchi, Kenneth J.; Marschilok, Amy C.; *Hayes, Sophia E.; *Szczepura, Lisa F. "Structural Investigation of Silver Vanadium Phosphorus Oxide (Ag₂VO₂PO₄) and its Reduction Products" *Chem. Mater.* **2021**, *33*, 4425-4434. DOI: 10.1021/acs.chemmater.1c00446
69. West, Michael E.; Sesti, Erika L.; Willmering, Matthew M.; Wheeler, Dustin D.; Ma, Zayd, L.; *Hayes, Sophia E. "Describing Angular Momentum Conventions in Circularly Polarized Optically Pumped NMR in GaAs and CdTe" *J. Magn. Reson.* **2021**, *327*, 106980. DOI: 10.1016/j.jmr.2021.106980
68. Henkelis, Susan; Judge, Patrick T.; Hayes, Sophia E.; *Nenoff, Tina M. "Preferential SO_x Adsorption in Mg-MOF-74 from a Humid Acid Gas Stream" *ACS Appl. Mater. Interfaces* **2021**, *13*, 7278-7284. DOI: 10.1021/acsami.0c21298.
67. Sun, He; Dwaraknath, Shyam; Ling, Handong; Qu, Xiaohui; Persson, Kristin; *Hayes, Sophia "Enabling Materials Informatics for ²⁹Si Solid-state NMR of Crystalline Materials" (*Nature Publishing Group*) *npj Computational Materials*. **2020**, *6*:53, 1-7. DOI: 10.1038/s41524-020-0328-3.
66. Zahan, Marufa; Sun, He; Hayes, Sophia E.; Krautscheid, Harald; Haase, Jürgen; *Bertmer, Marko "Influence of Alkali Metal Cations on the Photodimerization of Bromo Cinnamates Studied by Solid-State NMR" *J. Phys. Chem. C* **2020**, *124*, 27614-27620. DOI: 10.1021/acs.jpcc.0c09826.
65. Marti, Robert M.; Sarou-Kanian, Vincent; Moran, Colton M.; Walton, Krista S.; *Hayes, Sophia E. "NMR Crystallography of Aluminum Carbide: Impurities in the Reagent and Improved ²⁷Al NMR Tensors" *Inorg Chem.* **2020**, *124*, 7238-7243. DOI: 10.1021/acs.jpcc.9b11579.
64. Moran, Colton M.; Marti, Robert M.; Joshi, Jayraj; Hayes, Sophia E.; *Walton, Krista S. "Tuning Residual Metal in Partially Etched Carbide-Derived Carbons for Enhanced Acid Gas Adsorption" *Carbon* **2020**, *158*, 481-493. DOI: 10.1016/j.carbon.2019.11.016
63. Cui, Jinlei; Olmsted, David; Mehta, Anil K.; Asta, Mark; *Hayes, Sophia E. "NMR Crystallography: Evaluation of Hydrogen Positions in Hydromagnesite by ¹³C{¹H} REDOR Solid-State NMR and Density Functional Theory Calculation of Chemical Shielding Tensors" *Angew. Chem. Int. Ed.* **2019**, *58*, 4210-4216. DOI: 10.1002/anie.201813306.
62. Cui, Jinlei; Kast, Matthew G.; Hammann, Blake A.; Afriyie, Yvonne; Woods, Keenan N.; Plassmeyer, Paul N.; Perkins, Cory K.; Ma, Zayd L.; Keszler, Douglas A.; Page, Catherine J.; Boettcher, Shannon W.; *Hayes, Sophia E. "Aluminum Oxide Thin Films from Aqueous Solutions: Insights from Solid-State NMR and Dielectric Response" *Chem Mater.* **2018**, *30*, 7456-7463. DOI: 10.1021/acs.chemmater.7b05078
61. Lee, Jason J.; Yoo, Chunjae; Chen, Chia-Hsin; Hayes, Sophia E.; Sievers, Carsten; Jones, Christopher W. "Silica supported sterically hindered amines for CO₂ capture" *Langmuir* **2018**, *34*, 12279-12292. DOI: 10.1021/acs.langmuir.8b02472
60. Chen, Chia-Hsin; Shimon, Daphna; Lee, Jason J.; Mentink-Vigier, Frederic; Hung, Ivan; Sievers, Carsten; Jones, Christopher; *Hayes, Sophia E. "The 'Missing' Bicarbonate in CO₂ Chemisorption Reactions on Solid Amine Sorbents" *J. Am. Chem. Soc.* **2018** *140*, 8648-8651. DOI: 10.1021/jacs.8b04520

59. Moran, Colton M.; Joshi, Jayraj N.; Marti, Robert M., Hayes, Sophia E.; *Walton, Krista S. "Structured Growth of Metal-Organic Framework MIL-53(Al) from Solid Aluminum Carbide Precursor" *J. Am. Chem. Soc.* **2018** *140*, 9148-9153. DOI: 10.1021/jacs.8b04369
58. Moore, Jeremy K.; Marti, Robert M.; Guiver, Michael; Du, Naiying; Conradi, Mark S.; *Hayes, Sophia E. "CO₂ Adsorption on PIMs Studied with ¹³C NMR" *J. Phys. Chem. C*, **2018**, *122*, 4403-4408. DOI: 10.1021/acs.jpcc.7b12312
57. Shimon, Daphna; Chen, Chia-Hsin; Lee, Jason; Didas, Stephanie; Sievers, Carsten; Jones, Christopher W.; *Hayes, Sophia E. "¹⁵N Solid-state NMR Spectroscopic Study of Surface Amine Groups for Carbon Capture: 3-Aminopropyl Grafted to SBA15 Mesoporous Silica" *Environ. Sci. Technol.* **2018**, *52*, 1488-1495. DOI: 10.1021/acs.est.7b04555.
56. Willmering, Matthew M.; Sesti, Erika L.; Wood, Ryan; Sesti, Erika L.; Reyes, Arneil; Kuhns, Philip; Bowers, Clifford R.; Stanton, Christopher, J.; *Hayes, Sophia E. "Probing the magnetic field dependence of the light hole transition in GaAs/AlGaAs quantum wells using optically pumped NMR" *Phys Rev B* **2018**, *97*, 075303/1-9. DOI: 10.1103/PhysRevB.97.075303.
55. Marti, Robert M.; Howe, Joshua D.; Morelock, Cody R.; Conradi, Mark S.; Walton, Krista S.; Sholl, David S.; *Hayes, Sophia E. "CO₂ Dynamics in Pure and Mixed-Metal MOFs with Open Metal Sites for Carbon Capture" *J. Phys. Chem. C* **2017**, *121*, 25778-25787. DOI: 10.1021/acs.jpcc.7b07179. (journal cover Nov. 2017, <http://pubs.acs.org/toc/jpccck/121/46>)
54. Lee, Jason J; Chen, Chia-Hsin; Shimon, Daphna; Hayes, Sophia E.; *Sievers, Carsten; *Jones, Christopher W. "Effect of Humidity on the CO₂ Adsorption of Tertiary Amine Grafted SBA-15" *J. Phys. Chem. C* **2017**, *121*, 23480-23487. DOI: 10.1021/acs.jpcc.7b07930.
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52. Chen, Chia-Hsin; Shimon, Daphna; Lee, Jason J.; Didas, Stephanie A.; Mehta, Anil K.; Sievers, Carsten; Jones, Christopher W.; *Hayes, Sophia E. "Spectroscopic Characterization of Adsorbed ¹³CO₂ on 3-Aminopropylsilyl-Modified SBA15 Mesoporous Silica" *Environ. Sci Technol.* **2017**, *51*, 6553-6559. DOI: 10.1021/acs.est.6b06605.
51. Sesti, Erika L.; Willmering, Matthew M.; Ma, Zayd L.; Wheeler, Dustin D.; Conradi, Mark S.; *Hayes, Sophia E. "A Combined Experimental Setup for OP and ODNMR" *J. Magn Reson.* **2017** *281*, 172-187. DOI: 10.1016/j.jmr.2017.06.003
50. Willmering, Matthew M.; Ma, Zayd L.; Jenkins, Melanie A.; Conley, John F.; *Hayes, Sophia E. "Enhanced NMR with Optical Pumping (OPNMR) Yields ⁷⁵As Signals Selectively from a Buried GaAs Interface" *J. Am. Chem. Soc.* **2017** *139*, 3930-3933. DOI: 10.1021/jacs.6b08970.
49. Moran, Colton M.; Marti, Robert M.; Hayes, Sophia E.; *Walton, Krista S. "Synthesis and Characterization of Aluminum Carbide-Derived Carbon with Residual Aluminum Based Nanoparticles" *Carbon* **2017** *114*, 482-495. DOI: 10.1016/j.jmr.2016.09.020
48. Foo, Guo-Shiou; Lee, Jason J.; Chen, Chia-Hsin; Hayes, Sophia E.; Sievers, Carsten; *Jones, Christopher W. "Elucidation of Surface Species via *In-Situ* FTIR Spectroscopy of CO₂ Adsorption on Amine-Grafted SBA-15" *ChemSusChem.* **2017**, *10*, 266-276. DOI:10.1002/cssc.201600809.

47. Wells, Rachel K.; Xiong, Wei; Sesti, Erika; Cui, Jinlei; *Giammar, Daniel; Skemer, Philip; Hayes, Sophia E.; Conradi, Mark S. "Spatially-variable carbonation reactions in polycrystalline olivine" *Geochim. Cosmo. Acta* **2017**, *204*, 252-266. DOI: 10.1016/j.gca.2017.02.003.
46. Wheeler, Dustin D.; Sesti, Erika L.; Saha, Dipta; Pan, Xingyuan; Stanton, Christopher J.; *Hayes, Sophia E. "Modelling of OPNMR phenomena using photon energy-dependent $\langle Sz \rangle$ in GaAs and InP" *J. Magn. Reson.* **2016**, *273*, 19-26. DOI: 10.1016/j.jmr.2016.09.020
45. Cui, Jinlei; Sesti, Erika L.; Moore, Jeremy K.; Giammar, Daniel; *Hayes, Sophia E. "Evidence from ^{29}Si Solid-State Nuclear Magnetic Resonance of Dissolution Reactions of Forsterite" *Environmental Engineering Science*, **2016**, *33*, 799-805. DOI: 10.1089/ees.2016.0004.
44. Hammann, Blake A.; Marsh, David A.; Ma, Zayd L.; Wood, Suzannah R.; West, Michael E.; Johnson, Darren W.; *Hayes, Sophia E. "Synthetic Routes to a Nanoscale Inorganic Cluster $[\text{Ga}_{13}(\mu_3\text{-OH})_6(\mu_2\text{-OH})_{18}(\text{H}_2\text{O})](\text{NO}_3)_{15}$ Evaluated by Solid-State ^{71}Ga NMR" *J. Solid State Chem.* **2016**, *242* 193-198. DOI: 10.1016/j.jssc.2016.02.043.
43. Moore, Jeremy K.; Sakwa-Novak, Miles; Chaikittisilp, Watcharop; Mehta, Anil K.; Conradi, Mark S.; Jones, Christopher J.; * Hayes, Sophia E. "Characterization of a Mixture of CO_2 Adsorption Products in Hyperbranched Aminosilica Adsorbents by ^{13}C Solid-State NMR" *Environ. Sci. & Technol.* **2015**, *49*, 13684–13691. DOI: 10.1021/acs.est.5b02930
42. Hammann, Blake A.; Ma, Zayd, L.; Wentz, Katherine M.; Kamunde-Devonish, Maisha K.; Johnson, Darren W.; *Hayes, Sophia E. "Structural study by solid-state ^{71}Ga NMR of thin film transistor precursors" *Dalton Transact.* **2015**, *44*, 17652-17659. DOI: 10.1039/C5DT02967H
41. Milton N. Jackson, Jr., Maisha K. Kamunde-Devonish, Blake A. Hammann, Lindsay A. Wills, Lauren B. Fullmer, Sophia E. Hayes*, Paul H.-Y. Cheong*, William H. Casey*, May D. Nyman*, and Darren W. Johnson* "An overview of selected current approaches to the characterization of aqueous inorganic clusters" *Dalton Transact.* **2015**, *44*, 16982-17006. DOI: 10.1039/C5DT01268F
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39. Moore, Jeremy K.; Surface, J. Andrew; Brenner, Allison; Louis, Wang; Skemer, Philip; Conradi, Mark S.; *Hayes, Sophia E. "Quantitative Identification of Metastable Magnesium Carbonate Minerals by Solid-State ^{13}C NMR Spectroscopy" *Environ. Sci. Tech.* **2015**, *49*, 657-664. DOI: 10.1021/es503390d
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- Wells from Optically-Pumped NMR and Hanle Curve Measurements" *J. Magn Reson.* **2014**, 246, 130-135. DOI: 10.1016/j.jmr.2014.07.001
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19. Nieuwendaal, Ryan C.; Bertmer, Marko; *Hayes, Sophia E. "An unexpected phase transition during the [2+2] photocycloaddition reaction of cinnamic acid to truxillic acid: Changes in polymorphism monitored by solid-state NMR" *J. Phys. Chem. B* **2008**, *112*, 12920-12926. DOI: 10.1021/jp806218u
18. Fonseca, Isa; Hayes, Sophia E.; Blümich, Bernhard; *Bertmer, Marko "Temperature stability and photodimerization kinetics of β -cinnamic acid and comparison to its α - polymorph as studied by solid-state NMR spectroscopy techniques together with DFT calculations" *Phys. Chem. Chem. Phys.* **2008**, *10*, 5898-5907. DOI: 10.1039/b806861e
17. Mui, Stacy; Ramaswamy, Kannan; *Hayes, Sophia E. "Physical insights from a penetration depth model of optically-pumped NMR," *J. Chem. Phys.* **2008**, *128*, 052303/1-7. DOI:10.1063/1.2816783
16. *Hayes, Sophia E.; Mui, S.; Ramaswamy, K. "Optically pumped nuclear magnetic resonance of semiconductors," *J. Chem. Phys.* **2008**, *128*, 052203/1-17. DOI: 10.1063/1.2823131
15. Mui, S.; Ramaswamy, K.; *Hayes, S.E. "Effects of optical absorption on ^{71}Ga optically polarized NMR in semi-insulating GaAs: measurements and simulations," *Phys. Rev. B* **2007**, *75*, 195207/1-8. DOI:10.1103/PhysRevB.75.195207
14. Ramaswamy, K.; Tulsy, E.G.; Long, J.R.; Kao, J. L.-F.; *Hayes, S.E. "Determination of ^{77}Se - ^{77}Se and ^{77}Se - ^{13}C *J*-coupling Parameters for the Selenocyanide Clusters $[\text{Re}_5\text{OsSe}_8(\text{CN})_6]^{3-}$ and $[\text{Re}_4\text{Os}_2\text{Se}_8(\text{CN})_6]^{2-}$ " *Inorg. Chem.* **2007**, *46*, 1177-1186. DOI:10.1021/ic061571g
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10. Ma, G.; *Hayes, S.E. "Microwave-enhanced, solvent-free synthesis of singly and doubly ^{13}C -labelled *trans*-cinnamic acid at the α - and β -carbon positions" *J. Labelled Compd. Rad.* **2004**, *47*, 895-901. DOI: 10.1002/jlcr.878
9. Eickhoff, M.; Lenzman, B.; *Suter, D.; Hayes, S.E.; Wieck, A.D. "Mapping of Strain and Electric Fields in GaAs/Al_xGa_{1-x}As Quantum Well Samples by Laser Assisted NMR" *Phys. Rev. B* **2003**, *67*, 085308/1-5. DOI: 10.1103/PhysRevB.67.085308
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7. *Hayes, S.E.; Guidotti, R.; Even, W.R., Jr.; Hughes, P.J.; Eckert, H. " ^7Li solid-state nuclear Jetic resonance as a probe of lithium species in microporous carbon anodes" *J. Phys. Chem. A* **2003**, *107*, 3866-3876. DOI: 10.1021/jp021772f
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5. Rosenhahn, C.; Hayes, S.E.; Rosenhahn, B.; *Eckert, H. "Structural organization of arsenic selenide glasses: new results from liquid state NMR" *J. Non-Cryst. Solids* **2001**, *284*, 1-8. DOI: 10.1016/S0022-3093(01)00371-4
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Corporate Authorship

Hamers, Robert; **Hayes, Sophia**; Peaslee, Graham "Mid-Scale Instrumentation: Regional Facilities to Address Grand Challenges in Chemistry. A workshop sponsored by the National Science Foundation." <https://doi.org/10.7936/K71G0KF7>. Arlington, VA, September 29-30, **2016**. Web.

Bare, Simon R.; Lilly, Michael; Chermak, Janie; Eggert, Rod, Halperin William, Hannahs, Scott; **Hayes, Sophia**; Hendrich, Michael; Hurd, Alan; Osofsky, Mike; Tway, Cathy "Responding to the U.S. Research Community's Liquid Helium Crisis" (<https://www.aps.org/policy/reports/popa-reports/upload/HeliumReport.pdf> and <https://doi.org/10.7936/K7571B6D>). American Physical Society, Materials Research Society, American Chemical Society October **2016**. Web.

Patents

U.S. Patent (US8084374 B2) "Tuning of Photo-Absorption Materials through Use of Magnetic Fields" (2011) Hayes, S.E.; Ramaswamy, K.; Mui, S.

Provisional Patent "Spectroscopic Identification of Defects in Semiconductors through Optically-Pumped Nuclear Magnetic Resonance" Ref: 009039-PRO1 (2010) Hayes, S.E.; Ramaswamy, K.; Mui, S.

Research Support**Funded Support:**

- 7/22 – 6/27 **NSF NRT** "NRT: Training a diverse interdisciplinary workforce in applications of quantum technologies" (Hayes is lead-PI. Co-PIs: Sheretta Barnes, Erik Henriksen, Kater Murch)
- 9/20-8/23 **NSF DMR Condensed Matter Physics** "Development of Optically-pumped NMR Methods for Structural Characterization of Semiconductor Interfaces" (#2004915) (Hayes is PI. Sr. Personnel: Bill Brey, NHMFL and John Conley, OSU)
- 8/18 - 7/22 **DOE EFRC**, "Center for Understanding and Control of Acid Gas-induced Evolution of Materials for Energy" (Lead-PI: Krista Walton, GA Tech; Hayes is Senior Personnel)
- 10/16-9/22 **NSF Data Infrastructure Building Blocks: DIBBs Program, Div. of Adv. Cyberinfrastructure**, "CIF21 DIBBs: El: The Local Spectroscopy Data Infrastructure (#1640899) (Lead-PI: Kristin Persson, UC Berkeley, co-PIs: Mark Asta, UC Berkeley; Shyu Ping Ong, UCSD; Sophia Hayes)

Pending Support:

- 2022 – 2025 **Dreyfus Foundation** "Computation of NMR Spectra, Benchmarking, and Materials Informatics from Local Coordination Environments" (Hayes is sole PI)

Completed Support:

- 10/19-9/21 **NSF Quantum Leap Challenge Institute-Conceptualization Grant** "QLCI - CG: - Center for Quantum Sensors" (#1936526) (led by Kater Murch; Hayes is a co-PI)
- 9/16 – 8/19 **NSF Phase III Centers for Chemical Innovation**, "CCI Phase III: Center for Sustainable Materials Chemistry" (Lead-PI: Doug Keszler, OSU; Hayes is Senior Personnel)
- 8/14 - 7/18 **DOE Energy Frontiers Research Center, DE-FOA-0001010** "Center for Understanding and Control of Acid Gas-induced Evolution of Materials for Energy" (Lead PI: Krista Walton, GATech, Hayes is Sr. Personnel)
- 10/14-9/17 **DOE National Energy Technology Lab, DE-FOA-0001010** "Impact of microstructure on the containment and migration of CO₂ in fractured basalts" (Lead-PI: Dan Giammar; Co-PI's: Sophia Hayes; Phil Skemer; and Brian Ellis, Univ MI)
- 9/11 - 8/17 **NSF Phase II Centers for Chemical Innovation (CCI) (CHE-1102637)**, "Center for Sustainable Materials Chemistry" (lead-PI, Doug Keszler, OSU; Sophia Hayes is a member of the Executive team)
- 9/14-8/17 **NSF MRI** "MRI: Acquisition of an EPR Spectrometer for Variable Temperature Measurements" (# 1429711) (Lead-PI: Liviu Mirica, Co-PI: Blankenship, Buhro, d'Avignon, Hayes)

- 2016-2017 **NSF Chemistry Div.** (CHE-1644338), "Workshop: Needs and Opportunities for Mid-Scale Instrumentation in Chemistry" (Hayes is a lead/co-PI)
- 6/14 - 5/17 **NSF CBET (1403239)**, "Collaborative Research: In-situ Molecular Spectroscopy of CO₂ Adsorption/Desorption Processes on Supported Amine Adsorbents" (Co-PIs Chris Jones, GATech; Sophia Hayes, WU)
- 8/15-7/16 **NSF Supplement** "Data-Enabled Science for Computational Treatment of Solid-state NMR Spectra" (Hayes and Mark Asta, co-PIs)
- 7/12 - 6/16 **NSF Condensed Matter Physics (DMR-1206447)**, "Exploiting enhanced polarization from Optically-pumped NMR" (Hayes is sole PI)
- 2012-2014 **CCCU (WU)**, "Coupled geochemical and transport processes in geologic carbon sequestration: evolution of chemical gradients and flow properties in diffusion-limited zones" (co-PIs, Dan Giammar; Hayes; Catherine Peters, Princeton)
- 2011-2014 **DOE-BES #DE-FOA-0000412**, "In Situ NMR to Understand Hydrogen Storage Chemistry" (lead-PI Mark Conradi; co-PI Eric Majzoub; Sr. Personnel Hayes)
- 2012-2014 **Nat'l High Magnetic Field Lab, UCGP** "Optical NMR probes of high field optically-pumped NMR spectroscopy in semiconductor quantum structures" (lead-PI Russ Bowers; co-PI's: Hayes, Stephen McGill, Arneil Reyes, Chris Stanton)
- 2010-2013 **CCCU (WU)**, "Development of State-of-the-Art NMR Spectroscopy and Imaging for Utilization and Sequestration of CO₂" (co-PI's: Mark Conradi, Sophia Hayes; Sr. Personnel, Phil Skemer)
- 2009-2013 **NSF Major Research Instrumentation (0923413)**, "MRI: Development of Combined Optically-pumped and Optically-detected NMR of Bulk and Nanostructured Semiconductors (0923413)"
- 2010-2011 **ICARES (WU)**, "Optimization of Semiconductor Materials for Solar Energy through Characterization of Nanoscopic Defects and Dopant Sites" (co-PI's: Viktor Gruev, Sophia Hayes)
- 2007-2009 **Alfred P. Sloan Foundation Research Fellow.**
- 2007-2009 **National High Field Magnetic Laboratory, Los Alamos**, "Magneto-Absorption Studies of Semiconductors with Circularly Polarized Light" (time on special apparatus to measure optical properties at high static, variable, magnetic fields).
- 2008-2009 **ICARES (WU)**, "Understanding the role of defects in reducing photovoltaic efficiency of silicon solar cells—probed by optically pumped NMR"
- 2007-2009 **Center for Materials Innovation (WU)**, "Low Bandgap Semiconductor Materials for Multiple Exciton Generation" with Profs. Bill Buhro, Rich Loomis (Chemistry). Collaborative research to investigate surface chemistry of II-VI nanowires and study these by both NMR and optical spectroscopy for MEG applications.
- 2006-2007 **Army Research Office**, "Laser-Enhanced NMR of Semiconductor Nanostructures. (W911NF0610309)" Study initiated to study InP nanowires by OPNMR.
- 2003-2006 **Army Research Office**, Defense University Research Instrumentation Program (DURIP) "Design and construction of an apparatus for combined optically-polarized and optically-detected NMR to study semiconductor heterostructures. (DAAD19-03-1-0366)" Equipment funding to build an apparatus for combined OPNMR and ODNMR, for the study of semiconductor materials.
- 2004-2006 **Petroleum Research Fund**, Type G, "Study of topotactic photoconversion of cinnamic acid to truxillic acid via solid-state NMR with *in situ* optical irradiation." Research into topochemical solid-state photoreactions in organic molecular crystals and powders by ¹³C NMR.

- 2004-2007 **Center for Materials Innovation**, "Single-Nanostructure Spectroscopy and Transport," with Profs. Bill Buhro, Rich Loomis (Chemistry) and Stuart Solin (Physics). Collaborative research to synthesize III-V nanowires and characterize these by a combination of solid-state NMR and optical spectroscopy.
- 2004-2006 **Center for Materials Innovation**, "Environmental Impact of Nanoparticles," with Profs. Pratim Biswas and Dan Giammar, (Environmental Engineering). Collaborative research to study heavy metal sorption (Pb, U) by nanoparticles, especially TiO₂, for environmental remediation purposes.
- 2003-2008 **NSF/CAREER**, "Spectroscopic studies of interface structure and strain in low-dimensional semiconductor heterostructures by laser-enhanced nuclear magnetic resonance. (0239560)" Research to develop optically-polarized (-pumped) and optically-detected techniques to probe semiconductors, especially multilayered heterostructures.
- 2000-2001 (postdoc) **Lawrence Livermore National Laboratory Lab**-Directed Research Dollar Renewal, "Optically-polarized NMR of bulk and quantum-confined GaAs," (P.I.: Hayes).
- 1999-2000 (postdoc) **Lawrence Livermore National Laboratory Lab**-Directed Research Dollars Grant, "Optically-polarized NMR of semiconductor nanoclusters," (P.I.: Hayes).
- 1994-1998 (grad school) **Sandia National Laboratories** grant, "NMR studies of lithium intercalation of microporous carbons," (grant awarded to Hayes to fund 4 years of graduate study).

In the Media (selected)

Interviews and Podcasts:

BBC 5 Live on "Helium Shortages" Oct. 2021:

<https://www.thenakedscientists.com/articles/interviews/rising-worries-helium-shortages>

House Committee on Space, Science & Technology "Research and Innovation to Address the

Critical Materials Challenge" Dec. 2019: <https://youtu.be/26uD9LGt7oM>

NPR "Shortwave" Geoff Brumfiel podcast Oct. 2019:

<https://www.npr.org/2019/11/01/775554343/the-world-is-constantly-running-out-of-helium-heres-why-it-matters>

"Helium Hunters" Podcast, September 2019: <https://krlr.radio.com/media/podcast/helium-hunters>

(<https://omny.fm/shows/helium-hunters/show-1#description>)

BBC Newsday, May 2019: (recording link not available; mp3 file available upon request)

Knowledge @ Wharton, May 2019: (recording link not available; mp3 file available upon request)

NBC News, May 2019: <https://www.nbcnews.com/news/us-news/not-just-party-city-why-helium-shortages-worry-scientists-researchers-n1007151>

NBC News, Bay Area interview, May 2019: <https://www.facebook.com/NBCBayArea/posts/the-helium-shortage-has-hit-us-really-hard-sophia-hayes-a-professor-of-chemistry/10156088117146990/>

China News Daily, May 2019:

<http://www.chinadaily.com.cn/a/201905/21/WS5ce41450a3104842260bcf0c.html>

ACS Webinar, April 2019: <https://www.acs.org/content/acs/en/acs-webinars/popular-chemistry/helium.html>

Science Policy News, American Inst. of Physics, April 2019: <https://www.aip.org/fyi/2019/helium-users-grapple-supply-crunch>

Reactions – PBS and ACS's YouTube Channel, March 2019 (scientific consultant on content):

https://www.youtube.com/watch?v=h0Vz_AmKCPw

The Pulse, WHYY, Sept. 2017: <https://whyy.org/segments/recovering-and-recycling-a-critical-chemical-in-research/>

Quoted in the media:

WashU Ampersand: March 2020 "Communicating science with empathy and intention"

<https://artsci.wustl.edu/ampersand/communicating-science-empathy-and-intention>

Chemical & Engineering News, 2020: "How ACS local sections are supporting their communities during COVID-19" https://cen.acs.org/acs-news/programs/ACS-local-sections-supporting-communities/98/i16?utm_source=Twitter&utm_medium=Social&utm_campaign=CEN

Stereo Chemistry Podcast (Craig Bettenhausen, ACS) 2020: "Podcast: How helium shortages have changed science" https://cen.acs.org/business/specialty-chemicals/Podcast-helium-shortages-changed-science/98/web/2020/10?ref=search_results

Bloomberg, May 2019: <https://www.bloomberg.com/news/articles/2019-05-11/helium-shortage-is-hurting-parties-and-the-pharma-industry>

Time Magazine, May 2019: <https://time.com/5587690/helium-shortage-pharma/>

Radiology Business, May 2019: <https://www.radiologybusiness.com/topics/quality/helium-shortage-imaging-radiology-healthcare>

C&E News 2019: "Help for Helium Users is on the Way"

https://cen.acs.org/business/instrumentation/Help-helium-users-way/97/i46?ref=search_results

WashU Source, April 2019: "WashU Expert: The global helium shortage hits home"

<https://source.wustl.edu/2019/04/washu-expert-the-global-helium-shortage-hits-home/>

Physics Today, March 2019: "Helium users are at the mercy of suppliers"

<https://physicstoday.scitation.org/doi/full/10.1063/PT.3.4181>

Nature, July 2017: "https://www.nature.com/news/qatar-blockade-hits-helium-supply-1.22247"

<https://www.nature.com/news/qatar-blockade-hits-helium-supply-1.22247>

C&E News, 2017: "What could chemistry do with more expensive instruments?"

https://cen.acs.org/articles/95/i13/chemistry-expensive-instruments.html?ref=search_results

WashU Source, Nov. 2016: <https://source.wustl.edu/2016/11/hayes-helps-shape-national-helium-policy/>

C&E News, 2016: "Securing The Future Of NMR" https://cen.acs.org/articles/94/i7/Securing-Future-NMR.html?ref=search_results

C&E News, 2015: "As Helium Prices Rise, Universities Consider Recycling The Element"

https://cen.acs.org/articles/93/i30/Helium-Prices-Rise-Universities-Consider.html?ref=search_results

Invited Presentations (since 2001)

(Invited presentations "on hold" due to travel bans: Smarter7 Crystallography conference, Leuven Belgium; International Symposium on Non-Oxide and New Optical Glasses, China.)

103. Euromar July 2022. "Optically-pumped NMR as a quantum simulator" (invited plenary speaker)

102. Brazilian NMR Group (online) Nov. 2021. "The Materials Project: Creating a Database of NMR Tensors for Machine Learning" (invited plenary speaker).
101. M.I.T. NMR "Zoominar" (online) Aug. 2021 "Lessons Learned from Computed NMR Tensors of Crystalline Solids—Looking beyond 'Just' Isotropic Shift" (invited speaker).
100. ACS National Meeting, (online) April 2021 "²⁹Si chemical shift tensors: From NMR experiments to computational prediction" (invited speaker).
99. Alpine NMR Meeting, Chamonix, France September 2019 "Worldwide helium supply: price and supply issues" (special session, technical talk and discussion lead)
98. Practical Applications of NMR in Industry Conference, SC, February 2019. "Practical Applications of NMR Tensors – a Tale of Two Chemical Systems and NMR Crystallography" (invited talk)
97. Eastern Analytical Symposium, Princeton, NJ, Nov. 2018. "Structural details from quadrupolar solid-state NMR of solution-processed thin films from group 13 oxide molecular precursors" (invited talk, and separate Awards Session Chair).
96. Southeastern Magnetic Resonance Conference (SEMRC) Clemson, SC, October 2018. "Optically-Pumped NMR of Semiconductors and the Importance of NMR Tensors" (invited talk).
95. ACS Midwest Regional Meeting, Ames, IA October 2018. "NMR Spectroscopy and Computation of NMR Tensors and The Materials Project LSDI 'Library' " (invited talk)
94. National High Magnetic Field Lab, Tallahassee, FL, September 2018. (invited talk)
93. Clay Mineral Society Annual Meeting, Urbana, IL, June 2018. "Surprising Findings from Solid-state NMR of ¹³C in Carbonates: on the Pathway to 'NMR Crystallography' " (invited talk).
92. TSRC Town Talk (www.telluridescience.org/for-the-public/telluride-town-talks), Telluride, CO July 2017 "Fingerprinting CO₂ for Better, Safer Carbon Capture and Storage" (nominated informal science education lecture to the community, from the Telluride Science Research Conference workshops.)
91. Telluride Science Research Center workshop – Emerging Methodologies for Paramagnetic NMR and DNP, Telluride, CO July 2017. "Polarization via OPNMR reveals interface structure in semiconductor heterostructures and computing tensors for quadrupolar nuclei." (Invitation-only workshop, invited talk)
90. Duquesne University, Chemistry Department, Pittsburgh, PA April 2017 "NMR of Quadrupolar Nuclei: Opportunities for Materials Science" (student-nominated, invited seminar)
89. American Chemical Society National Meeting, San Francisco, CA April 2017 "Solid-state NMR of thin metal oxide films from prompt inorganic condensation" (invited talk and session chair: ACS Award in the Chemistry of Materials: Symposium in honor of Douglas A. Keszler)
88. Alexander von Humboldt Colloquium: *Global Research in the 21st Century: Perspectives of the U.S. Humboldt Network*, Washington D.C., March 2017, "Solid-state NMR for Materials Chemistry-- Cooperative Research Pushes the Cutting Edge in Metal Oxide Thin Films" (invited talk)
87. Sackler Award Symposium, Tel Aviv Univ., Tel Aviv, Israel Feb. 2017 "Interface Structure of Al₂O₃/GaAs by OPNMR" (invited talk)
86. Weizmann Institute of Science, Department of Chemical Physics Rehovot, Israel Feb. 2017 "NMR of Thin Films, OPNMR of Semiconductors – Methods" (NMR seminar)

85. Bruker Users' Meeting, Rocky Mountain Conference on Solid-state NMR, Breckenridge, CO July 2016 "Optical-pumping for signal enhancements in semiconductors" (invited talk).
84. Rutgers Univ., Dept. of Chemistry & Chemical Biology, New Brunswick, NJ, May 2016 "NMR of Quadrupolar Nuclei: Opportunities for Materials Science" (departmental seminar).
83. DOE EFRC Midterm Review, Gaithersburg, MD, Feb. 2016 "NMR Study of CO₂ Gas Dynamics and Structure of Metal Carbide-Derived Materials" (invited talk).
82. Physical Phenomena in High Magnetic Fields (PPHMF-8), Tallahassee, FL, Jan. 2016. "Group 13 (²⁷Al, ⁷¹Ga) Studies of Metal-oxide Clusters and Thin Films" (invited talk).
81. Ultra-high Magnetic Field workshop, NIH, Bethesda, MD, November 2015 "NMR of Half-Integer Quadrupolar Nuclei in Materials: Opportunities at Ultrahigh Fields" (invited talk)
80. NMR² meeting, Albuquerque, NM. Oct. 2015 "NMR and Other Misadventures in the Compton Basement—a Presentation in Honor of Prof. Mark S. Conradi" (invited talk).
79. Lausanne, Laboratory of NMR, Ecole Polytechnique Fédérale de Lausanne, September 2015. "Quadrupolar NMR of Group 13 Metals in Clusters and Thin Films"
78. Alpine Conference on Solid-state NMR, Chamonix, France Sept. 2015. "New Developments in Optically-pumped ¹¹³Cd NMR of CdTe and ⁷¹Ga NMR of AlGaAs/GaAs Quantum Wells" (invited talk).
77. Center for Understanding & Control of Acid Gas-Induced Evolution of Materials for Energy annual meeting, Atlanta, GA Sept. 2015 "Short course tutorial: Solid-state NMR for materials characterization and studies of gas sorption" (invited talk).
76. ACS National Meeting, Boston, August 2015. "*In situ* NMR reveals conversion of ¹³CO₂ to metal carbonates and pH monitoring for geosequestration studies", Presidential Session: "New Frontiers in Synthesis and Solid-state NMR Spectroscopy of Group 13 Clusters and Complexes" (invited talk, poster, respectively).
75. Euromar, Prague, Czechoslovakia, July 2015 "Group 13 (Al, Ga) Studies of Metal-oxide Clusters and Thin Films" (invited talk). "Materials for CO₂ Capture and Sequestration Studied by ¹³C NMR" (invited talk and contributed poster)
74. North American Solid State Chemistry Conference, Tallahassee, FL May 2015 "Solid-state NMR studies of Group 13 Oxides". "Materials for CO₂ Capture and Sequestration Studied by ¹³C NMR" (invited talk and contributed poster).
73. Keynote address to the 20th Annual Graduate Research Symposium, Washington Univ. Feb. 2015. "Collaborative Science: How Chemists, Engineers, and Physicists Come Together to Create the Next Generation of Electronic Materials"
72. Univ. of Oregon, Dept. of Chemistry, Eugene, OR October 2014 "Optically-pumped NMR as a Probe of Bandstructure and Defect Sites in GaAs/AlGaAs Quantum Wells and Direct-Gap Semiconductors" (departmental seminar).
71. McDonnell International Scholars Academy 5th Int'l Symposium, St. Louis, MO Oct. 2014 "*In Situ* ¹³C NMR to Develop Materials for the Capture and Sequestration of CO₂" (invited talk).
70. SACNAS Conference " 'It Takes a Village' How Chemists, Engineers, and Physicists Come Together to Create the Next Generation of Electronics", Los Angeles Oct. 2014 (invited talk).

69. DePauw Univ., Department of Chemistry, Indianapolis, October 2014 "Materials by Design: Solid-state NMR Investigations of Nanoscale Clusters, Metal Oxide Films and CO₂ Capture Materials" (invited talk).
68. Mathematics Dept., Washington University, St. Louis September 2014 "Chemistry Adventures in Group Theory" (departmental colloquium).
67. SPIE (Society of Photo-Optical Instrumentation Engineers), San Diego August 2014 "Experimental measurements of optically pumped NMR and spin polarization in bulk GaAs and AlGaAs/GaAs quantum wells" (invited talk).
66. UCSB, Santa Barbara, CA ITST colloquium June 2014 "OPNMR revealing Landau level in GaAs/AlGaAs quantum wells" (invited talk).
65. SACNAS (Society for Advancement of Hispanics/Chicanos and Native Americans in Science) Conference, San Antonio, TX, Oct 2013 "Living on the Edge—Chemistry at Interfaces" (invited talk).
64. CEA Saclay, France Oct. 2013 "NMR in materials science: optically-pumped NMR of semiconductors and CO₂ sequestration" (department seminar).
63. Int'l Society of Magnetic Resonance (ISMAR), Rio de Janeiro, Brazil, May 2013. "Unique Insights into Carbon Capture and Geosequestration of CO₂ from *In Situ* High-Pressure High-Temperature NMR" (invited talk). (Also: New Model of Electron Spin Polarization in GaAs and AlGaAs/GaAs Arising from Optical Pumping and Detection by OPNMR", invited poster).
62. Jost Chemical Company, May 2013 "High-Pressure High-Temperature NMR of CO₂ for Monitoring Geochemistry and Carbon Capture" (invited talk).
61. Center for Sustainable Materials Chemistry, Eugene, OR, April 2013 "Progress in ^{69/71}Ga and ²⁷Al NMR of Hydroxy- Hydrated 'M₁₃' Clusters" (progress-report talk).
60. First Solar, Sunnyvale, CA, April 2013 "Prospects of OPNMR for Solar Energy Materials" (invited talk).
59. Calera Corporation, Los Gatos, CA April 2013 "Characterization of Carbonates via High-Pressure High Temperature NMR" (invited talk).
58. Drexel University Dept of Materials Engineering, March 2013. "Optically-pumped NMR of GaAs: Examining Spin-Dependent Phenomena via the 69Ga and 71Ga Nuclear Spins" (invited talk).
57. NMRS (Nat'l NMR Society of India) Mumbai, India, Feb 2013. "Development of OPNMR for Studies of Semiconductor Bandstructure and Defects" (invited talk).
56. Texas A&M, Oct 2012. "Solid-state NMR at the Frontiers of Materials Science: CO₂ Sequestration and Spin-Dependent Splitting in Semiconductor Bandstructures" (departmental seminar).
55. Kopin Corporation, Aug 2012. "Development of OPNMR for Semiconductor Heterostructures" (invited seminar).
54. RMC (Rocky Mountain Conference on Analytical Chemistry), July 2012. "*In Situ* High-pressure Variable-temperature NMR for Studies of CO₂ Capture and Sequestration" (invited talk).
53. Samuel Weissman Memorial Symposium, St. Louis, May 2012. "Electron-nuclear Interactions--Still Fascinating Us ~60 Years (!) after Slichter's and Carver's Discoveries"
52. Ohio State Univ., May 2012. "Solid-state NMR at the Frontiers of Materials Science: CO₂ Sequestration and Spin-Dependent Splitting in Semiconductor Bandstructures" (departmental

seminar).

51. ENC (Experimental NMR Conference), April 2012, Miami, FL "Detection of Spin Polarization in Semiconductors with Optical Pumping" (invited talk). Poster: "In Situ High Pressure and Temperature
50. Michigan State Univ., April 2012. "Solid-state NMR at the Frontiers of Materials Science: CO₂ Capture and Semiconductor Bandstructures" (departmental seminar).
49. Pacifichem, Honolulu, HI, December 2010. "Optically-pumped NMR (OPNMR) as a monitor of the electronic structure of GaAs" (invited talk).
48. Univ. of Leipzig, Dept. of Experimental Physics, Germany, July 2010. "Optically-pumped NMR (OPNMR) as a New Tool for Spectroscopic Characterization of Semiconductor Structure and Bandstructure" (departmental seminar).
47. Univ. of MO St. Louis, Center for Nanoscience, St. Louis, MO, Nov. 2009. "Optically-pumped NMR: An Emerging Tool for the Study of Structure at the Nanoscale in Semiconductors" (departmental seminar).
46. NSF Workshop on Green Chemistry, Eugene, OR, Oct. 2009. "Applications of light+NMR to problems in the materials science of solids" (conference presentation).
45. Illinois State Univ., Dept. of Chemistry, Normal, IL, Oct. 2009. "Applications of light+NMR to problems in the materials science of solids" (departmental seminar).
44. Butler University, Dept. of Chemistry, Indianapolis, IN, Oct. 2009. "Applications of light+NMR to problems in the materials science of solids" (departmental seminar).
43. NNIN Inaugural Symposium on Nanotechnology for Public Health, Environment and Energy, St. Louis, MO Sept. 2009. "Optically-pumped NMR: An Emerging Tool for the Study of Structure at the Nanoscale in Semiconductors" (conference presentation).
42. Regitze R. Vold Memorial Lecture, Alpine Conference on Solid-state NMR, Chamonix, France, Sept. 2009. "A New Model of Optically-pumped NMR in Direct-Gap Semiconductors" (conference presentation)
41. Institute of Physical Chemistry, WWU Muenster, Germany, Sept. 2009 "OPNMR of GaAs: Roadmaps for New Routes through the Opto-Electronic 'Landscape'." (departmental seminar)
40. Gordon Research Conference, Magnetic Resonance, Biddeford, ME, June 2009. "OPNMR of GaAs: Roadmaps for New Routes through the Opto-Electronic 'Landscape'." (conference presentation)
39. Univ. of California, Santa Cruz, March 2009. "Studying defects and photogenerated carriers in semiconductors with light + NMR -- prospects for solar energy applications." (departmental seminar)
38. St. Olaf College, Dept. of Chemistry, MN, Feb. 2009. "Studying defects and photogenerated carriers in semiconductors with light + NMR -- prospects for solar energy applications." (departmental seminar, Pew Midstates Consortium-funded)
37. Kavli Foundation and Nat'l Academy of Sciences "Frontiers of Science" conference, Roscoff, France, Nov. 2008. "Electron-Nuclear Interactions in Semiconductors: Probed via Optically-Pumped NMR" (conference poster presentation)
36. MEMC, St. Peters, MO, Nov. 2008. "Optically-pumped NMR of semiconductors: a new analysis tool

for semiconductors.”

35. Northwestern Univ., Dept. of Chemistry, Evanston, IL, Oct. 2008. “Optically-Pumped NMR of Semiconductors: Probing Defect Sites and the Band Structure of GaAs” (departmental seminar).
34. Univ. of IL Chicago, Dept. of Chemistry, Chicago, IL, Oct. 2008. “Optically-Pumped NMR of Semiconductors: Probing Defect Sites and the Band Structure of GaAs” (departmental seminar).
33. Mt. Holyoke, Dept. of Chemistry, South Hadley, MA, Sept. 2008. “Solid-State NMR with Light Added -- Possibilities for Materials Science” (departmental seminar).
32. Dortmund University, Dept. of Physics, Ellha, Germany, May 2008. “Optically-pumped NMR of semiconductors: probing the bandstructure and defect sites in GaAs” (departmental seminar).
31. Univ. of Florida, Dept. of Chemistry, Gainesville, FL, Nov. 2007. “Laser-enhanced NMR of semiconductors” (departmental seminar).
30. M.I.T., Dept. of Chemistry, Cambridge, MA, Oct. 2007. “Optically-pumped NMR of semiconductors: probing the bandstructure and defect sites in GaAs” (departmental seminar).
29. Southern Illinois Univ. Carbondale, Dept. of Chemistry, Carbondale, IL, Sept. 2007. “Optically-pumped NMR of semiconductors” (departmental seminar).
28. Cornell University, Dept. of Chemistry, Ithaca, NY, Feb. 2007. “Electron-Nuclear Interactions Probed by ^{69}Ga and ^{71}Ga OPNMR of Semi-Insulating GaAs” (departmental seminar).
27. Ithaca College, Dept. of Chemistry, Ithaca, NY, Feb. 2007. “Solid-state Photodimerization of Cinnamic Acid--a Study of Topochemistry by ^{13}C NMR” (departmental seminar).
26. ACS Midwestern Regional Meeting, Quincy, IL, Oct. 2006. “Probing the Electronic Band Structure of GaAs with NMR” (invited talk).
25. Gordon Research Conference, Inorganic Chemistry, Newport, RI, June 2006. “OPNMR of ^{69}Ga in Bulk GaAs” (invited talk).
24. Univ. of Washington, Dept. of Chemistry, Seattle, WA, May 2006. “Optically-Induced Hyperfine Shifts in OPNMR of ^{69}Ga in Bulk Semi-insulating GaAs” (departmental seminar).
23. Hope College, Dept. of Chemistry, Holland, MI, March 2006. “Topochemical Reactions Monitored by Solid-State NMR” (departmental seminar).
22. Calvin College, Dept. of Chemistry, Grand Rapids, MI, March 2006. “Topochemical Reactions Monitored by Solid-State NMR” (departmental seminar).
21. Univ. of Calif. Santa Barbara, Materials Department & MRL, CA, March 2006. “OPNMR of ^{69}Ga in Bulk Semi-insulating GaAs” (interdepartmental IGERT seminar).
20. Univ. of Calif. Santa Barbara, Univ. of Calif. Santa Barbara, CA, March 2006. “Topochemical Reactions Monitored by Solid-State NMR” (departmental seminar).
19. High Field Solid State NMR Workshop, College of William & Mary, Williamsburg, VA, March 2006. “OPNMR of ^{69}Ga in Bulk Semi-insulating GaAs” (invited talk).
18. Alpine Conference on Solid-State NMR, Chamonix, France, Sept. 2005. “OPNMR of Ga-69 in GaAs in Bulk Single Crystals and in Heterostructured Devices” (invited talk).
17. Experimental NMR Conference (ENC), Providence, RI, April 2005. “OPNMR of Ga-69 in n-, p-, and Semi-Insulating-GaAs and Heterostructured InGaP/GaAs” (invited talk).

16. Univ. of Arkansas, Dept. of Physics, Fayetteville, AR, April 2005. "OPNMR of Ga-69 in n-, p-, and Semi-Insulating-GaAs and Heterostructured InGaP/GaAs" (departmental seminar).
15. St. Louis NMR Discussion Group, March, 2005. "OPNMR of ⁶⁹Ga spins in GaAs in Semi-insulating GaAs and In GaP/GaAs Heterostructures" (invited talk).
14. Univ. of Missouri St. Louis, Dept. of Chemistry, MO, Jan. 2005. "Solid Solid-state NMR of Crystalline Optical Memory/Optical Switch Materials" (departmental seminar).
13. Univ. of Missouri, Rolla, Dept. of Chemistry, MO, Nov. 2004. "Solid-state photochemistry combined with NMR--towards optical memory materials" (departmental seminar).
12. NSF Workshop on Materials Chemistry and Nanoscience, Broomfield, CO, Oct. 2004. "Laser Enhanced NMR of Semiconductor Nanostructures" (invited talk).
11. ISMAR, Triennial Conference for the Intl Society of Magnetic Resonance, Jacksonville, FL, Oct. 2004. "NMR with Optical Pumping of III-V Semiconductor Heterostructures" (invited talk).
10. Southern Illinois University Edwardsville, Dept. of Chemistry, IL, Sept. 2004. "Towards Materials for Optical Memory and Optical Switches: Nucleation and Growth Kinetics of [2+2] Cycloadditions Studied by Solid-state NMR" (departmental seminar).
9. Florida State University, Dept. of Chemistry, and Nat'l High Magnetic Field Lab (NHMFL), Tallahassee, FL, Sept. 2004. "Laser-enhanced NMR for the Study of Semiconductors" and "Optical Solid-state Nucleation and Growth Kinetics in a Model 'Optical Switch' Studied by Solid-state NMR" (departmental seminar).
8. Rocky Mountain NMR Conference, Denver, CO, July 2004. "Photo-induced nucleation and growth processes in crystalline [2+2] cycloadditions reactions—a model 'optical switch' compound" (invited talk).
7. RWTH Aachen University, Macromolecular Chemistry Dept., Aachen, Germany, May 2004. "Optical Pumping of GaAs—Some New Insights into Polarization" (departmental seminar).
6. Dortmund University, Dept. of Physics, Dortmund, Germany, May 2004. "Solid-state Nucleation and Growth Kinetics in a Model 'Optical Switch' Studied by Solid-state NMR" (Graduate College seminar).
5. Inst. of Physical Chemistry, University of Münster, Germany, May 2004. "Solid-state Nucleation and Growth Kinetics in a Model 'Optical Switch' Studied by Solid-state NMR" (departmental seminar).
4. Washington Univ., Dept. of Physics, St. Louis, MO, Dec. 2002. "Laser-enhanced NMR: New Tools for the Study of Semiconductors" (departmental seminar).
3. St. Louis University, Dept. of Chemistry, St. Louis, MO, Oct. 2002. "Laser-enhanced NMR of semiconductors" (departmental seminar).
2. Southwest Missouri State University, Dept. of Chemistry, Branson, MO, Oct. 2002. "Laser-enhanced NMR of semiconductors." (departmental seminar)
1. University of Missouri Columbia, Dept. of Chemistry, MO, Nov. 2001. "Laser-enhanced NMR of semiconductors" (departmental seminar).

Contributed Presentations (since 2001)

44. Chicago Area NMR Discussion Group, UWI Madison, November 2019. "Cataloguing ²⁹Si NMR

- Tensors, via DFT – for The Materials Project” (contributed talk).
43. Alpine NMR Meeting on Magnetic Resonance, Chamonix, France September 2019. “Measuring and Modeling Nuclear Spin Temperature Using ^{75}As OPNMR” (roundtable discussion)
 42. Missouri Inorganic Day, St. Louis, April 2019. “Use of NMR Tensors for Inorganic Structure Analysis.” (promoted talk)
 41. American Chemical Society, Orlando, FL, March 2019. “Hydromagnesite: Case study of solid-state NMR tensors and the development of the Local Spectroscopy Data Infrastructure (LSDI) NMR database” (promoted talk).
 40. American Physical Society (APS), Los Angeles, CA March 2018. “Optically-pumped ^{75}As NMR Reveals an Electric Field Gradient at an Al_2O_3 -GaAs Interface and Very Low Nuclear Spin Temperatures” (promoted talk).
 39. Experimental NMR Conference (ENC), Asilomar, CA March 2017 “ ^{75}As OPNMR Reveals Interface Structure in GaAs” (promoted talk)
 38. American Chemical Society, Boston, MA August 2015 “Materials for capture of CO_2 and acid gases studied via *in situ* and *ex situ* solid-state NMR”(contributed talk).
 37. Experimental NMR Conference, Asilomar, CA April 2015 {posters on CO_2 projects, OPNMR, quadrupolar NMR of M_{13} clusters, and calculations using CASTEP and Quantum Espresso} (contributed posters)
 36. Rocky Mountain NMR Conference, Copper Mtn, CO, July 2014 “Optically-pumped NMR of Multiple Quantum Wells of GaAs/AlGaAs and Hanle Curve Measurements” (contributed poster)
 35. Experimental NMR Conference, Boston, MA April 2014 “Assignment of Quantum Well Electronic States of ^{69}Ga OPNMR of AlGaAs/GaAs and New Observations in ^{113}Cd OPNMR of CdTe” (contributed poster)
 34. American Physical Society, Denver, CO March 2014 “Experimental Measurements of $^{69/71}\text{Ga}$ NMR in Optically-pumped NMR (OPNMR) of AlGaAs/GaAs Quantum Wells” (contributed talk)
 33. American Geophysical Union conference, San Francisco, CA, Dec 2013 “In Situ ^{13}C NMR at Elevated-Pressures and Temperatures Investigating the Conversion of CO_2 to Magnesium and Calcium Carbonate Minerals” (contributed poster)
 31. CCUS Meeting, Pittsburgh, PA, May, 2013 “Studies of CO_2 sequestration by *in situ* high-pressure high-temperature NMR.” (contributed poster).
 30. ACS National Meeting, San Diego, March 2012 “*In situ* variable pressure and variable temperature NMR of CO_2 and its reaction products in carbon capture applications.” (contributed talk).
 29. Alpine Conference on Solid-state NMR, Chamonix, France, Sept. 2011 (contributed poster).
 28. GRC, Magnetic Resonance, Biddeford, ME, June 2011, “Measurements and Simulations of the Photon Energy Dependence of OPNMR in Semi-insulating GaAs” (poster).
 27. ENC (Experimental NMR Conference), Asilomar, CA, April, 2011. (contributed posters).
 26. RMC (Rocky Mountain Conference on Analytical Chemistry), Snowmass, CO, July 2010. (contributed posters).

25. SPSSM, International Symposium on Structure-Property Relationships in Solid State Materials, Stuttgart, Germany, June 2010. "Optically-pumped NMR (OPNMR) as a New Tool for Spectroscopic Characterization of Semiconductor Structure and Bandstructure" (contributed talk).
24. APS (American Physical Society) March Meeting, Portland, OR, March 2010. " 'Optically Relevant Defects' in the Optically-pumped NMR of Semi-insulating GaAs" (contributed talk).
23. RMC, Snowmass, CO, Aug. 2009. "Spin-dependent Splitting of the GaAs Bandstructure: Fine Structure from a Combination of OPNMR, Magnetoabsorption, and Theoretical Calculations" (contributed talk).
22. ENC, Asilomar, CA, March 2009 "A New Model of Optical-Pumping Phenomena in Semiconductors" (contributed poster).
21. APS March Meeting, Pittsburgh, PA, March 2009 "A New Model of Optical-Pumping Phenomena in Semiconductors" (contributed talk)
20. ACS Nat'l Meeting, Philadelphia, PA, Aug. 2008 "Interrogation of the GaAs Electronic Bandstructure: Building on the 'Penetration Depth Model' of Optically-pumped $^{69/71}\text{Ga}$ NMR of GaAs" (promoted talk)
19. RMC, Breckenridge, CO, July 2008 "Probing the Band Structure and Landau Levels in GaAs via Optically-Pumped $^{69/71}\text{Ga}$ NMR" (promoted talk)
18. ENC, Asilomar, CA, March 2008 "Probing the Band Structure and Landau Levels in GaAs via Optically-Pumped $^{69/71}\text{Ga}$ NMR" (promoted talk) "Interrogation of the GaAs Electronic Bandstructure: Building on the "Penetration Depth Model" of Optically-pumped $^{69/71}\text{Ga}$ NMR of GaAs" (contributed poster), and "The [2+2] Photodimerization of α -trans-Cinnamic Acid to α -Truxillic Acid: 'Tail' irradiations and Polymorphism" (contributed poster).
17. Chicago Area NMR Meeting, Nov. 2007, "Laser-enhanced NMR of semiconductors: probing the bandstructure and defect sites in GaAs" (contributed talk).
16. GRC, Inorganic Chemistry, Newport, RI, July 2007, "Se-Se J -couplings in Hexarhenium Analogues" and "Surface- and Defect-Sensitive NMR of Semiconductors" (posters).
15. GRC, Magnetic Resonance, Biddeford, ME, June 2007, "Measurements and Simulations of the Photon Energy Dependence of OPNMR in Semi-insulating GaAs" (poster).
14. Canadian Society of Chemistry conference, Winnipeg, Canada, May 2007, "Measurements and Simulations of the Photon Energy Dependence of OPNMR in Semi-insulating GaAs" (contributed talk).
13. ENC, Daytona Beach, FL, April 2007 "Measurements and Simulations of the Photon Energy Dependence of OPNMR in Semi-insulating GaAs" (poster).
12. PCSI (Physics & Chemistry of Semiconductor Interfaces) Conference, Salt Lake City, UT, January 2007, "Measurements and Simulations of the Photon Energy Dependence of OPNMR in Semi-insulating GaAs" (poster).
11. RMC, Breckenridge, CO, July 2006, "Light Induced Hyperfine Shifts in OPNMR of ^{69}Ga in Semi-Insulating GaAs" (poster).

10. ENC Conference, Asilomar, CA, April 2006, "Knight Shifts in OPNMR of ^{69}Ga in Semi-Insulating GaAs" and "Solid-state Photochemistry: Topochemical (Stereochemical) Control of Products in Cycloaddition Reactions" (posters).
9. Missouri Inorganic Day, St. Louis, MO, May 2005, "Laser-Enhanced NMR of GaAs and Its Heterostructures" (contributed talk).
8. PCSI Conference, Bozeman, MT, January 2005, "Laser-enhanced NMR: Spectroscopy of Ga-69 Nuclear Spins in GaAs Semiconductor Heterostructures" (oral and poster).
7. GRC, Solid-State Chemistry, New London, NH, July 2004, "Monitoring topochemical solid-state photodimerizations via solid-state NMR" and "Determination of ^{77}Se - ^{77}Se and ^{77}Se - ^{13}C J -coupling parameters for the C_{4v} -symmetry selenocyanide cluster $[\text{Re}_5\text{OsSe}_8(\text{CN})_6]^{3-}$ " (posters).
6. PCSI Conference, Kona, HI, January 2004, "Nuclear Magnetic Resonance with Optical Pumping of III-V and II-VI Semiconductors" (oral and poster).
5. Chicago Area NMR Meeting, Chicago, IL, November 2003, "Solid-state NMR of photodimerizations in organic crystals" (contributed talk).
4. RMC Conference, Denver, CO, August 2003, "Investigation of Cinnamic Acid as a Powder and Single Crystal: H-1 and C-13 Spectra and Simulations" (poster).
3. PCSI Conference, Salt Lake City, UT, January 2003, "Laser-enhanced NMR: New Tools for the Study of Semiconductor Interfaces" (poster).
2. GRC, Solid-State Chemistry, New London, NH, July 2002, "Laser-enhanced NMR: New Tools for the Study of Semiconductors" (poster).
1. ENC Conference, Asilomar, CA, April 2002, "Advancements in optically detected NMR applied to nanoscopic heterostructures" and "Interaction between electric field gradients and the nuclear spin system observed by optically detected NMR in GaAs quantum wells" (posters).

Collaborators

- Prof. Chris Jones, Prof. Krista Walton, Prof. Carsten Sievers, Georgia Tech: studies of carbon capture polymers and solid supports, MOFs, other porous materials.
- Dr. Tina Nenoff, Sandia National Labs, studies of NOx binding and MOF structures
- Prof. Kristin Persson, Dr. Shyam Dwaraknath, Prof. Mark Asta for DFT computations of NMR spectra from crystalline inorganic structures
- Dr. Bill Brey, National High Magnetic Field Lab, Tallahassee, for new probe designs incorporating optical access and new detection schemes for NMR
- Prof. John Conley, Oregon State Univ. for semiconductor heterostructures.

Public Outreach

Science on Tap speaker (postponed) – on helium supply shortages

U.S. House of Representatives testimony, Committee on Science, Space & Technology (2019)

<https://science.house.gov/download/hayes-testimony>

Weidenbaum Center speaker (2020) – on CO₂ (carbon) capture and storage technologies

MLA Series speaker (University College, WU) (2020) – on "Hacking Climate Change"

Weidenbaum Center speaker (2020) – on helium supply issues

ACS Webinar: "Helium: An Irreplaceable Resource and Why We Must Conserve It"
<https://www.acs.org/content/acs/en/acs-webinars/popular-chemistry/helium/video.html>
 Reactions video (PBS & ACS): "Are We Running out of Helium?" (2019)
https://www.youtube.com/watch?v=h0Vz_AmKCPw
 Town Talk – Telluride Science Research Center (2017) – nominated lecture to general public in Colorado on CO₂ capture and sequestration
 Matter & Energy Transformations, Bio5925, 1-week outreach course (2015, 2017, 2019, 2021 postponed)
 Century Club Lecture (2010) – on CO₂ capture
 Celebrating Women Scholars in STEM, presentation and panel discussion (2010)
 Arts & Sciences National Council (2010) – on science communication
 Lab tours for Architecture 568B, "The Architecture of Medicine," Prof. Janet Baum (2009, 2010, 2011)
 "Alberti Scholars Program" outreach faculty speaker (2009)
 Outreach presentation at the St. Louis Science Center, on nanoscience (2006)
 Presentation "What's Next? Contemplating Life after College" Pew Midstates Science & Math Undergraduate Research Symposium (2004)
 WU Outreach "Materials Science Saturday" for grades 6-12 teachers (2004)

Chemistry Departmental Committees and Service

- Co-Chair, Chemistry Steering Committee (2021 – present)
- Chemistry Diversity, Equity, Inclusion committee member (2019 – present)
- Chemistry Website, Chair (2008-2021)
- Awards Committee (2004-present)
- NMR Committee (2001-present)
- Diversity & Inclusion Group, Lead (2015 – 2017): a reading/ discussion group of faculty and staff who meet periodically, to try to become more knowledgeable about issues related to underrepresented groups
- Search Committee, member (2021, 2019, 2017, 2007, 2004); Search Committee, Chair (2013-2014); Graduate Admissions and Recruiting (2002-2011); Chemistry External Chair Search Committee (2009); Graduate Work Committee (2003-2004, 2007-2009); Graduate Program – Minority Recruiting (2007-2008).
- Thesis Committees: Chemistry Department: 58 students
- Undergraduate Advising: 59 students,

University Service

- Arts & Sciences, WU Culture & Climate Working Group, 2021 -
- Arts & Sciences, WU Strategic Planning Group, 2021 -
- Arts & Sciences, WU Undergraduate Academic Affairs Committee, 2021 –
- Arts & Sciences, WU Envisioning Faculty Excellence Committee, 2021
- WU Faculty Committee for Tech Transfer, 2020 -
- WU Climate Change Program Steering Committee, 2020 -

- Arts & Sciences, Advisory Committee on Tenure, Promotion and Personnel (2018 – 2021)
- Washington University Diversity Programs Consortium (WUDPC)-STEM Focus (2012-2018): the focus of this group includes retention and recruitment of underrepresented minorities (URM) to professional (faculty) and students (graduate, undergraduate) at WashU. Some selected activities include mentoring faculty peers, and creating an environment welcoming to URM faculty, students, and staff.
- Washington University New Investigator Awards Committee (2015 – 2019)
- Physics department (astrophysics) search committee (2018-2019)
- Arts & Sciences, Academic Planning Committee (2010-2016): this committee is a group of faculty Arts & Sciences that act in an advisory role for the dean of A&S.
- Co-chair and creator of the “Washington U. Frontiers in Technology & Science” conference (2009, 2010): this is a grass-roots faculty-driven conference highlighting emerging research projects from young faculty, facilitating connections between departments and schools in STEM fields.
- Founder and Executive Board member of the Washington U. Family Network social network and on-line resource (2005 – 2009): this group established a website of St. Louis-based resources for families and those newly-locating to WashU. The purpose was to share information and advice such as schools, local doctors, etc.
- Graduate Fellowship Writing Workshop, Chemistry/STEM leader (2014)
- Olin Women’s Leadership Forum Program Scholarship Advisory committee (2013)
- Grant/Fellowship Writing Workshop leader (for grad students), College of Arts & Science (2013)
- Women in Innovation and Entrepreneurship (WIE) focus group (2013)
- WU Inst. of Materials Science & Engineering, Admissions Committee (2012)
- KIPP School Science Olympiad coach (2012-2013) (a charter school in St. Louis, grades 5-8)
- Office of the Provost, WU Postdoctoral Fellowship Program committee (2012-13)
- Mathematics Search Committee (2011-12)
- “Junior Jumpstart” faculty speaker (2009, 2010)
- Olin Fellows Selection Committee (2009, 2010, 2012)
- Physical Sciences Pre-Orientation (2007, 2008, 2009, 2010, 2011)
- Mechanical and Aerospace Engineering Search Committee (2008-09, 2009-10, 2010-11)
- Freshman Reading Program, Faculty Discussion Leader (2009)
- Israelow Selection Committee (2007)
- Panelist, Alumni Parents & Admission Program (APAP), (2004, 2005)
- WU Ph.D. Thesis Committees (Physics Department, IMSE, Engineering departments)--39 students
- External thesis committee member: University Dortmund, Dept. of Physics, Germany--2 students
Chemical Engineering, GA Tech—1 student

Professional Activities and Service

- Co-creator of the **Blue Skies Discussion Group** (via WashU’s Institute for School Partnership) – a reading and discussion group for K-12 educators, to address topics surrounding energy and the environment by capitalizing on university expertise, through talks and distribution of relevant materials. The aim is to provide teachers with cutting-edge knowledge about recent developments in research and technology that they can bring to the classroom. (<https://schoolpartnership.wustl.edu/event/blue-skies-discussion-group/>)
- TEDx St. Louis (formerly TEDx Gateway Arch) facilitator (2021 – present)
- Session Chair, ACS Award for Materials Chemistry (2017)

- NSF Workshop Lead on Opportunities for Mid-scale Instrumentation for Chemistry (2016-2017)
- Scientific Advisory Committee, Alpine Conference on Solid-state NMR (2016-2017)
- APS-MRS-ACS Helium Economics Study Committee (2015-2017)
- NSF Workshop on Ultrahigh-field NMR, participant (2015)
- Executive Committee, Experimental NMR Conference ("ENC"), 2014-2022
- Executive Committee, Rocky Mountain Conference on NMR ("RMC"), 2013-present
- External program reviewer of a Chemistry dept. (fall 2013)
- Co-organizer, SLINN Meeting (St. Louis Institute for Nanoscience & Nanomedicine), April 2013-2017.
- Editorial Board, *Solid-state Nuclear Magnetic Resonance*, published by Elsevier (2011-present)
- Vice Chair, Gordon Research Conference, Magnetic Resonance (2011)
- Executive Council, NSF Phase II Center for Sustainable Materials Chemistry (2011-2018)
 - NSF Phase II and Phase III Center for Sustainable Materials Chemistry: Lead for "Broadening Participation"--recruitment, retention, inclusion, and professional development of underrepresented group members (2015- 2018)
- Co-Chair, St. Louis NMR Discussion Group (2004-present)
- Chair, Midwest/Great Lakes Regional ACS Conference, Solid-state NMR session, St. Louis, MO (2011)
- ACS Midwest Award Jury member (2010-2014)
- Co-Chair, Pacificchem Meeting, Solid-state NMR and Inorganic Materials session, Honolulu, HI (2010)
- Host, Chicago Area NMR meeting (2008)
- Humboldt Foundation delegation to the German Embassy (2006)
- High school student summer research sponsor, STARS Summer Research Program (Patricia Denn 2017, Saqib Hassan 2014, Louis Wang 2012, Casey Zucarello 2011, Adam Brandt 2009, Spencer Wells 2008),
- Undergraduate research experience sponsor through NSF REU programs (Maria Vazquez de Vasquez 2014, Michael West 2013 and 2014, Britney Johnson 2010, Kimberly Hartstein 2009, Alexander Barnes 2003), and the Collaborative for Applied Experiences in Science Program (Ted Carnahan 2003)
- Tenure/Promotion Reviewer: Physics faculty (2004, 2017), ; Materials science faculty (2010); Chemistry faculty (2009, 2015, 2017, 2018, 2020, 2021)
- Ongoing: Reviewer for *Physical Review B*, *Physical Review Letters*, *Journal of the American Chemical Society*, *Chemistry of Materials*, *Inorganic Chemistry*, *Journal of Solid State Chemistry*, *Journal of Magnetic Resonance*, *Journal of Physics & Chemistry of Solids*, *Concepts in Magnetic Resonance*, *Solid-state Nuclear Magnetic Resonance*, *Canadian Journal of Chemistry*, and *Proceedings of the Materials Research Society*
- Proposal reviewer for NSF, DOE, Army Research Office, and U.S. Civilian R&D Foundation

Professional Memberships

ACS, American Chemical Society, Divisions of Inorganic Chemistry and Physical Chemistry
APS, American Physical Society, Division of Materials Physics
AAAS, American Association for the Advancement of Science

Teaching Experience

- Physics 534 (Chemistry 576), Magnetic Resonance:** inter-departmental graduate course, enrollments of 6-12, with 5-15 auditing students.
- Chemistry 465, Solid-state Chemistry:** upper division and graduate course, enrollments of ~8-30.
- Chemistry 461, Inorganic Chemistry:** 1-semester upper division course, enrollments of ~45-80.
- Chemistry 541, Advanced Physical Inorganic Chemistry:** graduate course on group theory and spectroscopy, upper division and graduate enrollments of ~7-20.
- Chemistry 470, Advanced Inorganic Laboratory:** advanced synthesis and characterization, upper division and graduate enrollments of ~10-24 students.
- Chemistry 182, "Chemistry for Concerned Citizens" Freshman Seminar:** non-majors course in critical analysis of issues in climate change, energy, and the environment. Enrollment of 6-8.
- Chemistry 181, First-Year Opportunity: Applications in Chemistry:** majors course, freshman seminar on chemistry research and professional development; training in the use of social media for professionals, enrollments of ~20.
- Chemistry 111, General Chemistry:** first-year chemistry, team-taught in 2-3 sections of ~250-330 students each.
- Bio 5925, Matter and Energy Transformations:** 1-week lecture and lab course, for the Master of Science in Biology for Biology Teachers, enrollment of ~20-30. (July 2015, July 2017, July 2019, July 2021 postponed)

Research Associates (current group members are shown in **bold**)

Postdoctoral Associates:

- Marko Bertmer: Aug. 2002-Sept. 2003, Feodor Lynen Fellow. He is currently a lecturer (Privatdozent) at University of Leipzig in Experimental Physics. Ph.D. Physical Chemistry, WWU-Münster, Germany, advisor: Prof. Hellmut Eckert. Habilitation, RWTH Aachen, advisor: Prof. Bernhard Blümich.
- Weijian Chen:** Aug. 2021 – present. Ph.D. in Physics with Kater Murch. Currently co-advised by faculty in Physics on quantum sensing themes.
- Julie Herberg: June 2002 - Jan. 2003. She is a Staff Physicist at LLNL, Livermore, CA. Ph.D. Physics, Washington Univ., advisor: Prof. Richard Norberg.
- Patrick Judge:** June 2021 – present. Ph.D. in Chemistry with Alexander Barnes. Currently working on EFRC NO_x and SO_x interactions with porous sorbent materials.
- Guibin Ma: Aug. 2003-Aug. 2005. He is currently at the University of Edmonton, Canada as a staff scientist researcher. Ph.D. Chemistry, KTH, Stockholm, Sweden, advisor: Prof. Julius Glaser.
- Zayd Ma: Nov. 2012-Oct. 2015. He worked jointly on OPNMR projects and on NMR of quadrupolar nuclei for the NSF Phase II CCI center. Ph.D. Physics, Univ. of Utah, advisor: Prof. Brian Saam. He currently works for the Air Force in Utah.
- Kannan Ramaswamy: May 2003 - Nov. 2008. He is an Assistant Professor of Physics at BITS-Pilani in Hyderabad, India. Ph.D. Physics, Indian Inst. of Science, Bangalore, advisor: Prof. J. Ramakrishna. Postdoctoral Researcher at the Weizmann Inst. Israel with Prof. Zeev Luz.
- Erika Sesti: Nov. 2014 – July 2016. Part-time Jan. 2019-Aug. 2019 Erika obtained her PhD in Chemistry from WashU under my supervision and is currently a staff member at Pfizer.

Daphna Shimon: Jan. 2016 – Sept. 2017. Daphna got her PhD at the Weizmann Inst. of Science with Prof. Shimon Vega in theory of dynamic nuclear polarization. Currently with Ilya Kaminker at Univ. of Tel Aviv, Israel.

Ph.D. Students:

Yvonne Afriyie (Aug. 2015 – Jan. 2019) Materials Science (IMSE) Ph.D. student. Research scientist at Intel, Arizona.

Chia-Hsin Chen (May 2014 – May 2019) Research Scientist, Johnson Matthey, U.K. Taiwanese Fellowship through the Ministry of Education, Taiwan.

Sarah (Gresham) Mattler (January 2007 – March 2012) Research Scientist, Exxon Mobil, Houston TX.

Jinlei Cui (Jan. 2015 – May 2019) Currently in a postdoc appointment with Prof. Marek Pruski, Ames Lab, Iowa.

Blake Hammann (January 2013 – December 2016) Research Scientist, Archer Daniels Midland

Robert Marti (January 2014 – July 2018) Staff scientist at PPG in Pittsburgh. Recipient of DOE Office of Science, Team Science Award, 2017, awarded to Robert Marti and Dr. Josh Howe (Sholl group).

Jeremy Moore (January 2011 – May 2015) Postdoc in MRI imaging at WU School of Medicine.

Stacy Mui (January 2005 – Oct. 2008) Currently with the IAEA, International Atomic Energy Agency, Vienna. Senior Member of the Technical Staff at Sandia Nat'l Labs, Livermore, CA, as a systems analyst (radiation and nuclear sector).

Ryan Nieuwendaal (January 2003 – March 2008), Staff Scientist, NIST, Maryland.

Erika Sesti (January 2009 – Oct. 2014). Research Scientist, Pfizer. 2012 Chemistry Dept. Teaching Award. 2013 ENC Student Travel Award. (Listed under postdocs).

He "Jason" Sun (January 2017 – present)

Andy Surface (January 2010 – August 2013) Staff scientist at PPG, Pittsburgh. Formerly, staff scientist at Albermarle, in Baton Rouge, LA.

Michael "Ike" West (January 2016 – June 2021) Postdoc, Cincinnati Children's Hospital

Dustin Wheeler (January 2009 – May 2014) CUNY Instrumentation/Facility Manager. Student leader of the Magnetic Resonance Gordon Research Symposium, June 2011.

Matt Willmering (January 2013 – May 2017) Staff Scientist, Cincinnati Children's Hospital 2014 Chemistry Dept. Teaching Award. Dean's Dissertation Fellowship, 2017.

M.A. Students:

Jhashanath "Subin" Adhikari, M.Sc. Physical Chemistry, Tribhuvan University, Kathmandu, Nepal. Attending Clark University, MA, for a Ph.D. in Chemistry.

Muhan Cao (January 2010 – Aug. 2011) Muhan is a Technical Consultant at Phenomenex, CA.

P. Curtis Carey, B.A. Chemistry, University of Wyoming. Present position unknown.

Kim Nguyen, B.S. Chemistry, University of Missouri St. Louis. She graduated from the group of Prof. Carolyn Anderson at WU Med School in 2011.

Katie Wentz. NSF Phase II CCI "Center for Sustainable Materials Chemistry" Hermiston Fellow for Chemistry outreach and informal science education. 2010 Chemistry Dept. Teaching Award. Teaching high school chemistry, Priory Academy

Undergraduate Students:

- Alexander Barnes: currently Professor, ETH Zurich; PhD Chemistry MIT; B.S. Whitman College, WA. *Honors:* 2006 NSF Graduate Fellowship; Phi Beta Kappa; 2003 NSF Summer Research Program in Solid-State Chemistry. (summers, 2003, 2004)
- John Beach: currently an engineering PhD student, UIUC. B.S. Chemical Engineering 2013 (Jan. 2012 – May 2013)
- Allison Brenner: A.B. Chemistry 2013. NSF Summer School in Solid-state Chemistry (Univ of OR). Applying to graduate school, Chemistry.
- Ted Carnahan: working in an MIS (computer) role in Columbia, MO.
- Julia Collins: A.B. Chemistry 2006. attending graduate school for chemistry, emphasis on chemical education, at Texas A&M. *Honors:* 2006 HyperCube Award. (2005-2006)
- Katie Cychosz: A.B. Chemistry 2005. Attending graduate school for chemistry at University of Michigan. *Honors:* 2005 Sowden Prize; 2004 Pfizer Summer Undergraduate Research Fellowship. (2004-2005)
- Dan Daranciang: A.B. Chemistry 2006. Attending graduate school for physical chemistry at Stanford. *Honors:* 2006 HyperCube Scholar Award. (2006)
- Nikhil Dharan: chemistry major (fall 2013 – Spring 2015) Recipient of a WU Undergraduate Research Fellowship, 2014.
- Kathleen Hagan: A.B. Chemical Engineering 2012. (2009)
- Kimberly Hartstein: A.B. Chemistry 2011. Currently a grad student at Univ. of WA, Seattle. Fulbright Fellow at WWU Münster, Germany in Physical Chemistry. *Honors:* 2011 Fulbright Fellow, 2011 WU Hypercube Award, 2009 NSF Summer Research Program in Solid-State Chemistry. (June 2009-Aug.2011)
- David Hirsh: A.B. Chemistry 2012. Currently a grad student with Rob Schurko at Univ. of Windsor, Canada. *Honors:* 2011 WU Summer Undergraduate Research Fellowship. Research paper selected for publication in the *WU Undergraduate Research Digest*, **2012**, one of 3 research articles from all undergraduate research activities at WU. (2010-2012)
- Michal Hyrc: A.B. Chemical Engineering 2013. *Honors:* selected for a WU Undergraduate Research Fellowship, 2009. Research published in the *Washington University Undergraduate Research Digest*, vol. 5, no. 2 spring **2010**, one of 3 research articles from all undergraduate research activities at WU. (2009)
- Adam Johnson: A.B. Chemistry 2009. Currently in graduate school for Food Science. Staff scientist at PepsiCo. (2008-2009)
- Britney Johnson: Currently a grad student at Washington Univ., Biochemistry Dept.. *Honors:* selected for NSF's Summer Research Program in Solid-State Chemistry, 2010. (2010)
- Vinay Kampalath: A.B. Chemistry 2007. Currently working for the Boston Urban Asthma Coalition, in a public health role. *Honors:* 2007 Merck Chemistry Award. (2005-2007)
- Yinuan Liu: She is currently a PhD student at UC Irvine
- Michael Mazza: WashU Chemistry and Environmental Studies double major. (May 2014-Spring 2016) Now at Caltech
- Chris McArdle: graduated 2005. Present position unknown.
- Emily Middlebrook: A.B. Chemistry 2012. (Fall 2010)
- Kelly Powderly: Northwestern Univ. Chemistry student. (Summer 2015)
- Jason Shields: A.B. Chemistry 2010. Currently attending graduate school at Princeton. *Honors:* Sowden Prize, Phi Beta Kappa, "Outstanding Junior Award" from ACS, Moog Scholar, nominee for the Goldwater Fellowship. Senior Honors presentation: "*Toward Shape*

Memory: Synthesis, Purification, and Polymerization of Cinnamoyloxyethyl Methacrylate"
(2008- May 2010)

Tammy Shirley: A.B. Chemistry 2005. M.D. candidate, WU Medical School. (2004-2005)

Nathan Soper: A.B. Chemistry 2020

Evan Stamper: A.B. Chemistry 2004. Ph.D. Northwestern University. Research scientist in the Chicago area. (2003-2004)

Vicky Su: recipient of a WashU Summer Undergraduate Research Fellowship. She is attending graduate school at Stanford.

Maria Vazquez de Vaxquez: Cal State Los Angeles chemistry major, CSMC Undergraduate Research fellow (summer 2014).

Michael West: Univ. of Arkansas, physics major. NNIN REU student fellow. (summer 2013), and CSMC Undergraduate Research fellow (summer 2014). Goldwater Scholar, Honorable Mention (2014).

Robin Wheelus: St. Olaf Physics student (Summer 2015)

Blair Winograd: A.B. Chemistry 2013. Currently, applying to chemistry PhD programs (Jan. 2012-May 2013)

Yanzhe Zhu: A.B. Chemical Engineering 2014. Currently in graduate school at Princeton (May 2012-May 2013)

High School Students:

Adam Brandt: (summer 2009) STARS student. Board of Governor's Scholarship, Missouri State Univ., Dept. of Physics.

Patricia Denn (summer 2017) STARS student.

Saqib Hassan (summer 2014) STARS student.

Daniel Martin (summer 2012).

Louis Wang: (summer 2012) STARS student. Honors: Moog Scholar (2013-) at Washington University; 2012 recipient of the LMI Aerospace Award for outstanding research. He is now a chemical engineering major at WU.

Spencer Wells: (summer 2008) STARS student. National Merit Finalist. Attending Univ. of IL, Urbana Champaign as an Engineering major.

Casey Zuccarello (summer 2011) STARS student.