Alexander J. Norquist

Curriculum Vitae

Professor of Chemistry
Haverford College

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Professional appointments

2017 – Present	Professor of Chemistry, Haverford College, Haverford PA
2010 – 2017	Associate Professor of Chemistry, Haverford College, Haverford PA
2003 – 2009	Assistant Professor of Chemistry, Haverford College, Haverford PA
2001 – 2003	Postdoctoral Research Assistant, University of Oxford, Oxford UK

Education

Ph.D, 1996 – 2000	Northwestern University, Evanston IL, Advisor Kenneth R. Poeppelmeier Ph.D. in Chemistry, Northwestern University
M.S., 1996 – 1997	Northwestern University, Evanston IL, Advisor Kenneth R. Poeppelmeier M.S. in Chemistry, Northwestern University
B.A., 1992 – 1996	Gustavus Adolphus College, St. Peter MN, Advisor Lawrence W. Potts B.A. in Chemistry

Grants and awards

2018 – 2021	DARPA, Discovering Reactions and Uncovering Mechanisms of Organohalide Hybrid Perovskite Formation, HR001118C0036, $5,969,851
2017 – 2020	National Science Foundation, 'The Dark Reactions Project: A machine learning approach to exploring structural diversity in solid state synthesis' DMR-1709351, $645,288
2013 – 2017	National Science Foundation, 'The Dark Reactions Project: A machine learning approach to materials discovery' DMR-1307801, $300,000
2013 – 2016	National Science Foundation, 'MRI Consortium: acquisition of a cyber-enabled single-crystal S-ray diffractometer for materials research at PUIs' DMR-1337296, Co-PI $470,000
2010 – 2015	Henry Dreyfus Teacher Scholar Award, 'Organically template vanadium tellurites: a new target for novel microporous materials' TH-10-013, $60,000.
2009 – 2013	National Science Foundation, 'RUI: Synthesis of organically templated gallium sulfites,' CHE-0911121, $160,000.
2005 – 2007	Research Corporation Cottrell College Science Award, 'Directed synthesis of noncentrosymmetric materials,' CC6418, $36,704.
2004 – 2007	American Chemical Society Petroleum Research Fund Type G Faculty Start-up Grant, 'Synthesis of organically templated molybdenum sulfates under hydrothermal condition,' $35,000.
2003 – 2008	Henry and Camille Dreyfus Foundation Faculty Start-up Award for Undergraduate Institutions, 'Synthesis of organically templated vanadium sulfates under hydrothermal conditions,' $20,000.

Current research interests.

My research interests are focused on the use of exploratory reactions in materials discovery. Mild hydrothermal conditions are used to prepare new organic inorganic hybrid materials, with specific attention being paid to organically templated transitional metal selenites and tellurites. I am interested in understanding and optimizing the way in which exploratory reactions are conducted, using cheminformatics and machine learning approaches.

Recent teaching responsibilities (post-tenure)

Chemistry 111 Chemical Structure and Bonding
Chemistry 112 Chemical Dynamics
Chemistry 115 Chemical Structure and Bonding with Inquiry lab
Chemistry 269 Research in Materials Science
Chemistry 301/302 Lab in Chemical Structure and Reactivity
Chemistry 320 Inorganic Chemistry
Chemistry 353 Topics in Materials Science
Chemistry 354 Solid State Chemistry
Chemistry 369 Research in Materials
Chemistry 391 Senior Seminar

Administrative duties at Haverford College (post-tenure)

- Chair, Chemistry department (2015 – 2017)
- Retirement and investment committee (2012 – Present)
- Honors committee (2015 – 2016)
- Committee on Student Standing and Programs, chair (2019 – 2020)
- Personnel reappointment case presenter (2015, 2019)
- Koshland Integrated Sciences Center machine shop faculty liaison (2014 - Present)
- Academic Council nature sciences representative (2013 – 2015)
- Administrative advisory committee (2011 – 2013, Chair 2012 – 2013)
- Alternate Academic Council, natural sciences representative (2011 – 2012)
- Teagle Systematic Improvement Grant team member (2010 – 2011)
- Goldwater / Beckman applicant reviewer, selection committee, committee chair (2012 – 2020)
- Haverford College department of chemistry ad-hoc search committee (2019)

Service to the wider scientific community

- Councilor in the Council on Undergraduate Research (CUR), Chemistry Division 2010 – 2016 (elected March 2010, re-elected March 2013)
- CUR-Quarterly chemistry division editor (2013 – 2016)
- American Chemical Society National meeting, August 2015, Building Innovative Solid State Materials Through Solution Chemistry co-organizer.
- Proposal reviews: National Science Foundation, American Chemical Society Petroleum Research Fund, Department of Energy Office of Basic Energy Sciences, Research Corporation.
- Ad hoc reviewer for Nature Communications, Inorganic Chemistry, Chemistry of Materials, the Journal of the American Chemical Society, the Journal of Solid State Chemistry, Crystal Growth and Design, Acta Crystallographica Section B and C, the European Journal of Inorganic Chemistry, the Journal of Molecular Structure and Nanotechnology.

Post-doctoral fellows mentored

Phil Adler	May 2015 – Dec 2016
Mansoor Ani Najeeb Nellikkal	May 2018 – present
Ian Pendleton	April 2018 – present

Selected peer-reviewed publications (83 total, undergraduate co-authors names are underlined)

1. Nisbet, M. L.; Pendleton, I. M.; Nolis, G. M.; Griffith, K. J.; Schrier, J.; Cabana, J.; Norquist, A. J.; Poepplemeier, K. R. Machine-learning-assisted synthesis of polar racemates. *J. Am. Chem. Soc.* **2020,** *142,* 7555-7566.

2. Jia, X.; Lynch, A.; Huang, Y.; Danielson, M.; Lang'at, I.; Milder, A.; Ruby, A. E.; Wang, H.; Friedler, S. A.; Norquist, A. J.; Schrier J. Anthropogenic biases in chemical reaction data and their detrimental effect on materials discovery, *Nature*, **2019,** *573,* 251-255.

3. Pendleton, I. M.; Cattabriga, G.; Li, Z.; Najeeb, M. A.; Friedler, S. A.; Norquist, A. J.; Chan, E.; Schrier, J. Experiment Specification, Capture and Laboratory Automation Technology (ESCALATE): a software pipeline for automated chemical experimentation and data management, *MRS Comm.* **2019**, *9*, 846-859.

4. Jia, X.; Dixon, J. L.; Zeller, M.; Schrier, J.; Norquist, A. J. Templated vanadium tellurites: identifying the effects of low density attractions on inorganic layer topology. *J. Solid State Chem.* **2019,** *273,* 158-165**.**

5. Xu, R. J.; Olshanksly, J. H.; Adler, P. D. F.; Huang, Y.; Smith, M. D.; Zeller, M.; Schrier, J.; **Norquist, A.** Understanding structural adaptability: a reactant informatics approach to experiment design. *Mol. Systems. Des. & Eng.* **2018.** *3*, 473-484.

6. Naili, H.; Francois, M.; **Norquist, A. J.**; Rekik, W. NCI calculations for understanding a physical phase transition in $(C_6H_{14}N_2)[Mn(H_2O)_6](SeO_4)_2$. *Solid State Sci.* **2017,** *74,* 44-55.

7. Salah A. M. S.; Sayari, N.; Naili, H.; **Norquist, A. J.** Conglomerate crystallization and chiral discrimination between four copper materials templated by methylbenzylamine. *RSC Advances* **2016,** *6*, 59055-59065.

8. Adler, P. D. F.; Xu, R.; Olshansky, J. H.; Smith, M. D.; Elbert, K. C.; Yang, Y.; Ferrence, G. M.; Zeller, M.; Schrier, J.; **Norquist, A. J.** Probing structural adaptability in templated vanadium selenites. *Polyhedron.* **2016,** *114*, 184-193.

9. Raccuglia, P.; Elbert K. C.; Adler, P. D. F.; Falk, C.; Wenny, M. B.; Mollo, A.; Zeller, M.; Friedler, S. A.; Schrier, J.; **Norquist, A. J.** Machine learning assisted materials discovery using failed experiments. *Nature,* **2016,** *533,* 73.

10. Nourmahnad, A.; Wenny, M. B.; Zeller, M.; Schrier, J.; **Norquist, A. J.** The role of inorganic acidity on templated vanadate composition and dimensionality. *J. Solid State Chem.* **2016,** *236,* 215-221.

11. Nourmahnad, A.; Smith, M. D.; Zeller, M.; Ferrence, G. M.; Schrier, J.; **Norquist, A. J**. The role of non-covalent interactions on vanadium tellurite chain connectivities. *Inorg. Chem.* **2015,** *54,* 694-703.

12. Olshansky, J. H.; Wiener, K. J.; Smith, M. D.; Nourmahnad, A.; Charles, M. J.; Zeller, M.; Schrier, J.; **Norquist, A. J**. Formation principles for vanadium selenites: the role of pH on product composition. *Inorg. Chem.* **2014,** *53*, 12027-12035.

13. Hajlaoui, F.; Naili, H.; **Norquist, A. J.;** Mhiri, T.; Bataille, T. The structural transformation of monoclinic $[(R)\text{-}C_5H_{14}N_2][Cu(H_2O)_4](SO_4)_2{\cdot}2H_2O$ into orthorhombic $[(R)\text{-}C_5H_{14}N_2]_2[Cu(H_2O)_6](SO_4)_3$; crystal structures and thermal behavior. *Phase Trans.* **2014,** *18,* 71-84.

14. Chang, K. B.; Smith, M. D.; Zeller, M.; **Norquist, A. J.** *catena*-Poly[2,2',2"-nitrilotris(ethan-aminium) [tri-□-oxido-tris[dioxidovanadate(V)]] monohydrate]. *Acta Crystallogr. Sect. E* **2013,** *69*, m570-m571.

15. Koffer, J. H.; Olshansky, J. H.; Smith, M. D.; Hernandez, K. J.; Zeller, M.; Ferrence, G. M.; Schrier, J.; **Norquist, A. J.** Formation principles for templated vanadium selenite oxalates. *Cryst. Growth. Des.* **2013,** *13,* 4504-4511.

16. Chang, K. B.; Smith, M. D.; Blau, S. M.; Glor, E. C.; Zeller, M.; Schrier, J.; **Norquist, A. J.** Steric induced layer flection in templated vanadium tellurites. *Cryst. Growth Des.* **2013,** *13*, 2190-2197.

17. Gautier, R.; **Norquist, A. J.;** Poeppelmeier, K. R. From racemic to polar materials. *Cryst. Growth Des.* **2012,** *51,* 6267-6271.

18. Olshansky, J. H.; Tran, T. T.; Hernandez, K. J.; Zeller, M.; Halasyamani, P. S.; Schrier, J.; **Norquist, A. J.** Role of hydrogen-bonding in the formation of polar achiral and nonpolar chiral vanadium selenite frameworks. *Inorg. Chem.* **2012,** *51,* 11040-11048.

19. Smith, M. D.; Blau, S. M.; Chang, K. B.; Tran, T. T.; Zeller, M.; Halasyamani, P. S.; Schrier, J.; **Norquist, A. J.** Inducing polarity in $[VO_3]_n^{n-}$ chain compounds using asymmetric hydrogen-bonding networks. *J. Solid State Chemistry* **2012,** *195,* 86-93.

20. Hajlaoui, F.; Naili, H.; Yahyaoui, S.; **Norquist, A. J.;** Mhiri, T.; Bataille, T. Synthesis, crystal structures and thermal behavior of organic-inorganic hybrids incorporating a chiral diamine. *J. Organometallic Chem.* **2012,** *700*, 110-116.

21. Smith, M. D.; Blau, S. M.; Chang, K. B.; Zeller, M.; Schrier, J.; Norquist, A. J. Beyond Charge Density Matching; the Role of C – H ⋯ O Interactions in the Formation of Templated Vanadium Tellurites. *Cryst. Growth Des.* **2011,** *11,* 4213-4219.

22. Olshansky, J. H.; Blau, S. M.; Zeller, M.; Schrier, J.; **Norquist, A. J.** Understanding an Order-Disorder Phase Transition in Ionothermally Synthesized Gallium Phosphates. *Cryst. Growth Des.* **2011,** *11*, 3065-3071.

23. Glor, E. C.; Blau, S. M.; Yeon, J.; Zeller, M.; Halasyamani, P. S.; Schrier, J.; **Norquist, A. J.** [*R*-$C_7H_{16}N_2$][$V_2Te_2O_{10}$] and [*S*-$C_7H_{16}N_2$][$V_2Te_2O_{10}$]; New Polar Templated Vanadium Tellurite Enantiomers. *J. Solid State Chem.* **2011,** *184*, 1445-1450.

24. Kaufman, E. A.; Zeller, M.; **Norquist, A. J.** A Slow Leak Synthetic Route to Organically Templated Gallium Sulfates. *Cryst. Growth Des.* **2010,** *10*, 4656-4661.

25. Chang, K. B.; Hubbard, D. J.; Zeller, M.; Schrier, J.; **Norquist, A. J.** The Role of Stereoactive Lone Pairs in Templated Vanadium Tellurite Charge Density Matching. *Inorg. Chem.* **2010,** *49*, 5167-5172.

26. Choyke, S. J.; Blau, S. M.; Larner, A. A.; Narducci Sarjeant, A.; Yeon, J.; Halasyamani, P. S.; **Norquist, A. J.** Noncentrosymmetry in New Templated Gallium Fluorophosphates. *Inorg. Chem.* **2009,** *48*, 11277-11282.

27. Sanchez Casalongue, H.; Choyke, S. J.; Narducci Sarjeant, A.; Schrier, J.; **Norquist, A. J.** Charge Density Matching in Templated Molybdates. *J. Solid State Chem.* **2009,** *182*, 1297-1303.

28. Hubbard, D. J.; Johnston, A. R.; Sanchez Casalongue H.; Narducci Sarjeant, A.; **Norquist, A. J.** Synthetic Approaches for Noncentrosymmetric Molybdates. *Inorg. Chem.* **2008,** *47*, 8518-8525.

29. Stover, A. K.; Gutnick, J. R.; Narducci Sarjeant, A.; **Norquist, A. J.** $[Mo_{16}O_{53}F_2]^{12-}$; a New Polyoxofluoromolybdate Anion. *Inorg. Chem.* **2007,** *46*, 4389-4391.

30. Welk, M. E.; Stern, C. L.; Poeppelmeier, K. R.; **Norquist, A. J.** The Effects of Reaction Gel Dehydration in the Synthesis of $Cu(NC_5H_5)_4VOF_4$ and $[Cu(NC_5H_5)_4VOF_4][\ Cu(NC_5H_5)_4(H_2O)VOF_4]\cdot H_2O$ *Cryst. Growth Des.* **2007,** *7*, 956-961.

31. Nelson, J. H.; Narducci Sarjeant, A.; **Norquist, A. J.** [Poly[tris(*p*-xylylenediaminium)[tetradeca-□-oxo-hexadecanonamolybdate(VI)]]] *Acta Crystallogr. Sect. E* **2007,** *63*, m1442-m1444.

32. Nelson, J. H.; Johnston, A. R.; Narducci Sarjeant, A.; **Norquist, A. J.** Composition Space Analysis of Templated Molybdates. *Solid State Sci.* **2007,** *9,* 472-484.

33. Nelson, J. R.; Narducci Sarjeant, A.; **Norquist, A. J.** Poly[tetrakis(4-aminopyridium) [hexadeca-□-decaoxooctamolybdate(VI)]]. *Acta Crystallogr. Sect. E*, **2006,** *62*, m1731-m1733.

34. Nelson, J. R.; Narducci Sarjeant, A.; **Norquist, A. J.** Poly[bis(4-aminopyridinium) decaoxotrimolybdate(VI)]. *Acta Crystallogr. Sect. E*, **2006,** *62*, m1448-m1450.

35. Veltman, T. R.; Stover, A. K.; Narducci Sarjeant, A.; Ok, K. M.; Halasyamani, P. S.; **Norquist, A. J.** Directed Synthesis of Noncentrosymmetric Molybdates Using Composition Space Analysis. *Inorg. Chem.* **2006,** *45*, 5529-5537.

36. Thorn, K. J.; Narducci Sarjeant, A.; **Norquist, A. J.** $[C_4H_{14}N_2]_2[Mo_8O_{26}]\cdot 2H_2O$: A New Molybdate Salt. *Acta Crystallogr. Sect. E,* **2005,** *61*, m1665-m1667.

37. Muller, E. A.; Cannon, R. J.; Narducci Sarjeant, A.; Ok, K. M.; Halasyamani, P. S.; **Norquist, A. J.** Directed Synthesis of Noncentrosymmetric Molybdates. *Cryst. Growth Des.* **2005,** *5*, 1913-1917.

38. Muller, E. A.; Narducci Sarjeant, A.; **Norquist, A. J.** $(C_6H_{16})_2[Mo_8O_{26}]$: A New □-Octamolybdate Salt. *Acta Crystallogr. Sect. E* **2005,** *61*, m730-m732.

39. Gutnick, J. G.; Muller, E. A.; Narducci Sarjeant, A.; **Norquist, A. J.** $[N_2C_5H_{14}][(MoO_3)_3(SO_4)]\cdot H_2O$: Sulfated □-Molybdena Chains. *Inorg. Chem.* **2004,** *43*, 6528-6530.

Popular press research highlights

1. 'The positive side of negative results' *Nature Podcast*, 05 May 2016 http://www.nature.com/nature/podcast/index-2016-05-05.html
2. 'Computer gleans chemical insight from lab notebook failures' Philip Ball, *Nature News* – 05 May 2016 http://www.nature.com/news/computer-gleans-chemical-insight-from-lab-notebook-failures-1.19866
3. 'Why machines should learn from failures' Daniela Hernandez *Wall Street Journal* 06 May 2016 http://www.wsj.com/articles/why-machines-should-learn-from-failures-1462538020
4. 'Computers trump chemists by studying failed experiments' Nick Summers *engadget.com* 06 May 2016 http://www.engadget.com/2016/05/05/machine-learning-algorithm-predict-chemical-reactions/
5. 'Lab failures turn to gold in search for new materials' Jordana Cepelewicz *Scientific American* 06 May 2016 http://www.scientificamerican.com/article/lab-failures-turn-to-gold-in-search-for-new-materials/
6. 'What scientists could learn from startups' Adam Marcus, Ivan Oransky, *The Week,* 22 May, 2016 http://theweek.com/articles/625377/what-scientists-could-learn-from-startups
7. 'Reproducibility crisis – why we need more dark reactions projects' Wade Miller, *Conceptual Revolutions*, June 26, 2016. http://conceptualrevolutions.com/2016/06/26/reproducibility-amgen-study-dark-reactions-project/
8. 'Machine learning can have human bias' Sam Lemonick, *Chemical and Engineering News,* 12 Sept. 2019. https://cen.acs.org/physical-chemistry/computational-chemistry/Machine-learning-human-bias/97/i36
9. 'Human biases cause problems for machines trying to learn chemistry' Kira Welter, *Chemistry World*, 13 Sept. 2019. https://www.chemistryworld.com/news/human-biases-cause-problems-for-machines-trying-to-learn-chemistry/3010970.article
10. 'Material concerns' *Nature*. 12 Sept. 2019, *573,* 164.
11. 'Chemists show how bias can crop up in machine learning algorithm results' Bob Yirka, 12 Sept. 2019 *Phys.org.* https://phys.org/news/2019-09-chemists-bias-cropmachine-algorithm.html

12. ‘Don’t let humans pick the experimental conditions?’ Derek Lowe *ScienceMag.org.* 16 Sept. 2019. https://blogs.sciencemag.org/pipeline/archives/2019/09/16/dont-let-humans-pick-the-experimental-conditions