James R. Neilson

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Research Vision

My research pertains to solid-state and materials chemistry; my interest lies in discovering and understanding emergent properties and reactivity of materials to achieve a paradigm of materials by design. As materials are key enablers of technology, the goal of this research is to design new functionality in materials, *i.e.,* control macroscopic electronic and magnetic properties through the competition of local interactions in materials. While we primarily perform experiments to make materials, characterize their structure and properties, we gain additional insight through numerical calculations and simulations.

Employment

2013–present Assistant Professor; Colorado State University, Fort Collins, CO USA
Department of Chemistry

2011–2013 Post-doctoral Associate; Johns Hopkins University, Baltimore, MD USA
Departments of Chemistry, Physics & Astronomy, and the Institute for Quantum Matter, with Professor Tyrel M. McQueen: *Development of low-temperature routes to inorganic materials and structure/property relationships in strongly correlated electron materials and superconductors.*

Education

2006–2011 University of California Santa Barbara, Santa Barbara, CA USA
Ph.D., Biomolecular Science & Engineering; Thesis title: *Kinetic Control of Aqueous Hydrolysis: Modulation of Structure/Property Relationships in Inorganic Crystals*. Advisor: Professor Daniel E. Morse

2005 University of Cambridge, Cambridge, U.K.
Undergraduate Research Fellowship, Summer 2005; Research: *Vibrational properties of disordered materials.* Advisor: Professor Stephen R. Elliot

2002–2006 Lehigh University, Bethlehem, PA USA
B.S., Materials Science & Engineering, June 2006. Minor in Spanish. Research: *Chalcogenide glasses and Nanolithography*. Research Advisor: Professor Himanshu Jain.

Graduate / Undergraduate Awards

National Science Foundation, Graduate Research Fellowship, 2007-2010
MRS Graduate Student Award, Silver Medalist, 2010
Barry M. Goldwater Scholar, 2005

Awards and Funding

- Alfred P. Sloan Foundation, Sloan Research Fellowship, $60,000 (USD), 2017-2019.
- Research Corporation for Scientific Advancement, Cottrell Scholar Award: *Materials Design Principles for Effective Light-Induced Charge Separation in Revolutionary Photovoltaics*, $100,000 (USD), 2017-2020.
- National Science Foundation, Early CAREER Award: *CAREER: Towards A Paradigm Of Molecular-Level Control Of Solid-State Chemistry* (PI), $520,000 (USD), 2017-2022.
- Department of Energy Early Career Award: *Informed Materials Design Principles From Local Structures and Dynamics In Hybrid Perovskites* (PI), $750,000 (USD), 2016-2021.
- W. M. Keck Foundation Science and Engineering Research Grant: *Property-selective Synthesis: Natural Selection for Transformative Chemically-Dynamic Materials* (Co-PI), $1,811,949 (USD), 2016-2019.
- Enercat-CSU Master Service Agreement (MSA): *Developing physical approaches to stabilize dispersion* (Co-PI), $46,632 (USD), 2016-2017.
- National Science Foundation, Research Experiences for Undergraduates: *REU: Chemistry Applied to Real World Problems – Chemical Sciences at CSU* (Co-PI and Co-Director), $300,000 (USD), 2015-2018.
- Oak Ridge National Laboratory (DOE), Seed LDRD: *Chemical Reactivity of Solids: Chemical Dynamics of the Atomic Structure of Solids Using Time-of-Flight Neutron Total Scattering* (Co-PI), $103,545 to CSU (USD), 2014-2016.
- Colorado State University Energy Institute Discovery Grant: *Relationships between synthesis, structure, and properties in new high-efficiency photovoltaic materials and devices: perovskites* (PI), $15,000 (USD), 2014-2015.

Group / Mentoring

Graduate Students: Victoria Combs (2016–current), Jewels Fallon (2016–current), Ethan Emerson (2015–current), Eve Mozur (2015–current), Paul Todd (2015–current), Loryn Killpack (2014–2016, M.S.), Arnold Paecklar (2014–current), Michael Tarne (2014–current), Mary Marisa (2013–current), Andrew Martinolich (2013–current), Annalise Maughan (2013–current), Greg Terho (2013–2014, M.S.).
Postdoctoral Associates: Dr. Josh Kurzman (2013–2015), Dr. Kate Ross (2014–2015).
Undergraduate Interns: Geordan Brickey (2013–2014), Mitchel Bordelon (2013–2016, *NSF Graduate Research Fellow at UCSB*), Juliette Granger (2015–2016), J. James Allen (2014–current), Mohammed Almaker (2016–current), Andrew Candia (2016–current), Erik Rognerud (2016–current), Julia Trowbridge (2016–current), Kyle Peterson (2016–current).

Publications (updated March 26, 2017)

With DOI links where available. Also listed at: http://sites.chem.colostate.edu/neilsonlab/research.html
Citation tracking at: Google Scholar.

In Press or Review (manuscripts available upon request)

J. R. Neilson, N. Drichko, A. Llobet, M. Balasubramanian, M. R. Suchomel, T. M. McQueen, Local increase of symmetry on cooling in KNi_2Se_2. [arXiv]

Awarded US Patents:

1. J. R. Neilson, T. M McQueen, *Magnetocaloric materials for cryogenic liquification.* United States Patent, 9,568,223 (Feb 14, 2017). [USPTO]

Appeared

39. D. Olds, K. Page, A. Paecklar, P. Peterson, J. Liu, G. Rucker, M. Ruiz-Rodriguez, M. Olsen, M. Pawel, S. Overbury, and J. R. Neilson, A high precision gas flow cell for performing in situ neutron studies of local atomic structure in catalytic materials. *Rev. Sci. Inst.* (2017) 88, 034101. [doi]

38. A. J. Martinolich, J. R. Neilson, Towards Reaction-By-Design: Achieving Kinetic Control of Solid State Chemistry with Metathesis. *Chem. Mater.* (2017) 29(2), 479-489. (*Invited perspective*) [doi]

37. M. E. Marisa, S. Zhou, B. C. Melot, G. F. Peaslee, J. R. Neilson, Paracrystalline Disorder from Phosphate Ion Orientation and Substitution in Synthetic Bone Mineral. *Inorg. Chem.* (2016) 55(23), 12290-12298. [doi]

36. A. J. Martinolich, J. A. Kurzman, J. R. Neilson, Circumventing Diffusion in Kinetically-Controlled Solid-State Metathesis Reactions, *J. Am. Chem. Soc.* (2016), 138(34), 11031-11037. [doi]

35. A. E. Maughan, A. M. Ganose, M. M. Bordelon, D. O. Scanlon, and J. R. Neilson, Defect tolerance to intolerance in the vacancy-ordered double perovskite semiconductors Cs_2SnI_6 and Cs_2TeI_6. *J. Am. Chem. Soc.* (2016), 138(27), 8453-8464. [doi]

34. A. J. Martinolich, R. J. Higgins, M. P. Shores, J. R. Neilson, Lewis Base Mediated Polymorph Selectivity of Pyrite $CuSe_2$ Through Atom Transfer In Solid State Metathesis. *Chem. Mater.* (2016), 26(6), 1854–1860. [doi]

33. J. A. Kurzman, A. J. Martinolich, and J. R. Neilson. Influence of interstitial Mn on local structure and magnetism in $Mn_{1+\delta}Sb$. *Phys. Rev. B* (2015), 92, 184414. [arXiv],[doi]

32. K. A. Ross, M. M. Bordelon, G. S. Terho, J. R. Neilson, Nanosized helical magnetic domains in strongly frustrated $Fe_3PO_4O_3$. *Phys. Rev. B*, (2015), 92, 134419. [arXiv],[doi]

31. J. R. Neilson, T. M. McQueen, Representational Analysis of Extended Disorder in Atomistic Ensembles Derived from Total Scattering Data. *J. Appl. Crystallogr.*, (2015), 48, 1560–1572. [arXiv],[doi]

30. M. Mourigal, S. Wu, M. B. Stone, J. R. Neilson, J. M. Caron, T. M. McQueen, C. L. Broholm, Block magnetic excitations in the orbitally-selective Mott insulator $BaFe_2Se_3$, *Phys. Rev. Lett.*, (2015), 115, 047401. [arXiv],[doi]

29. J. A. Kurzman, K. E. Dettelbach , A. J. Martinolich , C. P. Berlinguette , J. R. Neilson, Structural Characteristics and Eutaxy in the Photo-Deposited Amorphous Iron Oxide Oxygen Evolution Catalyst. *Chem. Mater.*, (2015), 27(9), 3462–3470. [doi]

28. A. J. Martinolich, J. A. Kurzman, J. R. Neilson, Polymorph Selectivity of Superconducting $CuSe_2$ Through Kinetic Control of Solid-State Metathesis. *J. Am. Chem. Soc.*, (2015), 137(11), 3827–3833. [doi]

27. A. E. Maughan, J. A. Kurzman, J. R. Neilson, Hybrid Inorganic-Organic Materials with an Optoelectronically Active Aromatic Cation: $(C_7H_7)_2SnI_6$ and $C_7H_7PbI_3$. *Inorg. Chem.*, (2015), 54(1), 370–378. [doi]

26. J. P. Sheckleton, J. R. Neilson, T. M. McQueen, Electronic tunability of the frustrated triangular-lattice cluster magnet $LiZn_{2-x}Mo_3O_8$, *Mater. Horiz.*, (2015), 2, 76–80. [doi]

25. A. J. Martinolich, J. R. Neilson, Pyrite Formation via Kinetic Intermediates Through Low-Temperature Solid-State Metathesis, *J. Am. Chem. Soc.*, (2014), 136(44) 15654–15659. [doi]

24. J. R. Neilson, N. C. George, M. M. Murr, R. Seshadri, D. E. Morse, Mesostructure from hydration gradients in demosponge biosilica, *Chem. Eur. J.*, (2014), 20(17) 4956-4965. [doi]

23. P. Cottingham, D. C. Miller, J. P. Sheckelton, J. R. Neilson, M. Feygenson, A. Huq, T. M. McQueen, Dynamic charge disproportionation in the 1D chain material PdTeI. *J. Mater. Chem. C*, (2014), 2, 3238–3246. [doi]

22. L. Tao, G. Rousse, J. R. Neilson, B. C. Melot, T. M. McQueen, C. Masquelier, Magnetic Structures of LiMBO$_3$ (M = Mn, Fe, Co) lithiated transition metal borates, *Inorg. Chem.*, (2013), 52 (20), 11966–11974. [doi]

21. W. A. Phelan, D. C. Wallace, K. E. Arpino, J. R. Neilson, K. J. Livi, C. R. Seabourne, A. J. Scott, T. M. McQueen, Stacking Variants and Superconductivity in the Bi-O-S System. *J. Amer. Chem. Soc.*, (2013), 135 (14) 5372–5374. [doi]

20. J. R. Neilson, A. Llobet, J. Wen, M. R. Suchomel, T. M. McQueen, Charge density wave fluctuations, heavy electrons, and superconductivity in KNi_2S_2, *Phys. Rev. B*, (2013), 87, 045124. [arXiv],[doi]

19. J. R. Neilson, A. Llobet, A. V. Stier, L. Wu, J.-J. Wen, J. Tao, Y. Zhu, Z. B. Tesanovic, N. P. Armitage, T. M. McQueen, Mixed-valence-driven heavy-fermion behavior and superconductivity in KNi_2Se_2, *Phys. Rev. B*, (2012), 86, 054512. [arXiv],[doi]

18. L. A. Bawazer, M. Izumi, D. Kolodin, J. R. Neilson, B. Schwenzer, D. E. Morse, Evolutionary selection of enzymatically synthesized semiconductors from biomimetic mineralization vesicles, *Proc. Natl. Acad. Sci. U.S.A.* (2012), 109 (26), E1705-E1714. [doi]

17. J. P. Sheckelton, J. R. Neilson, D. G. Soltan, T. M. McQueen, Possible valence bond condensation in the frustrated cluster magnet $LiZn_2Mo_3O_8$, *Nat. Mater.* (2012), 11, 493-496. [doi],[arXiv]

16. J. M. Caron, J. R. Neilson, D. C. Miller, K. Arpino, A. Llobet, T. M. McQueen, Orbital Selective Magnetism in the Spin-Ladder Iron Selenides $Ba_{1-x}K_xFe_2Se_3$, *Phys. Rev. B*, (2012), 85, 180405(R). [arXiv], [doi]

15. J. R. Neilson, T. M. McQueen, Bonding, ion mobility, and rate-limiting steps in deintercalation reactions with $ThCr_2Si_2$-type KNi_2Se_2, *J. Am. Chem. Soc.* (2012), 134 (18), 7750-7757. [doi]

14. J. M. Caron, J. R. Neilson, D. C. Miller, A. Llobet, T. M. McQueen, Iron displacements and magnetoelastic coupling in the spin-ladder compound $BaFe_2Se_3$, *Phys. Rev. B*, (2011), 84, 180409(R). [arXiv],[doi]

13. J. R. Neilson, J. A. Kurzman, R. Seshadri, D. E. Morse, Ordering double perovskite hydroxides by kinetically controlled aqueous hydrolysis, *Inorg. Chem.*, (2011), 50, 3003-3009. [doi]

12. J. R. Neilson, B. C. Melot, D. P. Shoemaker, J. Kurzman, R. Seshadri, D. E. Morse, Understanding complex magnetic order in disordered cobalt hydroxides through analysis of the local structure, *Phys. Rev. B*, (2011), 80, 094418. [arXiv],[doi]

11. B. Schwenzer, J. R. Neilson, S. M. Jeffries, D. E. Morse, $Cd_{1-x}Zn_xO$ [$0.05 \leq x \leq 0.26$] synthesized by vapor-diffusion induced co-nucleation from aqueous metal salt solutions, *Dalton Trans.*, (2011), 40 (6), 1295-1301. [doi]

10. H. L. Zhang, J. R. Neilson, D. E. Morse, Vapor-diffusion-controlled sol-gel synthesis of flaky lithium vanadium oxide and its electrochemical behavior, *J. Phys. Chem. C*, (2010), 114 (45), 19550-19555. [doi]

9. K. Niesz, C. Reji, J. R. Neilson, R. C. Vargas, D. E. Morse, Unusual evolution of ceria nanocrystal morphologies promoted by a low-temperature vapor diffusion based process, *Cryst. Growth Des.*, (2010), 10 (10), 4485-4490. [doi]

8. J. R. Neilson, J. A. Kurzman, R. Seshadri, D. E. Morse, Cobalt coordination and clustering in α-$Co(OH)_2$ revealed by synchrotron X-ray total scattering, *Chem. Eur. J.* (2010), 16 (33), 9998-10006. [doi]

7. J. R. Neilson, B. Schwenzer, R. Seshadri, D. E. Morse, Kinetic control of intralayer cobalt coordination in layered hydroxides: $Co^{oct}_{1-0.5x}Co^{tet}_{x}(OH)_2(Cl)_x(H_2O)_n$, *Inorg. Chem.* (2009), 48 (23), 11017-11023. [doi]

6. B. Schwenzer, J. R. Neilson, K. Sivula, C. Woo, J. M. J. Frechét, D. E. Morse, Nanostructured p-type cobalt layered double hydroxide/n-type polymer bulk heterojunction yields an inexpensive solar cell, *Thin Solid Films* (2009) 517, 5722-5727. [doi]

5. B. Schwenzer, L. Z. Pop, J. R. Neilson, T. Sbardellati, D. E. Morse, Nanostructured ZnS and CdS Films synthesized using Layered Double Hydroxide Films as Precursor and Template, *Inorg. Chem.* (2009), 48 (4), 1542-1550. [doi]

4. A. Kovalskiy, J. R. Neilson, A. C. Miller, F. C. Miller, M. Vlček, and H. Jain, Comparative study of electron- and photo-induced structural transformations on the surface of $As_{35}S_{65}$ amorphous thin films, *Thin Solid Films* (2008) 516, 7511-7518. [doi]

3. J. R. Neilson, A. Kovalskiy, M. Vlček, H. Jain, and F. Miller, Fabrication of nano-gratings in arsenic sulphide films, *J. Non-Cryst. Solids* (2007) 353, 1427–1430. [doi]

2. A. Kovalskiy, H. Jain, J. R. Neilson, M. Vlček, C. M. Waits, W. Churaman, M. Dubey, On the mechanism of gray scale patterning of Ag-containing As_2S_3 thin films, *J. Phys. Chem. Solids* (2007) 68, 920-925. [doi]

1. S. N. Taraskin, S. I. Simdyankin, S. R. Elliot, J. R. Neilson, and T. Lo, Universal features of terahertz absorption in disordered materials, *Phys. Rev. Lett.* (2006) 97, 055504. [doi]

Professional and Honor societies

American Chemical Society, American Physical Society, Materials Research Society, American Crystallographic Association, Neutron Scattering Society of America, *Phi Beta Kappa*, *Tau Beta Pi*.