

HANS-CONRAD ZUR LOYE

David W. Robinson Palmetto Professor of Chemistry and Carolina Distinguished Professor
Department of Chemistry and Biochemistry
University of South Carolina

EDUCATION

Postdoc	1988-89	Northwestern University	Chemistry
Ph.D.	1988	University of California, Berkeley	Chemistry
Sc. B.	1983	Brown University	Chemistry

EMPLOYMENT HISTORY

Joint Appointment	Savannah River National Laboratory in Radiochemistry and Materials Science	2020-present
Carolina Distinguished Professor	University of South Carolina	2018-present
Associate Dean for Research and Graduate Education	College of Arts and Sciences University of South Carolina	2015-2020
Associate Dean for Research	College of Arts and Sciences University of South Carolina	2011-2015
Interim Associate Dean for Research	College of Arts and Sciences University of South Carolina	2011
David W. Robinson Palmetto Professor of Chemistry	Department of Chemistry and Biochemistry University of South Carolina	2000-present
Professor	Department of Chemistry and Biochemistry University of South Carolina	2000-present
Associate Professor	Department of Chemistry and Biochemistry University of South Carolina	1996-2000
Associate Professor	Department of Chemistry Massachusetts Institute of Technology	1994-1996
Assistant Professor	Department of Chemistry Massachusetts Institute of Technology	1989-1994
Postdoctoral Fellow	Department of Chemistry Northwestern University	1988-1989

CURRENT RESEARCH INTERESTS

Synthesis of new hierarchical wasteform materials for the effective immobilization of nuclear waste in persistent architectures

Crystal growth of new oxide materials

Crystal growth of new fluorides

Crystal growth of new chalcogenides

Synthesis of new, structurally complex, scintillator materials

Investigation of optical, electronic and magnetic properties of new materials

Cooperative structure-property relationships

We investigate the crystal growth of new materials, including new scintillating and luminescing oxides and fluorides, and new uranium and thorium containing structures. In the latter case, we synthesize new hierarchical wasteform materials for the effective immobilization of nuclear waste in persistent architectures.

SUMMARY OF SCIENTIFIC ACCOMPLISHMENTS

Funding:	Over \$30 Million in research funding to date
Publications:	Over 500 publications in peer reviewed journals to date.
Patents:	6
Citations:	Over 19,000 citations; h-index = 69.
Undergraduates:	Over 50 undergraduate researchers trained to date.
Graduate Students:	Over 40 graduate student researchers trained to date.
Postdocs:	Over 13 postdoctoral researchers trained to date.
Research Seminars	> 200

I. HONORS AND AWARDS

Furman University John Albert Southern Lecturer, **2019**.
Carolina Distinguished Professor, **2018-present**.
Breakthrough Leadership in Research Award, **2016-2017**.
Charles H. Stone Award, ACS Carolina Piedmont Section, **2016**.
South Carolina Governor's Award for Excellence in Scientific Research, **2016**.
University of South Carolina Trustee Professorship Award, **2012**.
Southern Chemist Award, ACS Memphis Section, **2011**.
Elected to the rank of Fellow of the American Chemical Society, **2011**.
Guest Researcher at NIMS, Tsukuba, Japan, **2010**.
Outstanding South Carolina Chemist, ACS South Carolina Section, **2010**.
Elected to the rank of Fellow of the AAAS, **2009**.
IPMI Henry J. Albert Award, **2009**.
Invited Professor, Universite d'Angers, France, **2008**.
University of South Carolina Educational Foundation Award for Research in Science, Mathematics and Engineering, **2006**.
Elected full member of Sigma Xi, **2006**.
Visiting Professor Sun Yat-sen University, **2004-2006, 2008-2011**.
Visiting Professor at the ICMCB-CNRS-Bordeaux, France, **2003**.
Guest Professor Shandong Normal University, **2001**.
David W. Robinson Palmetto Professorship, **2000-present**.
Visiting Professor at the Université de Picardie, Jules Verne, France, **1999**.
Exxon Award in Solid State Chemistry, **1994**.
Paul M. Cook Career Development Professorship, **1993**.
Camille & Henry Dreyfus New Faculty Award, **1989**.
Raychem Fellowship, **1987**.
Earle C. Anthony Fellowship, **1984-1985**.
Chemistry Fellowship, UC Berkeley, **1983-1984**.
Graduated Magna Cum Laude with Honors, Brown University, **1983**.
Elected to Sigma Xi, **1981**.

II. PROFESSIONAL ACTIVITIES

Candidate for Executive Committee of the ACS Division of Fluorine Chemistry, **2021**.

UofSC SRNL Steering Committee, **2021-present**.

Inaugural Member American Association to Advance Powder Diffraction, **2020-present**.

Editorial Board Member – Inorganics, **2020-present**.

Director, DOE-EFRC “Center for Hierarchical Waste Form Materials” Renewed: **2020-2024**.

Member CAS Return to Work Planning and Management Team – UofSC, **2020**.

Member Future Planning Group – Research Subcommittee – UofSC, **2020**.

Member Battelle-SRNL-UofSC Team: SRNL Planning Committee, **2020**.

External Reviewer for the Notre Dame Center for Sustainable Energy, **2020**.

Chair, SSMC/EPM subcommittee of the NSF-DMR Committee of Visitors (COV). (SSMC = Solid State and Materials Chemistry; EPM = Electronic and Photonic Materials), **2019**.

Guest Editor – Frontiers in Chemistry – Special issue on Flux Crystal Growth, **2019**.

Institutional Director, NSF EPSCoR Track-1, **2017-present**.

Member International Advisory Board *Materials Issues in Nuclear Waste Treatment and Disposal*, CIMTEC, **2017-2018**.

Member External Review Committee of Savannah River National Laboratory (SRNL), **2017**.

External Reviewer of the FSU Chemistry Department, **2017**.

Director, DOE-EFRC “Center for Hierarchical Waste Form Materials” **2016-2020**.

Member Assistant/Associate Dean’s Graduate Council, **2016-present**.

Member External Review Committee of Savannah River National Laboratory (SRNL), **2016**.

Editorial Board Member - Solid State Sciences, **2016-present**.

Member International Advisory Board of the MAPEX Center for Materials and Processes, University of Bremen, Germany, **2015 – present**.

Technical Sessions Chair, 2016 South East Regional Meeting of the American Chemical Society (SERMACS), **2015-2016**.

Chair, Solid State Chemistry Gordon Conference, **2014-2016**.

Vice Chair, Solid State Chemistry Gordon Conference, **2012-2014**.

Breakthrough Magazine – Editorial Advisory Board, **2011-2013**.

Participant, NSF Materials Genome Initiative Workshop, Dec. 13, **2012**.

Oak Ridge National Laboratory (ORNL) SNS/HFIR User Group Executive Committee, **2011-2014**.

Associate Editor, Journal of Alloys and Compounds, **2011-2014**.

ORNL Neutron Scattering Science Review Committee, **2010-present**.

Director, Powder X-ray Diffraction Facility, **2008-present**.

Editor, Journal of the South Carolina Academy of Science, **2008-2012**.

Faculty Fellow, Office of Research and Health Sciences, USC, **2007-2008**.

Leader of the Polymer Nanocomposites Group at USC, **2006-2008**.

President South Carolina Academy of Science, **2006-2007**.

President-elect South Carolina Academy of Science, **2005**.

Vice-President South Carolina Academy of Science, **2004**.

Member Users Executive Committee, Brookhaven National Laboratory (BNL), Center for Functional Nanomaterials, **2004-2006**.

Sabbatical at Brookhaven National Laboratory, BNL-National Synchrotron Light Source, **2003**.

Chair: Solid State Chemistry Subdivision, American Chemical Society (ACS), Division of Inorganic Chemistry, **2003-2004**.

Editorial Board Member – Journal of the South Carolina Academy of Science, **2002-2008**.

Co-organizer of the NSF Summer Program in Solid State Chemistry, **2001-2007**.

Councilor to the South Carolina Academy of Science, **2000-2004**.

Editorial Board Member - Journal of Alloys and Compounds, **1998-2011**.

Associate Editor for Journal of Solid State Chemistry, **1997-2022**.

Editorial Board Member - Solid State Ionics, **1997-2002**.

Section Editor for CHEMTRACTS -Inorganic Chemistry, **1997-2007**.

III. SCHOLARSHIP

A. Thesis

“Magnetic, Chemisorption and Infrared Studies of Ni/TiO₂: An Example of an Epifacial Reaction”

Ph.D. thesis completed May 1988.

Supervisor: Prof. Angy Stacy

Institution: UC Berkeley

B. Publications

Submitted

Masachchi, L. W., Keerthisinghe, N., Morrison, G., Berseneva, A. A., Smith, M. D., zur Loye, H.-C., “Crystal Growth and Magnetism of Transition Metal Pyrochlore Fluorides”, *Inorg. Chem.*, **2023**, submitted.

Rai, B. K., Bretana, A., Morrison, G., Greer, R., Gofryk, K., zur Loye, H.-C., “Magnetism of Binary Actinide Oxides: A Review”, *Rep. Prog. Phys.*, **2023**, submitted.

In Print

1. K. C. Park, P. Kittikhunnatham, J. Lim, G. C. Thaggard, Y. Liu, C. R. Martin, G. A. Leith, D. J. Toler, A. T. Ta, N. Birkner, I. Lehman-Andino, A. Hernandez-Jimenez, G. Morrison, J. W. Amoroso, H.-C. zur Loye, D. P. DiPrete, M. D. Smith, K. S. Brinkman, S. R. Phillpot, N. B. Shustova, “f-block MOFs: A Pathway to Heterometallic Transuranics” *Angew. Chem. Int. Ed. Engl.* **2023**, *62*, e202216349. *
2. Fu, N., Hu, J., Feng, Y., Morrison, G., zur Loye, H.-C., Hu, J., “Composition based oxidation state prediction of materials using deep learning language models”, *Adv. Sci.*, **2023**, accepted.
Fu, N., Hu, J., Feng, Y., Morrison, G., zur Loye, H.-C., Hu, J., “Composition based oxidation state prediction of materials using deep learning”, arXiv preprint arXiv:2211.15895, **2022**.
3. Keerthisinghe, N., Ayer, G. B., Smith, M. D., zur Loye, H.-C., “Mild Hydrothermal Crystal Growth of a Series of Ternary Hafnium Fluorides”, *Inorg. Chem.*, **2023**, accepted.
4. Morrison, G., Jones, V. G., Zamorano, K. P., Greedan, J. E., zur Loye, H.-C., “Flux Synthesis, UV-vis Absorbance, and Magnetism of Cesium Copper Silicates with an Isolated Super-super Exchange Spin Dimer in $\text{Cs}_6\text{Cu}_2\text{Si}_9\text{O}_{23}$ ”, *Inorg. Chem.*, **2023**, accepted.
5. Berseneva, A. A., zur Loye, H.-C., “Advances in Chalcogenide Crystal Growth: Flux and Solution Syntheses, and Approaches for Post-Synthetic Modifications”, *Cryst. Growth Design*, **2023**, accepted.
6. Morrison, G., Masachchi, L. W., Tisdale, H. B., Chang, T., Jones, V. G., Zamorano, K. P., Breton, L. S., Chen, Y.-S., zur Loye, H.-C., “Polymorphism in A_3MF_6 (A = Rb, Cs; M = Al, Ga) Grown using Mixed Halide Fluxes”, DOI:10.1039/d3dt00352c. *Dalton*, **2023**, *52*, 8425-8433.
7. Breton, L. S., Smith, M. D., zur Loye, H.-C., “Synthesis of Uranium Mixed Anion Compounds Synthesized using the Boron-Chalcogen Mixture Method: $\text{Ba}_6\text{Co}_6\text{U}_{0.91}\text{S}_{13.5}\text{O}_{0.5}$ and $\text{Ba}_{5.47}\text{K}_{0.53}\text{Zn}_6\text{US}_{13.5}\text{O}_{0.5}$ ”, DOI: 10.1016/j.solidstatesciences.2023.107207. *Solid State Sci.*, **2023**, *140*, 107207.
8. King, A. A., Breton, L. S., Morrison, G., Smith, M. D., Liang, M., Halasyamani, P. S., zur Loye, H.-C., “Crystal Structures and Property Measurements of Novel Rare Earth Magnesium Thiosilicates Synthesized via Flux Crystal Growth Utilizing the Boron Chalcogenide Mixture Method”, DOI:10.1021/acs.inorgchem.3c00708. *Inorg. Chem.*, **2023**, *62*, 7446-7452.
9. Deason, T. K., Hines, A. T., Morrison, G., Smith, M. D., Besmann, T. M., Mofrad, A. M., Fondeur, F. F., Lehman-Andino, I., Amoroso, J. W., DiPrete, D. P., zur Loye, H.-

- C., “Flux Crystal Growth of the Extended Structure Pu(V) Borate $\text{Na}_2(\text{PuO}_2)(\text{BO}_3)$ ”, DOI:10.1021/jacs.2c11355. *J. Am. Chem. Soc.*, **2023**, 145, 10007-10014. *
10. Usman, M., Christian, M., Smith, M. D., Besmann, T., zur Loye, H.-C., “DFT-Guided Flux Synthesis of a Family of Layered Titanates Crystallizing in the Lepidocrocite Structure Type”, DOI: 10.1016/j.solidstatesciences.2023.107161. *Solid State Sciences*, **2023**, 139, 107161.
 11. Berseneva, A. A., Klepov, V. V., Tisdale, H. B., zur Loye, H.-C., “Flux-assisted polytypism in the $[\text{Na}_2\text{Cl}]\text{GaQ}_2$ heterolayered salt-inclusion chalcogenide family”, DOI:10.1039/D3CE00074E. *CrystEngComm*, **2023**, 25, 2307-2312. *
 12. Hines, A. T., Morrison, G., Yabrough, B. J., Shustova, N. B., Jacobsohn, L. G., zur Loye, H.-C., “Luminescence of alkali rare earth borates $\text{A}_3\text{Ln}(\text{BO}_3)_2$ (A = Na, K; Ln = Eu, Tb)”, DOI:10.1016/j.solidstatesciences.2023.107130. *Solid State Sci.*, **2023**, 138, 107130.
 13. Berseneva, A. A., Masachchi, L. W., Jacobsohn, L. G., zur Loye, H.-C., “Tunable Salt-Inclusion Chalcogenides for Ion-exchange, Photoluminescence, and Scintillation”, DOI:10.1021/acs.chemmater.2c03592 *Chem. Mater.*, **2023**, 35, 1417-1431. *
 14. Deason, T. K., Morrison, G., Mofrad, A., Tisdale, H., Amoroso, J., DiPrete, D. P., Was, G., Sun, Kai; Besmann, T. M., zur Loye, H.-C., “Developing Waste Forms for the Transuranic Elements: Quaternary Neptunium Fluorides of the type $\text{Na}_x\text{MNP}_6\text{F}_{30}$ (M = Ti, V, Cr, Mn, Fe, Co, Ni, Al, Ga)”, DOI:10.1021/jacs.2c10669. *J. Am. Chem. Soc.*, **2023**, 145, 465-475. *
 15. Proust, V., Gossard, A., Schaeperkoetter, J., Vannier, S., David, T., Thomas, D., Barre, Y., Misture, S., Grandjean, A., zur Loye, H.-C., “Design and characterization of hierarchical aluminosilicate composite materials for Cs entrapment: ionic exchange efficiency tied to microstructure”, DOI:10.1016/j.jwpe.2022.103381 *J. Water Process.*, **2023**, 51, 103381.
 16. Park, K. C., Kittikhunnatham, P., Lim, J., Thaggard, G. C., Liu, Y., Martin, C. R., Leith, G. A., Toler, D. J., Ta, A. T., Birkner, N., Lehman-Andino, I., Hernandez-Jimenez, A., Morrison, G., Amoroso, J. W., zur Loye, H.-C., DiPrete, D. P., Smith, M. D., Brinkman, K. S., Phillipot, S. R., Shustova, N. B., “f-block MOFs: A Pathway to Heterometallic Transuranics”, DOI:10.1002/anie.202216349. *Angew. Chem.*, **2023**, 62, e202216349. *
 17. Li, Y., Hu, S., Montgomery, R., Grandjean, A., Besmann, T. M., zur Loye, H.-C., “Effect of Charge and Anisotropic Diffusivity on Ionic Exchange Kinetics in Nuclear Waste Form Materials”, DOI:10.1016/j.jnucmat.2022.154077. *J. Nuclear Mater.*, **2022**, 572, 154077.

18. Berseneva, A. A., Aziziha, M., Schorne-Pinto, J., Besmann, T. M., zur Loye, H.-C., “All-Inorganic Open-Framework Chalcogenides, $A_3Ga_5S_9 \cdot xH_2O$ ($A = Rb$ and Cs), Exhibiting Ultrafast Uranyl Remediation and Illustrating a Novel Post-Synthetic Preparation of Open-Framework Oxychalcogenides”, DOI:10.1021/acs.chemmater.2c02059. *Chem. Mater.*, **2022**, *34*, 8366-8378. *
19. Usman, M., Christian, M. S., Morrison, G., Smith, M. D., Zhang, W., Besmann, T. M., Halasyamani, P. S., zur Loye, H.-C., “Flux Crystal Growth of Rubidium-Iron Silicates and Germanates and their Ion-Exchange Using Alkali Nitrate Salts”, DOI:10.1016/j.solidstatesciences.2022.106995. *Solid State Sci.*, **2022**, 106995.
20. Berseneva, A. A., Klepov, V. V., Pal, K., Seeley, K., Koury, D., Schaeperkoetter, J., Wright, J., Misture, S. T., Kanatzidis, M. G., Wolverton, C., Gelis, A. V., zur Loye, H.-C., “Transuranium Sulfide via the Boron Chalcogen Mixture Method and Reversible Water Uptake in the $NaCuTS_3$ Family”, DOI:10.1021/jacs.2c04783. *J. Am. Chem. Soc.*, **2022**, *144*, 13773-13786. *
21. Breton, L. S., Baumbach, R., Tisdale, H. B., zur Loye, H.-C., “Structures and Magnetic Properties of $K_2Pd_4U_6S_{17}$, $K_2Pt_4U_6S_{17}$, $Rb_2Pt_4U_6S_{17}$, and $Cs_2Pt_4U_6S_{17}$ Synthesized using the Boron-Chalcogen Mixture Method”, DOI:10.1021/acs.inorgchem.2c01363. *Inorg. Chem.*, **2022**, *61*, 10502-10508. *
22. Hines, A. T., Morrison, G., Tisdale, H. B., Smith, M. D., Besmann, T. S., Mofrad, A., Sun, K., Was, G., zur Loye, H.-C., “Crystallization of $A_3Ln(BO_3)_2$ ($A = Na, K$; $Ln =$ lanthanide) from a Boric Acid Containing Hydroxide Melt: Synthesis and Investigation of Lanthanide Borates as Potential Nuclear Waste Forms”, DOI:10.1021/acs.inorgchem.2c01301. *Inorg. Chem.*, **2022**, *61*, 11232-11242. *
23. Breton, L. S., Morrison, G., Lacroix, M., R., Halasyamani, P.S., zur Loye, H.-C., “Lanthanide Thioborates, an Emerging Class of Nonlinear Optical Materials, Efficiently Synthesized Using the Boron-Chalcogen Mixture Method”, DOI:10.1039/D2CC01260J. *Chem. Commun.*, **2022**, *58*, 7992-7995. *
24. Carone, D., Klepov, V. V., Thompson, S. A. J., Hines, A. T., zur Loye, H.-C., “Luminescence and Scintillation in the Niobium Doped Oxyfluoride $Rb_4Ge_5O_9F_6:Nb$ ”, DOI:10.3390/inorganics10060083. *Inorganics*, **2022**, *10*, 83.
25. Novikov, S. A., Lu, Y., Zhang, W., Halasyamani, P. S., Hariyani, S., Brgoch, J., Klepov, V. V., zur Loye, H.-C., Mozharivskiy, Y., “Phosphorescence in Mn^{4+} -doped R^+ / R^{2+} germanates ($R^+ = Na^+$ or K^+ , $R^{2+} = Sr^{2+}$)”, DOI:10.1021/acs.inorgchem.2c01364. *Inorg. Chem.*, **2022**, *61*, 9364-9374.
26. Usman, M., Smith, M. D., zur Loye, H.-C., “A Complex Mayenite-Type Strontium Oxy-chloride Exhibiting Three-Component Site Mixing: $Sr_{12}Al_{3.44}Fe_{8.16}Ge_{2.38}O_{32}Cl_{14.34}$ ”, DOI:10.1016/j.jssc.2022.123285. *J. Solid State Chem.*, **2022**, *313*, 123285.

27. Aslani, C. K., Klepov, V. V., zur Loye, H.-C., “Hydrothermal Synthesis of new Mixed-Oxoanion Materials: Rare Earth Iodate Sulfates $\text{Sm}(\text{IO}_3)(\text{SO}_4)$ and $\text{Ln}_2(\text{IO}_3)_3(\text{SO}_4)\text{OH}\cdot 3\text{H}_2\text{O}$ ($\text{Ln} = \text{Sm}, \text{Eu}, \text{Dy}$)”, DOI:10.1016/j.solidstatesciences.2022.106918. *Solid State Sci.*, **2022**, *129*, 106918.
28. Tisdale, H., Christian, M. S., Morrison, G., Besmann, T. M., Sun, K., Was, G., zur Loye, H.-C., “Investigation of Rare Earth Containing Double Phosphates of the Type $\text{A}_3\text{Ln}(\text{PO}_4)_2$ ($\text{Ln} = \text{Y}, \text{La}, \text{Pr}, \text{Nd}, \text{Sm-Lu}$) as Potential Nuclear Waste Forms”, DOI:10.1021/acs.chemmater.2c00326. *Chem. Mater.*, **2022**, *34*, 3819-3830. *
29. Carone, D., Morrison, G., Smith, M. D., zur Loye, H.-C., “Crystal Growth of New Germanate framework structures: Impact of the presence of square planar copper species and mixed Ge/Mn sites on the overall structures of $\text{Rb}_2\text{Cu}_3\text{Ge}_5\text{O}_{14}$, $\text{Cs}_2\text{Cu}_3\text{Ge}_5\text{O}_{14}$, $\text{Cs}_7\text{Cu}_2\text{Ge}_{11}\text{O}_{27}\text{F}$, and $[(\text{Cs}_6\text{F})(\text{Cs}_3\text{AgF})][\text{Ge}_{12}\text{Mn}_2\text{O}_{32}]$ ”, DOI:10.1021/acs.cgd.2c00133. *Cryst. Growth Design*, **2022**, *22*, 3319-3325.
30. Carone, D., Jacobsohn, L. G., Breton, L. S., zur Loye, H.-C., “Synthesis, structure, and scintillation of $\text{Rb}_4\text{Ta}_2\text{Si}_8\text{O}_{23}$ ” DOI:10.1016/j.solidstatesciences.2022.106861. *Solid State Sci.*, **2022**, *127*, 106861.
31. Hines, A. T., Morrison, G., Smith, M. D., zur Loye, H.-C., “Solvothermal Synthesis of $\text{BiCuI}_5(\text{phen})_2$, a Novel Metal-Organic Halobismuthate”, DOI:10.1007/s10870-022-00932-6. *J. Chem. Cryst.*, **2022**, *52*, 394-398.
32. Ayer, G., Morrison, G., Smith, M., Jacobsohn, zur Loye, H.-C., “Luminescence and Scintillation of $[\text{Nb}_2\text{O}_2\text{F}_9]^{3-}$ dimer Containing Oxide-Fluorides: $\text{Cs}_{10}(\text{Nb}_2\text{O}_2\text{F}_9)_3\text{F}$, $\text{Cs}_{9.4}\text{K}_{0.6}(\text{Nb}_2\text{O}_2\text{F}_9)_3\text{F}$, and $\text{Cs}_{10}(\text{Nb}_2\text{O}_2\text{F}_9)_3\text{Cl}$ ”, DOI:10.1021/acs.inorgchem.1c03787. *Inorg. Chem.*, **2022**, *61*, 3256-3262.
33. Morrison, G. zur Loye, H.-C., “Uranyl titanate silicates: Syntheses, structures, and family relations”, DOI:10.1021/acs.cgd.1c01180. *Cryst. Growth Design*, **2022**, *22*, 1221-1228.
34. Keerthisinghe, N., Christian, M. S., Berseneva, A. A., Morrison, G., Klepov, V. V., Smith, M. D., zur Loye, H.-C., “Investigation of Metastable Low Dimensional Halometallates”, DOI:10.3390/molecules27010280. *Molecules*, **2022**, *27*, 280.
35. Ayer, G. B., Smith, M. D., Jacobsohn, L. G., Morrison, G., Breton, L. S., Zhang, W., Halasyamani, P. S., zur Loye, H.-C., “Synthesis of Hydrated Ternary Lanthanide-Containing Chlorides Exhibiting X-ray Scintillation and Luminescence”, DOI:10.1021/acs.inorgchem.1c02004. *Inorg. Chem.*, **2021**, *60*, 15371-15382.
36. Keerthisinghe, N., Berseneva, A. A., Klepov, V. V., Morrison, G., zur Loye, H.-C., “A Geometrically Frustrated Family of $\text{M}^{\text{II}}\text{M}^{\text{III}}\text{F}_5(\text{H}_2\text{O})_2$ Mixed-Metal Fluorides with Complex Magnetic Interactions”, DOI:10.1021/acs.inorgchem.1c01889. *Inorg. Chem.*,

2021, *60*, 14318-14329.

37. Glaser, P., Steward, O., Atif, R., Asuigui, D. R., Swanson, J., Biacchi, A., Hight Walker, A., Morrison, G., zur Loye, H.-C., Stoll, S., “Synthesis of Mixed-Valent Lanthanide Sulfide Nanoparticles”, DOI:10.1002/anie.202108993. *Angew. Chem. Int. Ed.* **2021**, *60*, 23134-23141.
38. Christian, M., Pace, K. A., Klepov, V. V., Morrison, G., zur Loye, H.-C., Besmann, T., “A New Database Approach for Discovery of Novel Actinide Waste Forms”, DOI:10.1021/acs.cgd.1c00494. *Cryst. Growth Design*, **2021**, *21*, 5100-5107.
39. Klepov, V. V., Pace, K. A., Berseneva, A. A., Felder, J. B., Calder, S., Morrison, G., Zhang, Q., Kirkham, M. J., Parker, D. S., zur Loye, H.-C., “Chloride Reduction of Mn^{3+} in Mild Hydrothermal Synthesis of a Charge Ordered Defect Pyrochlore, $CsMn^{2+}Mn^{3+}F_6$, a Canted Antiferromagnet with a Hard Ferromagnetic Component”, DOI:10.1021/jacs.1c04245. *J. Am. Chem. Soc.*, **2021**, *143*, 11554-11567.
40. DeVore II, M. A., Villa-Aleman, E., Felder, J. B., Yeon, J., zur Loye, H.-C., Wellons, M. S., “Vibrational Spectroscopy of Uranium Tetrafluoride Hydrates”, DOI:10.1016/j.vibspec.2021.103277. *Vibrational Spectroscopy*, **2021**, *115*, 103277.
41. Kutahyali Aslani, C., Klepov, V. V., Aslani, M. A. A., zur Loye, H.-C., “Hydrothermal Synthesis of new Iodates $Ln_2(IO_3)_3(IO_4)$ ($Ln=La, Nd, Pr$) Containing the Tetraoxoiodate(V) Anion: Creation of Luminescence Properties by Doping with Eu, Dy, Tb”, DOI: 10.1021/acs.cgd.1c00545. *Cryst. Growth Design*, **2021**, *21*, 4707-4712.
42. Breton, L. S., Smith, M. D., zur Loye, H.-C., “Trends in Rare Earth Thiophosphate Syntheses: $Rb_3Ln(PS_4)_2$ ($Ln = La, Pr, Ce$), $Rb_{3-x}Na_xLn(PS_4)_2$ ($Ln = Pr, Ce; x = 0.50, 0.55$), and $RbEuPS_4$ Obtained by Molten Flux Crystal Growth”, DOI:10.1039/D1CE00703C. *CrystEngComm*, **2021**, *23*, 5241-5248.
43. Ferreira, T., Calder, S., Parker, D. S., Athena, S. S., zur Loye, H.-C., “Relationship between A-site cation and magnetic structure in 3d-5d-4f double perovskite iridates Ln_2NiIrO_6 ($Ln = La, Pr, Nd$)”, DOI:10.1103/PhysRevMaterials.5.064408. *Physical Review Materials*, **2021**, *5*, 064408.
44. Morrison, G., Pace, K. A., zur Loye, H.-C., “Mild Hydrothermal Synthesis of Potassium Uranyl Phosphates with Layered and Framework Structures”, DOI:10.1016/j.jssc.2021.122293. *J. Solid State Chem.*, **2021**, *301*, 122293.
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C. Patents and Invention Disclosures

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