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Education and Training:

Johns Hopkins University, Baltimore, MD	Ph.D.	2010	Materials Science
Tsinghua University, Beijing, China	M.S.	2005	Physics
Tsinghua University, Beijing, China	B.S.	2002	Electronic Engineering

Professional Experience:

2014-present Neutron Scattering Scientist, Oak Ridge National Laboratory
2011-2014 Clifford G. Shull Fellow, Oak Ridge National Laboratory
2010-2011 Postdoc, Johns Hopkins University

Professional Honors, Awards:

Outstanding Staff Service Award, Oak Ridge National Laboratory, 2021
Clifford G. Shull Fellowship, Oak Ridge National Laboratory, 2011
Wolman Fellow of Whiting School of Engineering, Johns Hopkins University, 2006

Scientific Activities

Reviewer:

Nature Materials, Nature Communications, Physical Review Letters, Physical Review B, Physical Review E, Physical Review Materials, Applied Physics Letters, Journal of Materials Chemistry A, Acta Materialia, Scripta Materialia, Journal of Applied Physics, Journal of Physics and Chemistry of Solids, Modelling and Simulation in Materials Science and Engineering, Intermetallics, Journal of Alloys and Compounds, Journal of Materials Science, Metallurgical and Materials Transactions A, Philosophical Magazine, Physica A, etc.

Organizer:

Workshop: Tutorial on modern modeling methods in neutron spectroscopy, April 2019
Workshop: Atomistic modeling on neutron scattering, June 2017

PI:

LDRD: Atomistic modeling and machine learning for neutrons, FY21-23
LDRD: Hyperspectral Compressive neutrOn Lensless (HyperCOOL) Imaging with VISION, FY18-19

Co-PI:

LDRD: Containerized, heterogenous software environment for Neutron Scattering Data Analysis, Interpretation and Automation, FY20-22
LDRD: ICE-MAN, the Integrated Computational Environment-Modeling & Analysis for Neutrons, FY17-19
LDRD: Virtual Experiments in Neutron Spectroscopy, FY16-17
LDRD: An Integrated Approach to the Design and Discovery of Fast Ionic Conducting Materials, FY15-17

Publications [(1-174)]

Google Scholar: https://scholar.google.com/citations?user=pV_StB0AAAAAJ&hl=en
As of 10/19/2021, total publications: 174; total citations: 12723; h-index: 51

1. Zuo T, Cheng Y, Chen P, Gao Z, Zhang Y, Liaw PK. Structural and magnetic transitions of CoFeMnNiAl high-entropy alloys caused by composition and annealing. *Intermetallics*. 2021;137.
2. Zheng Q, Feng T, Hachtel JA, Ishikawa R, Cheng Y, Daemen L, et al. Direct visualization of anionic electrons in an electride reveals inhomogeneities. *Science Advances*. 2021;7(15).
3. Zhang J, Cheng Y, Kolesnikov AI, Bernholc J, Lu W, Ramirez-Cuesta AJ. Study of anharmonicity in zirconium hydrides using inelastic neutron scattering and ab-initio computer modeling. *Inorganics*. 2021;9(5).
4. Yang G, Li X, Cheng Y, Wang M, Ma D, Sokolov AP, et al. Distilling nanoscale heterogeneity of amorphous silicon using tip-enhanced Raman spectroscopy (TERS) via multiresolution manifold learning. *Nature Communications*. 2021;12(1).
5. Ramirez-Cuesta AJ, Cheng YQ. The ICEMAN, a heterogeneous platform for analysis of neutron scattering data. *Neutron News*. 2021;32(1):15-6.
6. Nikolic M, Daemen L, Ramirez-Cuesta AJ, Xicohtencatl RB, Cheng Y, Putnam ST, et al. Neutron Insights into Sorption Enhanced Methanol Catalysis. *Topics in Catalysis*. 2021;64(9-12):638-43.
7. Moura NS, Bajgiran KR, Roman CL, Daemen L, Cheng Y, Lawrence J, et al. Catalytic Enhancement of Inductively Heated Fe₃O₄ Nanoparticles by Removal of Surface Ligands. *ChemSusChem*. 2021;14(4):1122-30.
8. Moon J, Cheng Y, Daemen L, Novak E, Ramirez-Cuesta AJ, Wu Z. On the Structural Transformation of Ni/BaH₂ During a N₂-H₂ Chemical Looping Process for Ammonia Synthesis: A Joint In Situ Inelastic Neutron Scattering and First-Principles Simulation Study. *Topics in Catalysis*. 2021;64(9-12):685-92.
9. Marsh C, Han X, Li J, Lu Z, Argent SP, Da Silva I, et al. Exceptional Packing Density of Ammonia in a Dual-Functionalized Metal-Organic Framework. *Journal of the American Chemical Society*. 2021;143(17):6586-92.
10. Mamontov E, Cheng Y, Daemen LL, Kolesnikov AI, Ramirez-Cuesta AJ, Ryder MR, et al. Low rotational barriers for the most dynamically active methyl groups in the proposed antiviral drugs for treatment of SARS-CoV-2, apilimod and tetrandrine. *Chemical Physics Letters*. 2021;777.
11. Ma Y, Han X, Xu S, Wang Z, Li W, Da Silva I, et al. Atomically Dispersed Copper Sites in a Metal-Organic Framework for Reduction of Nitrogen Dioxide. *Journal of the American Chemical Society*. 2021;143(29):10977-85.
12. Liu X, Garcia-Mendez R, Lupini AR, Cheng Y, Hood ZD, Han F, et al. Local electronic structure variation resulting in Li 'filament' formation within solid electrolytes. *Nature Materials*. 2021.
13. Liu S, Han X, Chai Y, Wu G, Li W, Li J, et al. Efficient Separation of Acetylene and Carbon Dioxide in a Decorated Zeolite. *Angewandte Chemie - International Edition*. 2021;60(12):6526-32.
14. Lin L, Fan M, Sheveleva AM, Han X, Tang Z, Carter JH, et al. Control of zeolite microenvironment for propene synthesis from methanol. *Nature Communications*. 2021;12(1).

15. Li J, Han X, Kang X, Chen Y, Xu S, Smith GL, et al. Purification of Propylene and Ethylene by a Robust Metal–Organic Framework Mediated by Host–Guest Interactions. *Angewandte Chemie - International Edition*. 2021;60(28):15541-7.
16. Larsen GS, Cheng Y, Daemen LL, Lamichhane TN, Hensley DK, Hong K, et al. Polymer, Additives, and Processing Effects on N95 Filter Performance. *ACS Applied Polymer Materials*. 2021;3(2):1022-31.
17. Hanus R, George J, Wood M, Bonkowski A, Cheng Y, Abernathy DL, et al. Uncovering design principles for amorphous-like heat conduction using two-channel lattice dynamics. *Materials Today Physics*. 2021;18.
18. Han X, Lu W, Chen Y, Da Silva I, Li J, Lin L, et al. High Ammonia Adsorption in MFM-300 Materials: Dynamics and Charge Transfer in Host-Guest Binding. *Journal of the American Chemical Society*. 2021;143(8):3153-61.
19. de Falco G, Florent M, Jagiello J, Cheng Y, Daemen LL, Ramirez-Cuesta AJ, et al. Alternative view of oxygen reduction on porous carbon electrocatalysts: the substance of complex oxygen-surface interactions. *iScience*. 2021;24(3).
20. Chapman CW, Ramić K, Hu X, Brown JM, Arbanas G, Kolesnikov AI, et al. Thermal neutron scattering measurements and modeling of yttrium-hydrides for high temperature moderator applications. *Annals of Nuclear Energy*. 2021;157.
21. Bone AN, Widener CN, Moseley DH, Liu Z, Lu Z, Cheng Y, et al. Applying Unconventional Spectroscopies to the Single-Molecule Magnets, $\text{Co}(\text{PPh}_3)_2\text{X}_2$ (X=Cl, Br, I): Unveiling Magnetic Transitions and Spin-Phonon Coupling. *Chemistry - A European Journal*. 2021;27(43):11110-25.
22. Billeter E, Sterzi A, Sambalova O, Wick-Joliat R, Grazioli C, Coreno M, et al. Hydrogen in tungsten trioxide by membrane photoemission and density functional theory modeling. *Physical Review B*. 2021;103(20).
23. Al-Qasir II, Cheng Y, Lin JYY, Campbell AA, Sala G, Ramić K, et al. Neutron thermalization in nuclear graphite: A modern story of a classic moderator. *Annals of Nuclear Energy*. 2021;161.
24. Zhang L, Zhang X, Qian K, Li Z, Cheng Y, Daemen LL, et al. Activation and surface reactions of CO and H₂ on ZnO powders and nanoplates under CO hydrogenation reaction conditions. *Journal of Energy Chemistry*. 2020;50:351-7.
25. Yoshida HK, Dissanayake SE, Christianson AD, Dela Cruz CR, Cheng YQ, Okamoto S, et al. Static and dynamic spin properties in the quantum triangular lattice antiferromagnet Ag_2CoO_2 . *Physical Review B*. 2020;102(2).
26. Xiang Y, Li X, Cheng Y, Sun X, Yang Y. Advanced characterization techniques for solid state lithium battery research. *Materials Today*. 2020;36:139-57.
27. Wu P, Tan S, Moon J, Yan Z, Fung V, Li N, et al. Harnessing strong metal–support interactions via a reverse route. *Nature Communications*. 2020;11(1).
28. Wang J, Dolyniuk JA, Krenkel EH, Niedziela JL, Tanatar MA, Timmons EI, et al. Clathrate BaNi_2P_4 : An Interplay of Heat and Charge Transport Due to Strong Host-Guest Interactions. *Chemistry of Materials*. 2020;32(18):7932-40.
29. Moseley DH, Th+–baud SJ, Lindsay LR, Cheng Y, Abernathy DL, Manley ME, et al. Temperature-dependent lattice dynamics in iridium. *Physical Review Materials*. 2020;4(11).
30. Moseley DH, Stavretis SE, Zhu Z, Guo M, Brown CM, Ozerov M, et al. Inter-Kramers Transitions and Spin-Phonon Couplings in a Lanthanide-Based Single-Molecule Magnet. *Inorganic Chemistry*. 2020;59(7):5218-30.
31. Moon J, Cheng Y, Daemen LL, Li M, Polo-Garzon F, Ramirez-Cuesta AJ, et al. Discriminating the Role of Surface Hydride and Hydroxyl for Acetylene Semihydrogenation over Ceria through in Situ Neutron and Infrared Spectroscopy. *ACS Catalysis*. 2020;10(9):5278-87.

32. Mamontov E, Cheng Y, Daemen LL, Kolesnikov AI, Ramirez-Cuesta AJ, Ryder MR, et al. Hydration-Induced Disorder Lowers the Energy Barriers for Methyl Rotation in Drug Molecules. *Journal of Physical Chemistry Letters*. 2020;11(23):10256-61.
33. Mamontov E, Cheng Y, Daemen LL, Keum JK, Kolesnikov AI, Pajerowski D, et al. Effect of Hydration on the Molecular Dynamics of Hydroxychloroquine Sulfate. *ACS Omega*. 2020;5(33):21231-40.
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35. Li X, Wang J, Bai N, Zhang X, Han X, da Silva I, et al. Refinement of pore size at sub-angstrom precision in robust metal-organic frameworks for separation of xylenes. *Nature Communications*. 2020;11(1).
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37. Kammert J, Moon J, Cheng Y, Daemen L, Irle S, Fung V, et al. Nature of Reactive Hydrogen for Ammonia Synthesis over a Ru/C12A7 Electride Catalyst. *Journal of the American Chemical Society*. 2020;142(16):7655-67.
38. Jafari A, Klobes B, Sergueev I, Moseley DH, Manley ME, Dronskowski R, et al. Phonon Spectroscopy in Antimony and Tellurium Oxides. *Journal of Physical Chemistry A*. 2020;124(39):7869-80.
39. Hood ZD, Cheng Y, Evans SF, Adhikari SP, Parans Paranthaman M. Unraveling the structural properties and dynamics of sulfonated solid acid carbon catalysts with neutron vibrational spectroscopy. *Catalysis Today*. 2020;358:387-93.
40. Duong TD, Sapchenko SA, da Silva I, Godfrey HGW, Cheng Y, Daemen LL, et al. Observation of binding of carbon dioxide to nitro-decorated metal-organic frameworks. *Chemical Science*. 2020;11(20):5339-46.
41. Dajnowicz S, Cheng Y, Daemen LL, Weiss KL, Gerlits O, Mueser TC, et al. Substrate Binding Stiffens Aspartate Aminotransferase by Altering the Enzyme Picosecond Vibrational Dynamics. *ACS Omega*. 2020;5(30):18787-97.
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43. Cheng YQ, Ramirez-Cuesta AJ. Calculation of the Thermal Neutron Scattering Cross-Section of Solids Using OCLIMAX. *Journal of Chemical Theory and Computation*. 2020;16(8):5212-7.
44. Cheng YQ, Kolesnikov AI, Ramirez-Cuesta AJ. Simulation of Inelastic Neutron Scattering Spectra Directly from Molecular Dynamics Trajectories. *Journal of Chemical Theory and Computation*. 2020;16(12):7702-8.
45. Chapman CW, Hu X, Brown J, Arbanas G, Kolesnikov AI, Cheng Y, et al., editors. Thermal neutron scattering measurements of YHx for the transformational challenge reactor. *Transactions of the American Nuclear Society*; 2020.
46. Chai Y, Han X, Li W, Liu S, Yao S, Wang C, et al. Control of zeolite pore interior for chemoselective alkyne/olefin separations. *Science*. 2020;368(6494):1002-6.
47. Borgschulte A, Terreni J, Billeter E, Daemen L, Cheng Y, Pandey A, et al. Inelastic neutron scattering evidence for anomalous H-H distances in metal hydrides. *Proceedings of the National Academy of Sciences of the United States of America*. 2020;117(8):4021-6.
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50. Wu L, Evans SF, Cheng Y, Navrotsky A, Moyer BA, Harrison S, et al. Neutron Spectroscopic and Thermochemical Characterization of Lithium-Aluminum-Layered Double Hydroxide Chloride: Implications for Lithium Recovery. *Journal of Physical Chemistry C*. 2019;123(34):20723-9.
51. Stavretis SE, Moseley DH, Fei F, Cui HH, Cheng Y, Podlesnyak AA, et al. Spectroscopic Studies of the Magnetic Excitation and Spin-Phonon Couplings in a Single-Molecule Magnet. *Chemistry - A European Journal*. 2019;25(69):15846-57.
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55. Sato T, Daemen LL, Cheng Y, Ramirez-Cuesta AJ, Ikeda K, Aoki T, et al. Hydrogen-Release Reaction of a Complex Transition Metal Hydride with Covalently Bound Hydrogen and Hydride Ions. *ChemPhysChem*. 2019;20(10):1392-7.
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63. Liu X, Chen Y, Hood ZD, Ma C, Yu S, Sharafi A, et al. Elucidating the mobility of H⁺ and Li⁺ ions in (Li_{6.25}: XH_xAl_{0.25})La₃Zr₂₀12 via correlative neutron and electron spectroscopy. *Energy and Environmental Science*. 2019;12(3):945-51.
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