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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

Organizer:

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

Lecturer:

National School on Neutron and X-Ray Scattering, since 2018

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 [1-188]

Google Scholar: https://scholar.google.com/citations?user=pV_StB0AAAAAJ&hl=en
As of 7/27/2022, total publications: 188; total citations: 14826; h-index: 54

1. Schneeloch, J. A.; Tao, Y.; Cheng, Y.; Daemen, L.; Xu, G.; Zhang, Q.; Louca, D., Gapless Dirac magnons in CrCl₃. *npj Quantum Materials* **2022**, 7 (1).
2. Novak, E.; Daemen, L.; Ramirez-Cuesta, A. J.; Cheng, Y.; Smith, R.; Egami, T.; Jalarvo, N., Uncovering the hydride ion diffusion pathway in barium hydride via neutron spectroscopy. *Scientific Reports* **2022**, 12 (1).
3. Cladek, B. R.; Ramirez-Cuesta, A. J.; Everett, S. M.; McDonnell, M. T.; Daemen, L.; Cheng, Y.; Brant Carvalho, P. H. B.; Tulk, C.; Tucker, M. G.; Keffer, D. J.; Rawn, C. J., In situ inelastic neutron scattering of mixed CH₄-CO₂ hydrates. *Fuel* **2022**, 327.
4. Chen, J.; Mei, Q.; Chen, Y.; Marsh, C.; An, B.; Han, X.; Silverwood, I. P.; Li, M.; Cheng, Y.; He, M.; Chen, X.; Li, W.; Kippax-Jones, M.; Crawshaw, D.; Frogley, M. D.; Day, S. J.; García-Sakai, V.; Manuel, P.; Ramirez-Cuesta, A. J.; Yang, S.; Schröder, M., Highly Efficient Proton Conduction in the Metal-Organic Framework Material MFM-300(Cr)-SO₄(H₃O)₂. *Journal of the American Chemical Society* **2022**, 144 (27), 11969-11974.
5. Drake, H. F.; Xiao, Z.; Day, G. S.; Vali, S. W.; Daemen, L. L.; Cheng, Y.; Cai, P.; Kuszynski, J. E.; Lin, H.; Zhou, H. C.; Ryder, M. R., Influence of Metal Identity on Light-Induced Switchable Adsorption in Azobenzene-Based Metal-Organic Frameworks. *ACS Applied Materials and Interfaces* **2022**, 14 (9), 11192-11199.
6. Mu, S.; Dixit, K. D.; Wang, X.; Abernathy, D. L.; Cao, H.; Nagler, S. E.; Yan, J.; Lampen-Kelley, P.; Mandrus, D.; Polanco, C. A.; Liang, L.; Halász, G. B.; Cheng, Y.; Banerjee, A.; Berlijn, T., Role of the third dimension in searching for Majorana fermions in α -RuCl₃ via phonons. *Physical Review Research* **2022**, 4 (1).
7. Klein, R. A.; Balderas-Xicohténcatl, R.; Maehlen, J. P.; Udovic, T. J.; Brown, C. M.; Delaplane, R.; Cheng, Y.; Denys, R. V.; Ramirez-Cuesta, A. J.; Yartys, V. A., Neutron vibrational spectroscopic evidence for short H-H contacts in the RNiInH_{1.4}; 1.6 (R = Ce, La) metal hydride. *Journal of Alloys and Compounds* **2022**, 894.
8. Kneller, D. W.; Gerlits, O.; Daemen, L. L.; Pavlova, A.; Gumbart, J. C.; Cheng, Y.; Kovalevsky, A., Joint neutron/molecular dynamics vibrational spectroscopy reveals softening of HIV-1 protease upon binding of a tight inhibitor. *Physical Chemistry Chemical Physics* **2022**, 24 (6), 3586-3597.
9. Albers, P. W.; Leich, V.; Ramirez-Cuesta, A. J.; Cheng, Y.; Hömig, J.; Parker, S. F., The characterisation of commercial 2D carbons: graphene, graphene oxide and reduced graphene oxide. *Materials Advances* **2022**, 3 (6), 2810-2826.
10. Ma, Y.; Lu, W.; Han, X.; Chen, Y.; Da Silva, I.; Lee, D.; Sheveleva, A. M.; Wang, Z.; Li, J.; Li, W.; Fan, M.; Xu, S.; Tuna, F.; McInnes, E. J. L.; Cheng, Y.; Rudić, S.; Manuel, P.; Frogley, M. D.; Ramirez-Cuesta, A. J.; Schröder, M.; Yang, S., Direct Observation of Ammonia Storage in UiO-66 Incorporating Cu(II) Binding Sites. *Journal of the American Chemical Society* **2022**.
11. Guo, L.; Han, X.; Ma, Y.; Li, J.; Lu, W.; Li, W.; Lee, D.; da Silva, I.; Cheng, Y.; Rudić, S.; Manuel, P.; Frogley, M. D.; Ramirez-Cuesta, A. J.; Schröder, M.; Yang, S., High capacity ammonia adsorption in a robust metal-organic framework mediated by reversible host-guest interactions. *Chemical Communications* **2022**.
12. Klein, R. A.; Balderas-Xicohténcatl, R.; Maehlen, J. P.; Udovic, T. J.; Brown, C. M.; Delaplane, R.; Cheng, Y.; Denys, R. V.; Ramirez-Cuesta, A. J.; Yartys, V. A., Neutron

Vibrational Spectroscopic Evidence for Short H-H Contacts in the RNiInH_{1.4};1.6 (R = Ce, La) Metal Hydride. *Neutron News* **2022**, 33 (2), 7-9.

13. Brubaker, Z. E.; Miskowicz, A.; Cheng, Y. Q.; Daemen, L.; Niedziela, J. L., Inelastic neutron spectra of polyacrylonitrile-based carbon fibers. *Physical Review Materials* **2022**, 6 (1).
14. Lin, L.; Fan, M.; Sheveleva, A. M.; Han, X.; Tang, Z.; Carter, J. H.; da Silva, I.; Parlett, C. M. A.; Tuna, F.; McInnes, E. J. L.; Sastre, G.; Rudić, S.; Cavaye, H.; Parker, S. F.; Cheng, Y.; Daemen, L. L.; Ramirez-Cuesta, A. J.; Attfield, M. P.; Liu, Y.; Tang, C. C.; Han, B.; Yang, S., Control of zeolite microenvironment for propene synthesis from methanol. *Nature Communications* **2021**, 12 (1).
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16. Yu, L.; Han, X.; Wang, H.; Ullah, S.; Xia, Q.; Li, W.; Li, J.; Da Silva, I.; Manuel, P.; Rudić, S.; Cheng, Y.; Yang, S.; Thonhauser, T.; Li, J., Pore Distortion in a Metal-Organic Framework for Regulated Separation of Propane and Propylene. *Journal of the American Chemical Society* **2021**, 143 (46), 19300-19305.
17. Juneja, R.; Thébaud, S.; Pandey, T.; Polanco, C. A.; Moseley, D. H.; Manley, M. E.; Cheng, Y. Q.; Winn, B.; Abernathy, D. L.; Hermann, R. P.; Lindsay, L., Quasiparticle twist dynamics in non-symmorphic materials. *Materials Today Physics* **2021**, 21.
18. Liu, X.; Garcia-Mendez, R.; Lupini, A. R.; Cheng, Y.; Hood, Z. D.; Han, F.; Sharafi, A.; Idrobo, J. C.; Dudney, N. J.; Wang, C.; Ma, C.; Sakamoto, J.; Chi, M., Local electronic structure variation resulting in Li 'filament' formation within solid electrolytes. *Nature Materials* **2021**, 20 (11), 1485-1490.
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20. Al-Qasir, I. I.; Cheng, Y.; Lin, J. Y. Y.; Campbell, A. A.; Sala, G.; Ramic, K.; Islam, F. F.; Qteish, A.; Marsden, B.; Abernathy, D. L.; Stone, M. B., Neutron thermalization in nuclear graphite: A modern story of a classic moderator. *Annals of Nuclear Energy* **2021**, 161.
21. Mamontov, E.; Cheng, Y.; Daemen, L. L.; Kolesnikov, A. I.; Ramirez-Cuesta, A. J.; Ryder, M. R.; Stone, M. B., 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.
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23. Nikolic, M.; Daemen, L.; Ramirez-Cuesta, A. J.; Xicohtencatl, R. B.; Cheng, Y.; Putnam, S. T.; Stadie, N. P.; Liu, X.; Terreni, J.; Borgschulte, A., Neutron Insights into Sorption Enhanced Methanol Catalysis. *Topics in Catalysis* **2021**, 64 (9-12), 638-643.
24. Moon, J.; Cheng, Y.; Daemen, L.; Novak, E.; Ramirez-Cuesta, A. J.; 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), 685-692.
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27. Chapman, C. W.; Ramić, K.; Hu, X.; Brown, J. M.; Arbanas, G.; Kolesnikov, A. I.; Abernathy, D. L.; Daemen, L.; Ramirez-Cuesta, A. T. J.; Cheng, Y.; Stone, M. B.; Liu, L. E.; Danon, Y., Thermal neutron scattering measurements and modeling of yttrium-hydrides for high temperature moderator applications. *Annals of Nuclear Energy* **2021**, *157*.
28. Billeter, E.; Sterzi, A.; Sambalova, O.; Wick-Joliat, R.; Grazioli, C.; Coreno, M.; Cheng, Y.; Ramirez-Cuesta, A. J.; Borgschulte, A., Hydrogen in tungsten trioxide by membrane photoemission and density functional theory modeling. *Physical Review B* **2021**, *103* (20).
29. Marsh, C.; Han, X.; Li, J.; Lu, Z.; Argent, S. P.; Da Silva, I.; Cheng, Y.; Daemen, L. L.; Ramirez-Cuesta, A. J.; Thompson, S. P.; Blake, A. J.; Yang, S.; Schröder, M., Exceptional Packing Density of Ammonia in a Dual-Functionalized Metal-Organic Framework. *Journal of the American Chemical Society* **2021**, *143* (17), 6586-6592.
30. Hanus, R.; George, J.; Wood, M.; Bonkowski, A.; Cheng, Y.; Abernathy, D. L.; Manley, M. E.; Hautier, G.; Snyder, G. J.; Hermann, R. P., Uncovering design principles for amorphous-like heat conduction using two-channel lattice dynamics. *Materials Today Physics* **2021**, *18*.
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32. de Falco, G.; Florent, M.; Jagiello, J.; Cheng, Y.; Daemen, L. L.; Ramirez-Cuesta, A. J.; Badosz, T. J., Alternative view of oxygen reduction on porous carbon electrocatalysts: the substance of complex oxygen-surface interactions. *iScience* **2021**, *24* (3).
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36. Larsen, G. S.; Cheng, Y.; Daemen, L. L.; Lamichhane, T. N.; Hensley, D. K.; Hong, K.; Meyer, H. M.; Monaco, S. J.; Levine, A. M.; Lee, R. J.; Betters, E.; Sitzlar, K.; Heineman, J.; West, J.; Lloyd, P.; Kunc, V.; Love, L.; Theodore, M.; Paranthaman, M. P., Polymer, Additives, and Processing Effects on N95 Filter Performance. *ACS Applied Polymer Materials* **2021**, *3* (2), 1022-1031.
37. Zhang, J.; Cheng, Y.; Kolesnikov, A. I.; Bernholc, J.; Lu, W.; Ramirez-Cuesta, A. J., Study of anharmonicity in zirconium hydrides using inelastic neutron scattering and ab-initio computer modeling. *Inorganics* **2021**, *9* (5).

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39. Cheng, Y. Q.; Kolesnikov, A. I.; Ramirez-Cuesta, A. J., Simulation of Inelastic Neutron Scattering Spectra Directly from Molecular Dynamics Trajectories. *Journal of Chemical Theory and Computation* **2020**, 16 (12), 7702-7708.
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