

# Marshall McDonnell

Application Engineering Group  
Advanced Computing Systems Section  
Computer Science and Mathematics Division  
Computing and Computational Sciences Directorate  
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## SUMMARY

Since April 2019 I have been working as a research software engineer at Oak Ridge National Laboratory. My main research interest is developing software with sound engineering practices with a focus on applications in materials research. I am the co-author of 16 refereed publications with 7 manuscripts forthcoming (accepted, under review, submitted, or in preparation), co-author of 37 presentations (oral and poster), an active open-source software developer, and co-instructor for 4 workshops around the world.

## PROFESSIONAL EXPERIENCE

- 2019- **Research Software Engineer**  
Computer Science and Mathematics Division  
Oak Ridge National Laboratory, Oak Ridge, TN
- 2016-2019 **Postdoctoral Research Associate**  
Neutron Scattering Division  
Oak Ridge National Laboratory, Oak Ridge, TN  
Advisor: Matthew Tucker
- 2011-2016 **Graduate Student Research Assistant**  
Computational Materials Research Group  
Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, TN  
Advisor: David Keffer

## EDUCATION

- 2011-2016 **Doctor of Philosophy**, University of Tennessee Knoxville, TN  
Chemical and Biomolecular Engineering  
Thesis: *Mass and Charge Transport in Hydrated Polymeric Membranes*  
Advisor: David J. Keffer  
Interdisciplinary Graduate Minor in Computational Science  
Graduate Certificate in Sustainability Science
- 2006-2010 **Bachelor of Science**, Lincoln Memorial University Harrogate, TN  
Mathematics and Chemistry, *Magna Cum Laude*  
Salutatorian

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## RESEARCH INTERESTS AND EXPERIENCE

- Software Development
- Neutron total scattering data reduction.
  - Advancing reverse Monte Carlo modeling methods
  - Parallel analysis programs for MD trajectories
  - Distributed and linked data management software
  - Embedded systems and Internet-of-Things (IoT)
  - Development operations: version control, continuous integration and deployment
- Materials Research
- Amorphous, glass, and high-temperature liquid materials
  - Irradiation effects on nuclear materials
  - Polymeric membrane materials for sustainable energy and food packaging
  - Charge transport in aqueous solutions and membranes
  - Structure and energetics in battery electrode materials
- Multiscale Modeling
- Molecular dynamics (MD): *ab initio*, classical, and reactive
  - Reverse Monte Carlo modeling
  - Electronic structure calculations (density-functional theory)
  - Monte Carlo (MC) methods and statistical mechanical modeling
- Neutron and X-ray Scattering
- Structural characterization via both neutron and X-ray diffraction and total scattering
  - Help Users conduct neutron total scattering experiments on the Nanoscale-Ordered Materials Diffractometer ([NOMAD](#)) at the Spallation Neutron Source
  - Study of atomic-level dynamics with neutron inelastic scattering
  - Analysis and interpretation of data using Rietveld refinements, reverse Monte Carlo (RMC) modeling, and complimentary multiscale modeling techniques.

## SOFTWARE DEVELOPMENT EXPERIENCE

- RMCPProfile
- Reverse Monte Carlo software for fitting multiple experimental data types simultaneously
  - Role: Developer, Development Operations
  - <http://www.rmcpfile.org>
- Mantid
- Data reduction, analysis, and visualization framework for neutron and muon datasets
  - Role: Developer, Code Reviewer
  - <http://www.mantidproject.org>
  - <https://github.com/mantidproject/mantid>
- ADDIE
- Graphical user interface for reduction and analysis of neutron total scattering data
  - Role: Project Manager, Developer
  - <https://github.com/neutrons/addie>
- ICE-MAN
- Integrated computer environment for modeling and analysis for neutron data
  - Role: Developer
- LAMMPS
- A massively parallel molecular dynamics software with Monte Carlo capabilities
  - Role: Contributor
  - <https://lammmps.sandia.gov>
  - <https://github.com/lammmps/lammmps>
- ASE
- Atomic Simulation Environment: Python modules for atomistic simulations
  - Role: Contributor
  - <https://wiki.fysik.dtu.dk/ase/>
  - <https://gitlab.com/ase/ase>

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## MILITARY SERVICE

General Staff Sergeant, U.S. Army Reserve  
Time of Service May 2003 - June 2015  
Occupation Experience Platoon Sergeant, Squad Leader, Combat Engineer, Heavy Equipment Operator,  
Demolition & Explosives Trainer, Explosive Ordnance Clearing Agent  
Deployments December 2004 - December 2005 Kuwait & Southern Iraq  
March 2009 - April 2010 Central Iraq  
Notable Awards De Fleury Medal (Bronze), Meritorious Service Medal, four Army Achievement Medals  
Best Warrior Competition - Winner - 2010 (844<sup>th</sup> Battalion Level)  
Best Warrior Competition - Runner Up - 2010 ( 412<sup>th</sup> Theater Engineer Command Level)

## PROFESSIONAL SERVICE

Memberships American Chemical Society (ACS)  
Materials Research Society (MRS)  
American Institute of Chemical Engineers (AIChE)  
American Crystallographic Association (ACA)  
US Research Software Engineering (US-RSE)  
Reviewer Computational Materials Science  
Journal of Open Source Software  
Journal of Physical Chemistry  
Molecular Simulation

## ACADEMIC AWARDS

2011-2015 **NSF-IGERT Fellowship** with STAIR program: Sustainability Technology through  
Advanced Interdisciplinary Research  
2010 **Award** American Chemical Society Undergraduate Senior Award  
2008 **1st Place Oral Presentation** 118th Tennessee Academy of Science in Chemistry  
2007-2009 **Award** Lincoln Ambassador Award  
2007-2009 **Scholarship** Mildred A. Murray Scholarship  
2006 **Scholarship** Algernon Sydney Sullivan Scholarship

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## SKILLS

### *Software*

Languages	Python, Java, C/C++, Fortran, Ruby, MATLAB, Bash, Perl, JavaScript, Tcl/Tk, MySQL, IDL
Web Frameworks	Flask, Ruby on Rails
Frontend	React.js, Next.js, Vue.js, Three.js
Cloud Computing	OpenStack, Amazon Web Services, Microsoft Azure
Database	PostgreSQL, MySQL, MongoDB, etcd, Consul
Infrastructure as Code	Terraform
Security Management	Vault
Virtualization	ProxMox, Virtual Box
Containerization	Docker, docker-compose, Podman
Version Control	Git, GitHub, GitLab
Continuous Integration	Jenkins, Travis-CI, GitLab-CI
Operating Systems	Linux (Ubuntu, Red Hat, Fedora, CentOS), Mac OS, Windows

### *Computational*

Simulation Techniques	Ab Initio, Classical, and Reactive Molecular Dynamics Simulations, Monte Carlo Simulations, Reverse Monte Carlo Modeling, Electronic Structure Calculations (Density Functional Theory), Finite Element Methods
Simulation Software	LAMMPS, Quantum ESPRESSO, Atomic Simulation Environment, NWChem, CP2K, HOOMD-Blue, GROMACS, PackMol, Moltemplate, Deal.II
Parallel Computing	MPI, OpenMP, CUDA, MapReduce-MPI
Math Libraries	LAPACK, ScaLAPACK, BLAS, MKL, PETSc, NumPy, SciPy
Profiling	PAPI, HPCToolkit
Debugging Software	Valgrind, GDB, TotalView
Visualization Tools	VMD, Ovito, AtomEye, XCrysDen, Matplotlib, Gnuplot, Grace

### *Experimental*

Techniques	Neutron and X-ray Powder Diffraction and Total Scattering, Neutron Inelastic Scattering, Aerodynamic Levitation, Chemical Synthesis
Data Reduction Software	ADDIE, Mantid, GudrunN, GudrunX, PDFgetN, PDFgetX2
Data Analysis Software	RMCPProfile, GSAS, GSAS-II, PDFgui

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## PROPOSALS

### *Software*

2021-2022 **Co-Investigator** "Smart Spectral Matching for Nonproliferation", Awarded \$500,000 for Laboratory Director's Research and Development Funding Program under National Security Sciences call. PI: Ashley Shields

### *Computational*

2017-2018 **User** "Computational Resources for the Interpretation of Neutron Scattering Data from the Spallation Neutron Source and HFIR", Allocation on [Cori](#) and [Edison](#) at [NERSC](#). PI: Thomas Proffen, Proxy: Vickie Lynch, (8M hours).

2016 **Co-author and User** "Multiscale Materials Modeling of Polymer Effects on Charge Transport", [XSEDE](#) allocation on [Comet](#) and [Gordon](#) at [SDSC](#). PI: David Keffer, (100k hours).

2014-2016 **Co-author and User** "Multiscale Materials Modeling", [NICS](#) allocation on [Darter](#). PI: David Keffer, (2M hours).

### *Experimental*

2016-2019 **Author or Co-author**, Awarded 35 individual neutron beamtimes through proposal submission process for Oak Ridge National Laboratory's Neutron Sciences User Program.  
- Multiple beamlines: [NOMAD](#), [VISION](#), [SEQUOIA](#), [CORELLI](#), and [Powder](#)

## WORKSHOPS, OUTREACH, AND MENTORSHIPS

9. **Instructor**, RMCProfile tutorial at Hot Topics in Contemporary Crystallography III Workshop, Bol, Croatia, September 2018.
8. **Instructor and Lecturer**, 2nd US School on Total Scattering Analysis, Oak Ridge National Laboratory, TN, August 2018.
7. **Lecturer**, "Evaluating Chemical Potential in Molecular Simulations" for MSE 614 - *Modeling & Simulation in Materials Science & Engineering : Classical Mechanics* graduate course.  
Course Instructor : David Keffer  
April 2018.
6. **Instructor and Lecturer**, 1st US School on Total Scattering Analysis, Oak Ridge National Laboratory, TN, May 2017.
5. **Instructor**, RMCProfile tutorial at the Annual Meeting on Liquid and Amorphous Materials, Tokyo, Japan, March 2017.
4. **Lecturer**, "Evaluating Free Energy and Chemical Potential in Molecular Simulation" for MSE 614 - *Modeling & Simulation in Materials Science & Engineering : Classical Mechanics* graduate course.  
Course Instructor : David Keffer  
April 2016.
3. **Mentor**, Summer Materials Camp (High School Program) at University of Tennessee, May 2013.
2. **Teacher**, Geometry and Pre-calculus for Upward Bound Summer Program, Douglas-Cherokee Economic Authority  
May 2010 - August 2010.
1. **Tutor**, Mathematics and Chemistry at Lincoln Memorial University,  
August 2007 - January 2009.

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## PUBLICATIONS

### *Forthcoming*

23. Salmon, P. S., Onodera, Y., Kohara, S., Hirata, A., Nishiyama, N., Kitani, S., Zeidler, A., Shiga, M., Masuno, A., Inoue, H., Tahara, S., Polidori, A., Fischer, H., Mori, T., Kojima, S., Kawaji, H., Kolesnikov, A. I., Stone, M. B., Tucker, M. G., **McDonnell, M. T.**, Hannon, A. C., Hiraoka, Y., Obayashi, I., Nakamura, T., Akola, J., Fujii, Y., Ohara, K., Taniguchi, T., Sakata, O., "Structure and properties of densified silica glass: Characterizing the order within disorder", *NPG Asia Materials*, **accepted**.
22. Peterson, P. F., Olds, D., **McDonnell, M. T.**, Page, K., "Unified conversions between total scattering data formalisms", *Journal of Applied Crystallography, Teaching and Education*. *under review*.
21. Cladek, B. R., Everett, S. M., **McDonnell, M. T.**, Tucker, M. G., Keffer, D. J., Rawn, C. J., "Local Structure and Distortions of Mixed CH<sub>4</sub> – CO<sub>2</sub> Hydrates", *Communications Chemistry*, *under review*.
20. Koch, R. J., Sinclair, R., **McDonnell, M. T.**, Yu, R., Abeykoon, M., Tucker, M. G., Tselik, A. M., Billinge, S. J. L., Zhou, H. D., Yin, W.-G., Bozin, E. S., "Dual orbital degeneracy lifting in a strongly correlated electron system", *Physical Review E*, *submitted*.
19. Cladek, B. R., Everett, S. M., **McDonnell, M. T.**, Tucker, M. G., Keffer, D. J., Rawn, C. J., "Analysis of in situ Low-temperature Neutron Pair Distribution Function Coupled with Molecular Dynamics Simulations of CH<sub>4</sub> and CO<sub>4</sub> Hydrates", *Physical Review X*, *submitted*.
18. Nicholson, D. M., Gao, C. Y., **McDonnell, M. T.**, Keffer, D. J., "Entropy Pair Functional Theory: Direct Entropy Evaluation Spanning Phase Transitions", *ready for submission*. *Draft available upon request*.
17. **McDonnell, M. T.**, Olds, D., Page, K., Neufeind, J., Tucker, M. G., Bilheux, J. C., Zhou, W., Peterson, P. F., "ADDIE: ADvanced DIffraction Environment - A Software Environment for Analyzing Neutron Diffraction Data", *in preparation*.

### *Published*

16. Zhang, Y., **McDonnell, M. T.**, Tucker, M. G., Liu, W., "Reverse Monte Carlo Modeling for Low Dimensional Systems", *Journal of Applied Crystallography*, 52(5) 2019. doi: [10.1107/S160057671901080X](https://doi.org/10.1107/S160057671901080X).
15. Cladek, B. R., Everett, S. M., **McDonnell, M. T.**, Tucker, M. G., Keffer, D. J., Rawn, C. J., "Molecular Rotational Dynamics in Mixed CH<sub>4</sub> – CO<sub>2</sub> Hydrates: Insights from Molecular Dynamics Simulations", *Journal of Physical Chemistry C*, 123(43) 2019. pp.26251-26262, doi: [10.1021/acs.jpcc.9b06242](https://doi.org/10.1021/acs.jpcc.9b06242).
14. Mangelis, P., Koch, R. J., Lei, H., Neder, R. B., **McDonnell, M.T.**, Feygenson, M., Petrovic, C., Lappas, A., Bozin, E. S. "Correlated disorder to order crossover in the local structure of K<sub>x</sub>Fe<sub>2y</sub>Se<sub>2-z</sub>S<sub>z</sub>", *Physical Review B*, 100(9) 2019. pp.094108, doi: [10.1103/PhysRevB.100.094108](https://doi.org/10.1103/PhysRevB.100.094108).
13. Zhang, Y., Scholz, T., Dronskowski, R., **McDonnell, M. T.**, Tucker, M. G., "Local magnetic cluster size identified by neutron total scattering in site-diluted spin-glass Sn<sub>0.88</sub>Fe<sub>3.12</sub>N", *Physical Review B*, 100(1) 2019, pp. 014419, doi: [10.1103/PhysRevB.100.014419](https://doi.org/10.1103/PhysRevB.100.014419).
12. Palomares, R. I., **McDonnell, M. T.**, Yang, L., Yao, T., Szymanowski, J. E., Neufeind, J., Sigmon, G. E., Lian, J., Tucker, M. G., Wirth, B. D., Lang, M., "Oxygen point defect accumulation in single-phase UO<sub>2+x</sub>", *Physical Review Materials*, 3(5) 2019, pp. 053611, doi: [10.1103/PhysRevMaterials.3.053611](https://doi.org/10.1103/PhysRevMaterials.3.053611).
11. Zhang, Y., **McDonnell, M. T.**, Calder, S., Tucker, M. G., "Mechanistic insights into the superexchange-interaction driven negative thermal expansion in CuO", *Journal of American Chemical Society*, 141(15) 2019, pp. 6310-6317, doi: [10.1021/jacs.9b00569](https://doi.org/10.1021/jacs.9b00569).
10. **McDonnell, M. T.**, Keffer, D. J., "Reactive Molecular Dynamics Simulations of an Excess Proton in Polyethylene Glycol-Water Solutions", *Molecular Simulation*, 45(4-5) 2019, pp. 381-393, doi: [10.1080/08927022.2018.1557328](https://doi.org/10.1080/08927022.2018.1557328).
9. Usher, T., Forrester, J. S., **McDonnell, M. T.**, Neufeind, J., Page, P., Peterson, P. F., Levin, I., Jones, J. L., "Time-of-flight neutron total scattering with applied electric fields: *Ex situ* and *in situ* studies of ferroelectric materials", *Review of Scientific Instruments*, 89(092905), 2018, pp. 1-7, doi: [10.1063/1.5037609](https://doi.org/10.1063/1.5037609).
8. Olds, D., Mills, R. A., **McDonnell, M. T.**, Liu, J., Kim, J. R., Dunstan, M. T., Gaultois, M. W., Everett, S. M., Tucker, M. G., Page, K., "A high temperature gas flow environment for neutron total scattering studies of complex materials", *Review of Scientific Instruments*, 89(092906), 2018, pp. 1-7, doi: [10.1063/1.50334648](https://doi.org/10.1063/1.50334648).
7. Cladek, B. R., Everett, S. M., **McDonnell, M. T.**, Tucker, M. G., Keffer, D. J., Rawn, C. J., "Guest-Host Interactions in Mixed CH<sub>4</sub> – CO<sub>2</sub> Hydrates: Insights from Molecular Dynamics Simulations", *Journal of Physical Chemistry C*, 122, 2018, pp. 19575-19583. doi: [10.1021/acs.jpcc.8b05228](https://doi.org/10.1021/acs.jpcc.8b05228).
6. Mangelis, P., Lei, H., **McDonnell, M.T.**, Feygenson, M., Petrovic, C., Bozin, E. S., Lappas, A. "On the Nanoscale Structure of K<sub>x</sub>Fe<sub>2y</sub>Ch<sub>2</sub> (Ch = S, Se): A Neutron Pair Distribution Function View", *Condensed Matter*, 3(20), 2018, pp. 1-10. doi: [10.3390/condmat3030020](https://doi.org/10.3390/condmat3030020).
5. McNutt, N.W., **McDonnell, M.T.**, Rios, O., Keffer, D.J., "Li-ion Localization and Energetics as a Function of Anode Structure", *ACS Applied Materials & Interfaces*, 9(8), 2017, pp. 6988-7002. doi: [10.1021/acsami.6b13748](https://doi.org/10.1021/acsami.6b13748).

4. **McDonnell, M.T.**, Greeley, D.A., Kit, K.M., Keffer, D.J., "Molecular Dynamics Simulations of Hydration Effects on Solvation, Diffusivity, and Permeability in Chitosan/Chitin Films", *Journal of Physical Chemistry B*, 120(34), 2016, pp. 8997-9010. doi: 10.1021/acs.jpcc.6b05999.
3. **McDonnell, M.T.**, Xu, H., Keffer, D.J., "Ab initio molecular dynamics simulations of an excess proton in a triethylene glycol-water solution: solvation structure, mechanism and kinetics", *Journal of Physical Chemistry B*, 120(23), 2016, pp. 5223-5242. doi: 10.1021/acs.jpcc.6b02445.
2. Deng, S., Hassan, M.K., Nalawade, A., Perry, K.A., More, K.L., Mauritz, K.A., **McDonnell, M.T.**, Keffer, D.J., Mays, J.W., "High Temperature, Low Humidity Proton Exchange Membranes with Enhanced Conductivities based on Poly(1,3-cyclohexadiene) and Polyethylene Glycol", *Polymer*, 77, 2015, pp. 208-217. doi: 10.1016/j.polymer.2015.09.033.
1. **McDonnell, M.T.**, Keffer, D.J., "Intrinsic Relationships between Proton Conductivity and Nanopore Size and Functionalization", *Microporous and Mesoporous Materials*, 177, 2013, pp. 1724. doi: 10.1016/j.micromeso.2013.04.007.

#### Other Papers

**McDonnell, M.T.**, "Supercomputer Design: An Initial Effort to Capture the Environmental, Economic, and Societal Impacts", TRACE: Tennessee Research and Creative Exchange, [http://trace.tennessee.edu/utk\\_chembiopubs/93](http://trace.tennessee.edu/utk_chembiopubs/93), 2013.

### PRESENTATIONS

#### \*presenter

37. **\*McDonnell, M. T.**, Olds, D., Page, K., Neufeind, J., Tucker, M. G., Bilheux, J. C., Zhou, W., Peterson, P. F., ADDIE: ADvanced DIffraction Environment, SciPy Virtual Conference, Austin, TX, 2020. **Poster Presentation**
36. Cladek, B. R., Everett, S. M., Tucker, M. G., **McDonnell, M. T.**, Keffer, D. J., Rawn, C. J., "In Situ Low-temperature Pair Distribution Function (PDF) Analysis and Molecular Dynamics (MD) Simulations of CH<sub>4</sub> and CO<sub>2</sub> Hydrates", Pittsburgh Diffraction Conference, Oak Ridge National Laboratory, TN, October 2019. **Poster Presentation (Won Chung Soo Yoo Graduate Student Best Poster Award)**
35. **\*McDonnell, M. T.**, Olds, D., Page, K., Neufeind, J., Tucker, M. G., Bilheux, J. C., Zhou, W., Peterson, P. F., "ADDIE: ADvanced DIffraction Environment", ORNL Software Expo, Oak Ridge National Laboratory, TN, May 2019. **Poster Presentation**
34. Sluss, C. C., Nicholson, D. M., Gao, C. Y., **McDonnell, M. T.**, Keffer, D. J., "Direct Entropy Calculation From Molecular Dynamics Simulation", South-Eastern Theoretical Chemistry Association Meeting, Knoxville, Tennessee, May 2019. **Poster Presentation**
33. Cladek, B. R., Everett, S. M., Tucker, M. G., **McDonnell, M. T.**, Keffer, D. J., Rawn, C. J., "In Situ Low-temperature Pair Distribution Function (PDF) Analysis of CH<sub>4</sub> and CO<sub>2</sub> Hydrates", South-Eastern Theoretical Chemistry Association Meeting, Knoxville, Tennessee, May 2019. **Poster Presentation**
32. Palomares, R. I., Cureton, W., Yang, L., Wirth, B., Lang, M., **\*McDonnell, M. T.**, Tucker, M. G., Neufeind, J., and Ramirez-Cuesta, A., "Unraveling the Defect Structure in Irradiated Nuclear Materials using the ORNL Integrated Computational Environment-Modeling & Analysis for Neutrons (ICE-MAN)", 1st University of Tennessee JDRD Symposium, Knoxville, Tennessee, February 2019. **Oral Presentation**
31. Cladek, B. R., **\*McDonnell, M. T.**, Everett, S. M., Keffer, D. J., Rawn, C. J., Tucker, M. G., "Guest-Host Interactions in Mixed CH<sub>4</sub>-CO<sub>2</sub> Hydrates: Neutron Total Scattering and Computational Modeling", 7th Reverse Monte Carlo Modelling Meeting, Budapest, Hungary, September 2018. **Oral Presentation**
30. **\*McDonnell, M. T.**, "Combining Neutron Total Scattering and Molecular Dynamics Simulations: Understanding Atomistic Origins of Structure-Property Relations in Materials", 2nd US School on Total Scattering Analysis, Oak Ridge National Laboratory, TN, August 2018. **Oral Presentation**
29. **\*McDonnell, M. T.**, "Data Reduction and Corrections for Neutron Total Scattering", 2nd US School on Total Scattering Analysis, Oak Ridge National Laboratory, TN, August 2018. **Oral Presentation**
28. **\*McDonnell, M. T.**, Olds, D., Page, K., Neufeind, J., Tucker, M. G., Bilheux, J. C., Zhou, W., Peterson, P. F., "ADDIE: ADvanced DIffraction Environment", 2018 Basic Energy Science Review of the High Flux Isotope Reactor and the Spallation Neutron Source, Oak Ridge National Laboratory, TN, August 2018. **Poster Presentation**
27. **\*McDonnell, M. T.**, Olds, D., Page, K., Neufeind, J., Tucker, M. G., Bilheux, J. C., Zhou, W., Peterson, P. F., "ADDIE: ADvanced DIffraction Environment", ORNL Postdoctoral Research Symposium, Oak Ridge National Laboratory, TN, August 2018. **Poster Presentation**
26. **\*McDonnell, M. T.**, Olds, D., Page, K., Neufeind, J., Tucker, M. G., Bilheux, J. C., Zhou, W., Peterson, P. F., "ADDIE: ADvanced DIffraction Environment", 9th American Conference on Neutron Scattering, College Park, Maryland, June 2018. **Oral Presentation**

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25. \***McDonnell, M. T.**, Olds, D., Page, K., Neufeind, J., Tucker, M. G., Bilheux, J. C., Zhou, W., Peterson, P. F., "ADDIE: ADvanced Diffraction Environment", ORNL Software Expo, Oak Ridge National Laboratory, TN, May 2018. **Poster Presentation**
  24. Cladek, B. R., Everett, S. M., Tucker, M. G., **McDonnell, M. T.**, Keffer, D. J., Rawn, C. J., "In Situ Low-temperature Pair Distribution Function (PDF) Analysis of CH<sub>4</sub> and CO<sub>2</sub> Hydrates ", Gordon Research Conference for Natural Gas Hydrate Systems, Galveston, TX, March 2018. **Oral Presentation (Won GRC Student Award)**
  23. \***McDonnell, M. T.**, Olds, D., Page, K., Neufeind, J., Tucker, M. G., Bilheux, J. C., Zhou, W., Peterson, P. F., "ADDIE: ADvanced DIffraction Environment", ORNL Neutron Sciences Software Review, Oak Ridge National Laboratory, TN, May 2018. **Poster Presentation**
  22. \***McDonnell, M. T.**, "Live Demonstraion of ADDIE: Data Reduction for Total Scattering", Mantid Users Workshop, Oak Ridge National Laboratory, TN, January 2018. **Live Demonstration**
  21. Cladek, B. R., Everett, S. M., **McDonnell, M. T.**, Tucker, M. G., Keffer, D. J., Rawn, C. J., "In Situ Low-temperature Pair Distribution Function (PDF) Analysis of CH<sub>4</sub> and CO<sub>2</sub> Hydrates ", American Geophysical Union Fall Meeting, TN, December 2017. **Oral Presentation**
  20. Cladek, B. R., Everett, S. M., Tucker, M. G., **McDonnell, M. T.**, Keffer, D. J., Rawn, C. J., "In Situ Low-temperature Pair Distribution Function (PDF) Analysis of CH<sub>4</sub> and CO<sub>2</sub> Hydrates ", Joint Nanoscience and Neutron Scattering User Meeting, Oak Ridge National Laboratory, TN, August 2017. **Oral Presentation**
  19. \***McDonnell, M. T.**, Olds, D., Page, K., Neufeind, J., Tucker, M. G., Bilheux, J. C., Zhou, W., Peterson, P. F., "AD-DIE: ADvanced DIffraction Environment", Joint Nanoscience and Neutron Scattering User Meeting, Oak Ridge National Laboratory, TN, August 2017. **Oral Presentation**
  18. \***McDonnell, M. T.**, Olds, D., Page, K., Neufeind, J., Tucker, M. G., Bilheux, J. C., Zhou, W., Peterson, P. F., "ADDIE: ADvanced DIffraction Environment", 67th Annual Meeting of the American Crystallographic Association, New Orleans, LA, May 2017. **Oral Presentation**
  17. \***McDonnell, M. T.**, "Postdoctoral Experience with Total Scattering at the Spallation Neutron Source", 1st US School on Total Scattering Analysis, Oak Ridge National Laboratory, TN, May 2017. **Oral Presentation**
  16. \***McDonnell, M. T.**, "Data Reduction on NOMAD using ADDIE", 1st US School on Total Scattering Analysis, Oak Ridge National Laboratory, TN, May 2017. **Oral Presentation**
  15. \***McDonnell, M. T.**, "Live Demonstraion of ADDIE: Data Reduction for Total Scattering", Neutron Day Seminar Series: Data and Instrument Software, Oak Ridge National Laboratory, TN, March 2017. **Live Demonstration**
  14. \***McDonnell, M. T.**, Xu, H., Keffer, D.J., "Effect of Triethylene Glycol on Proton Transport in Aqueous Solution", University of Tennessee Department of Material Science & Engineering Seminar Series, Knoxville, TN, October 2015. **Oral Presentation**
  13. \***McDonnell, M. T.**, Mays, J., Keffer, D.J., "Modeling and Characterization of Novel PEM Fuel Cell Membranes for Hot, Dry Operating Conditions", Foundations of Molecular Modeling and Simulation Meeting, Mt. Hood, OR, July 2015. **Poster Presentation**
  12. \***McDonnell, M. T.**, Mays, J., Keffer, D.J., "Modeling and Characterization of Novel PEM Fuel Cell Membranes for Hot, Dry Operating Conditions", Materials Research Society Spring Meeting, San Francisco, CA, April 2015. **Poster Presentation**
  11. McNutt, N., **McDonnell, M. T.**, Rio, O., Feygenson, M., Proffen, T., Keffer, D., "Structural Analysis of Lithiated Lignin-Derived Carbon Composite Anodes", American Institute for Chemical Engineers Annual Meeting, Atlanta, GA, November 2014. **Oral Presentation**
  10. \***McDonnell, M. T.**, Mays, J., Keffer, D.J., "Multiscale Modeling of Proton Transport in Novel PEM Fuel Cell Membranes", American Institute for Chemical Engineers Annual Meeting, Atlanta, GA, November 2014. **Oral Presentation**
  9. McNutt, N., **McDonnell, M. T.**, Rio, O., Feygenson, M., Proffen, T., Keffer, D., "A Mechanistic Understanding of Lithium-Ion Diffusion and Intercalation in Novel Lignin-Derived Carbon Composite Anodes", American Institute for Chemical Engineers Annual Meeting,, Atlanta, GA, November 2014. **Oral Presentation**
  8. \***McDonnell, M. T.**, Greeley, D., Kit, K., Keffer, D., "Modeling Oxygen Permeability in Biodegradable Polymer Films", American Institute for Chemical Engineers Annual Meeting, Atlanta, GA, November 2014. **Poster Presentation**
  7. \***McDonnell, M. T.**, Mays, J., Keffer, D.J., "Multiscale Modeling of Proton Transport in Novel PEM Fuel Cell Membranes", Gordon Research Seminar and Conference for Computational Chemistry, Mt. Snow, VT, July 2014. **Poster Presentation**
  6. \***McDonnell, M. T.**, Mays, J., Keffer, D.J., "Multiscale Modeling of Proton Transport in Novel PEM Fuel Cell Membranes", Workshop for Structure and Dynamics of Confined Interfacial Fluids: Blending, Scattering, Spectroscopy and Computer Modeling Techniques, Oak Ridge National Laboratory, TN, July 2014. **Oral and Poster Presentation**



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