

Jamie J. Molaison

833 Dorset Drive, Knoxville, TN 37923

Mobile: (865) 235-4114 email: molaisonjj@ornl.gov

EDUCATION

- M.S., Chemistry (Inorganic), University of Tennessee, Knoxville, TN, 2006
- B.S., Chemistry, Nicholls State University, Thibodaux, LA, 2002

EXPERIENCE

Scientific Associate, Spallation Neutron Source Science Support Group, Instrument and Source Division, Oak Ridge National Laboratory, Oak Ridge, TN
2006-Present

- Assisted in the oversight and coordination of the Spallation Neutrons And Pressure (SNAP) high-pressure neutron diffractometer construction, installation, and maintenance activities
- Performed high-pressure neutron-diffraction experiments, which included sample preparation, data collection, and data analysis.
- Held the role of lab space manager for the SNAP beamline
- Coordinated upgrade and repair efforts of instrument support groups with the goal of maintaining reliable beamline operations and minimizing downtime
- Performed user-related activities including sample environment setup/troubleshooting/operation, sample preparation and disposition, instrument-specific training
- Maintained instrument documentation and chemical and sample inventories
- Participated in user-proposal feasibility reviews and scheduled approved experiments
- Co-organized SNAP Instrument Development Team meetings and the 2010 meeting of the IUCr Commission on High Pressure
- Designed numerous items using Creo 3D modeling software each having a varying degree of impact on the operational and scientific success of SNAP.
- Aided in the design, procurement, testing and implementation of several custom sample environments and components that significantly increased SNAP's capabilities and data quality. These include:
 - New diamond-anvil cells (DACs) and associated components used to collect refinable data at a sample pressure of 80 GPa, which supplanted the previous world record (for refinable neutron diffraction data) of 30 GPa
 - Multiple low- and high-temperature apparatuses that allow for simultaneous exploration of P-T space
 - Nested Kirkpatrick-Baez supermirrors designed to increase signal/background for small samples by focusing neutron beams down to >100 μm .
 - Various collimation and shielding pieces required to reduce neutron background levels to those suitable for obtaining quality data from $\sim .03 \text{ mm}^3$ samples

Research Assistant, Professor John F. C. Turner, University of Tennessee, Knoxville, TN
2002–2006

Thesis title: *Structural and dynamical studies of superacids and superacidic solutions using neutron and high energy X-ray scattering*

- Manipulated air and moisture sensitive compounds using inert gas and high vacuum techniques
- Determined liquid structures through acquisition of neutron and high energy X-ray diffraction data followed by subsequent analysis using the ATLAS suite of programs
- Synthesized and purified molecular inorganic compounds to ultra-pure levels with respect to chemical and isotopic composition
- Characterized inorganic and organic compounds by NMR, IR, and Raman spectroscopy
- Determined the structure of inorganic and organic compounds using single crystal x-ray crystallography using a SMART 1000 diffractometer and the SHELXTL suite of programs
- Constructed custom glassware using standard freehand scientific glass-blowing techniques
- Wrote proposals for the acquisition of experiment time at neutron sources and synchrotron facilities
- Co-authored papers for publication in peer-reviewed journals

Graduate Teaching Assistant, General Chemistry, University of Tennessee,
2002–2005

- Instructed during labs and recitations, administered exams

PUBLICATIONS

1. Zheng, H. Y.; Wang, L. J.; Li, K.; Yang, Y. Y.; Wang, Y. J.; Wu, J. J.; Dong, X.; Wang, C. H.; Tulk, C. A.; Molaison, J. J.; Ivanov, I. N.; Feygenson, M.; Yang, W. G.; Guthrie, M.; Zhao, Y. S.; Mao, H. K.; Jin, C. Q., Pressure induced polymerization of acetylide anions in CaC₂ and 10(7) fold enhancement of electrical conductivity. *Chem. Sci.* **2017**, *8* (1), 298-304.
2. Sun, J. M.; Dong, X.; Wang, Y. J.; Li, K.; Zheng, H. Y.; Wang, L. J.; Cody, G. D.; Tulk, C. A.; Molaison, J. J.; Lin, X. H.; Meng, Y. F.; Jin, C. Q.; Mao, H. K., Pressure-Induced Polymerization of Acetylene: Structure-Directed Stereoselectivity and a Possible Route to Graphane. *Angew. Chem.-Int. Edit.* **2017**, *56* (23), 6553-6557.
3. Song, G.; Lin, J.; Bilheux, J.; Xie, Q.; Santodonato, L.; Molaison, J.; Skorpenske, H.; M. Dos Santos, A.; Tulk, C.; An, K.; Stoica, A.; Kirka, M.; Dehoff, R.; Tremsin, A.; Bunn, J.; Sochalski-Kolbus, L.; Bilheux, H., Characterization of Crystallographic Structures Using Bragg-Edge Neutron Imaging at the Spallation Neutron Source †. *Journal of Imaging* **2017**, *3* (4), 65.
4. Li, X.; Baldini, M.; Wang, T.; Chen, B.; Xu, E. S.; Vermilyea, B.; Crespi, V. H.; Hoffmann, R.; Molaison, J. J.; Tulk, C. A.; Guthrie, M.; Sinogeikin, S.; Badding, J. V., Mechanochemical Synthesis of Carbon Nanothread Single Crystals. *J Am Chem Soc* **2017**, *139* (45), 16343-16349.
5. Hester, B. R.; Dos Santos, A. M.; Molaison, J. J.; Hancock, J. C.; Wilkinson, A. P., Synthesis of Defect Perovskites (He_{2-x} squarex)(CaZr)F₆ by Inserting Helium into the Negative Thermal Expansion Material CaZrF₆. *J Am Chem Soc* **2017**, *139* (38), 13284-13287.

6. Haberl, B.; Dissanayake, S.; Ye, F.; Daemen, L. L.; Cheng, Y.; Li, C. W.; Ramirez-Cuesta, A. J.; Matsuda, M.; Molaison, J. J.; Boehler, R., Wide-angle diamond cell for neutron scattering. *High Pressure Res.* **2017**, *37* (4), 495-506.
7. Guthrie, M.; Pruteanu, C. G.; Donnelly, M. E.; Molaison, J. J.; dos Santos, A. M.; Loveday, J. S.; Boehler, R.; Tulk, C. A., Radiation attenuation by single-crystal diamond windows. *J. Appl. Crystallogr.* **2017**, *50*, 76-86.
8. Guguchia, Z.; Adachi, T.; Shermadini, Z.; Ohgi, T.; Chang, J.; Bozin, E. S.; von Rohr, F.; dos Santos, A. M.; Molaison, J. J.; Boehler, R.; Koike, Y.; Wieteska, A. R.; Frandsen, B. A.; Morenzoni, E.; Amato, A.; Billinge, S. J. L.; Uemura, Y. J.; Khasanov, R., Pressure tuning of structure, superconductivity, and novel magnetic order in the Ce-underdoped electron-doped cuprate $T' - \text{Pr}_{1.3-x}\text{La}_{0.7}\text{Ce}_x\text{CuO}_4$ ($x=0.1$). *Phys. Rev. B* **2017**, *96* (9), 094515.
9. Cai, W. Z.; Dunuwille, M.; He, J. G.; Taylor, T. V.; Hinton, J. K.; MacLean, M. C.; Molaison, J. J.; dos Santos, A. M.; Sinogeikin, S.; Deemyad, S., Deuterium Isotope Effects in Polymerization of Benzene under Pressure. *J. Phys. Chem. Lett.* **2017**, *8* (8), 1856-1864.
10. Boehler, R.; Molaison, J. J.; Haberl, B., Novel diamond cells for neutron diffraction using multi-carat CVD anvils. *Rev. Sci. Instrum.* **2017**, *88* (8), 083905.
11. Zheng, H. Y.; Li, K.; Cody, G. D.; Tulk, C. A.; Dong, X.; Gao, G. Y.; Molaison, J. J.; Liu, Z. X.; Feyngenson, M.; Yang, W. G.; Ivanov, I. N.; Basile, L.; Idrobo, J. C.; Guthrie, M.; Mao, H. K., Polymerization of Acetonitrile via a Hydrogen Transfer Reaction from CH_3 to CN under Extreme Conditions. *Angew. Chem.-Int. Edit.* **2016**, *55* (39), 12040-12044.
12. Tulk, C. A.; dos Santos, A. M.; Neufeind, J. C.; Molaison, J. J.; Sales, B. C.; Honkimaki, V., Density driven structural transformations in amorphous semiconductor clathrates. *Appl. Phys. Lett.* **2015**, *106* (2), 5.
13. Schaeffer, A. M.; Cai, W. Z.; Olejnik, E.; Molaison, J. J.; Sinogeikin, S.; dos Santos, A. M.; Deemyad, S., Boundaries for martensitic transition of Li-7 under pressure. *Nat. Commun.* **2015**, *6*, 6.
14. Rivin, O.; Broide, A.; Maskova, S.; Lucas, M. S.; Hen, A.; Orion, I.; Salhov, S.; Shandalov, M.; Moreira Dos Santos, A.; Molaison, J.; Chen, Z.; Halevy, I., High pressure neutron powder diffraction study of $\text{Fe}_{1-x}\text{Cr}_x$ with and without hydrogen exposure. *Hyperfine Interact.* **2015**, *231* (1), 29-36.
15. Makowska, M. G.; Kuhn, L. T.; Cleemann, L. N.; Lauridsen, E. M.; Bilheux, H. Z.; Molaison, J. J.; Santodonato, L. J.; Tremsin, A. S.; Grosse, M.; Morgano, M.; Kabra, S.; Strobl, M., Flexible sample environment for high resolution neutron imaging at high temperatures in controlled atmosphere. *Rev. Sci. Instrum.* **2015**, *86* (12), 9.
16. Li, K.; Zheng, H. Y.; Wang, L. J.; Tulk, C. A.; Molaison, J. J.; Feyngenson, M.; Yang, W. G.; Guthrie, M.; Mao, H., $\text{K}_3\text{Fe}(\text{CN})_6$ under External Pressure: Dimerization of CN^- Coupled with Electron Transfer to $\text{Fe}(\text{III})$. *J. Phys. Chem. C* **2015**, *119* (39), 22351-22356.
17. Li, K.; Zheng, H.; Hattori, T.; Sano-Furukawa, A.; Tulk, C. A.; Molaison, J.; Feyngenson, M.; Ivanov, I. N.; Yang, W.; Mao, H.-k., Synthesis, Structure, and Pressure-Induced Polymerization of $\text{Li}_3\text{Fe}(\text{CN})_6$ Accompanied with Enhanced Conductivity. *Inorganic Chemistry* **2015**, *54* (23),

11276-11282.

18. Haravifard, S.; Banerjee, A.; van Wezel, J.; Silevitch, D. M.; dos Santos, A. M.; Lang, J. C.; Kermarrec, E.; Srajer, G.; Gaulin, B. D.; Molaison, J. J.; Dabkowska, H. A.; Rosenbaum, T. F., Reply to Zayed: Interplay of magnetism and structure in the Shastry-Sutherland model. *Proc. Natl. Acad. Sci. U. S. A.* **2015**, *112* (5), E383-E384.
19. Chatterji, T.; dos Santos, A. M.; Molaison, J. J.; Hansen, T. C.; Klotz, S.; Tucker, M.; Samanta, K.; Saha-Dasgupta, T., Anomalous breakdown of Bloch's rule in the Mott-Hubbard insulator MnTe₂. *Phys. Rev. B* **2015**, *91* (10), 7.
20. Ye, F.; Bao, W.; Chi, S. X.; dos Santos, A. M.; Molaison, J. J.; Fang, M. H.; Wang, H. D.; Mao, Q. H.; Wang, J. C.; Liu, J. J.; Sheng, J. M., High-Pressure Single-Crystal Neutron Scattering Study of Magnetic and Fe Vacancy Orders in (Tl, Rb)(₂)Fe₄Se₅ Superconductor. *Chin. Phys. Lett.* **2014**, *31* (12), 4.
21. Tulk, C. A.; Machida, S.; Klug, D. D.; Lu, H.; Guthrie, M.; Molaison, J., The structure of CO₂ hydrate between 0.7 and 1.0 GPa. *J. Chem. Phys.* **2014**, *141* (17), 8.
22. Haravifard, S.; Banerjee, A.; van Wezel, J.; Silevitch, D. M.; dos Santos, A. M.; Lang, J. C.; Kermarrec, E.; Srajer, G.; Gaulin, B. D.; Molaison, J. J.; Dabkowska, H. A.; Rosenbaum, T. F., Emergence of long-range order in sheets of magnetic dimers. *Proc. Natl. Acad. Sci. U. S. A.* **2014**, *111* (40), 14372-14377.
23. Chheda, T. D.; Mookherjee, M.; Mainprice, D.; dos Santos, A. M.; Molaison, J. J.; Chantel, J.; Manthilake, G.; Bassett, W. A., Structure and elasticity of phlogopite under compression: Geophysical implications. *Phys. Earth Planet. Inter.* **2014**, *233*, 1-12.
24. Hirai, S.; dos Santos, A. M.; Shapiro, M. C.; Molaison, J. J.; Pradhan, N.; Guthrie, M.; Tulk, C. A.; Fisher, I. R.; Mao, W. L., Giant atomic displacement at a magnetic phase transition in metastable Mn₃O₄. *Phys. Rev. B* **2013**, *87* (1), 6.
25. Guthrie, M.; Boehler, R.; Tulk, C. A.; Molaison, J. J.; dos Santos, A. M.; Li, K.; Hemley, R. J., Neutron diffraction observations of interstitial protons in dense ice. *Proc. Natl. Acad. Sci. U. S. A.* **2013**, *110* (26), 10552-10556.
26. Boehler, R.; Guthrie, M.; Molaison, J. J.; dos Santos, A. M.; Sinogeikin, S.; Machida, S.; Pradhan, N.; Tulk, C. A., Large-volume diamond cells for neutron diffraction above 90GPa. *High Pressure Res.* **2013**, *33* (3), 546-554.
27. Tulk, C. A.; Klug, D. D.; Molaison, J. J.; dos Santos, A. M.; Pradhan, N., Structure and stability of an amorphous water-methane mixture produced by cold compression of methane hydrate. *Phys. Rev. B* **2012**, *86* (5), 8.
28. Tulk, C. A.; Klug, D. D.; dos Santos, A. M.; Karotis, G.; Guthrie, M.; Molaison, J. J.; Pradhan, N., Cage occupancies in the high pressure structure H methane hydrate: A neutron diffraction study. *J. Chem. Phys.* **2012**, *136* (5), 6.
29. Guthrie, M.; Tulk, C. A.; Molaison, J.; dos Santos, A. M., Local structural motifs and extended-range order in liquid and solid ammonia under pressure. *Phys. Rev. B* **2012**, *85* (18), 9.

30. Stone, M. B.; Tulk, C. A.; dos Santos, A.; Molaison, J. J.; Chang, S.; Leao, J. B.; Samulon, E. C.; Shapiro, M. C.; Fisher, I. R., Pressure Dependent Diffraction and Spectroscopy of a Dimerized Antiferromagnet. *J. Phys. Soc. Jpn.* **2011**, *80*, 4.
31. Yang, L.; Tulk, C. A.; Klug, D. D.; Chakoumakos, B. C.; Ehm, L.; Molaison, J. J.; Parise, J. B.; Simonson, J. M., Guest disorder and high pressure behavior of argon hydrates. *Chem. Phys. Lett.* **2010**, *485* (1-3), 104-109.
32. Tremsin, A. S.; McPhate, J. B.; Vallerger, J. V.; Siegmund, O. H. W.; Feller, W. B.; Bilheux, H. Z.; Molaison, J. J.; Tulk, C. A.; Crow, L.; Cooper, R. G.; Penumadu, D.; Iop, Transmission Bragg edge spectroscopy measurements at ORNL Spallation Neutron Source. In *International Conference on Neutron Scattering 2009*, Iop Publishing Ltd: Bristol, 2010; Vol. 251.
33. Ice, G. E.; Choi, J. Y.; Takacs, P. Z.; Khounsary, A.; Puzyrev, Y.; Molaison, J. J.; Tulk, C. A.; Andersen, K. H.; Bigault, T., Nested neutron microfocusing optics on SNAP. *Appl. Phys. A-Mater. Sci. Process.* **2010**, *99* (3), 635-639.
34. Zhang, C.; Yi, W.; Sun, L. L.; Chen, X. J.; Hemley, R. J.; Mao, H. K.; Lu, W.; Dong, X. L.; Bai, L. G.; Liu, J.; Dos Santos, A. F. M.; Molaison, J. J.; Tulk, C. A.; Chen, G. F.; Wang, N. L.; Zhao, Z. X., Pressure-induced lattice collapse in the tetragonal phase of single-crystalline Fe_{1.05}Te. *Phys. Rev. B* **2009**, *80* (14), 5.
35. Ice, G. E.; Pang, J. W. L.; Tulk, C.; Molaison, J.; Choi, J. Y.; Vaughn, C.; Lytle, L.; Takacs, P. Z.; Andersen, K. H.; Bigault, T.; Khounsary, A., Design challenges and performance of nested neutron mirrors for microfocusing on SNAP. *J. Appl. Crystallogr.* **2009**, *42*, 1004-1008.
36. McLain, S. E.; Soper, A. K.; Molaison, J. J.; Benmore, C. J.; Dolgos, M. R.; Yarger, J. L.; Turner, J. F. C., On the structure of liquid antimony pentafluoride. *J. Mol. Liq.* **2007**, *131*, 239-245.
37. Fernandez-Alonso, F.; Bermejo, F. J.; McLain, S. E.; Turner, J. F. C.; Molaison, J. J.; Herwig, K. W., Observation of fractional Stokes-Einstein behavior in the simplest hydrogen-bonded liquid. *Phys. Rev. Lett.* **2007**, *98* (7), 4.
38. McLain, S. E.; Benmore, C. J.; Siewenie, J. E.; Molaison, J. J.; Turner, J. F. C., On the variation of the structure of liquid deuterium fluoride with temperature. *J. Chem. Phys.* **2004**, *121* (13), 6448-6455.

REFERENCES

- Dr. Bianca Haberl, Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN (865) 805-4065 haberlb@ornl.gov
- Dr. Antonio Moreira dos Santos, Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN (865) 235-3343 dossantosam@ornl.gov
- Dr. Malcolm Guthrie, European Spallation Source, Lund, Sweden +46 721 79 22 83 Malcolm.Guthrie@esss.se