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AFFILIATIONS: Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831
University of Tennessee, Knoxville, TN 37996: Bredesen Center for Interdisciplinary Research and Graduate Education; Biochemistry & Cellular & Molecular Biology Department; Genome Science and Technology Graduate Program

PRESENT POSITION: Senior Staff scientist

FIELD OF SPECIALIZATION: Structural biology, biodeuteration, renewable energy, bio-nanotechnology

PROFESSIONAL PREPARATION

Post-Doctoral: Oak Ridge National Laboratory, TN (1998-2002).
Department of Biochemistry, University College Dublin (1997-1998).
Ph.D. Degree: Department of Biochemistry, University College Dublin (1997) Advisor Prof. Stephen G. Mayhew.
B.Sc. Degree: University College Dublin (1992). Major in biochemistry, minor in chemistry.

POSITIONS AND APPOINTMENTS

April 2021 – Present: Distinguished R&D Staff, Neutron Scattering Division, ORNL
Nov 2020 – Present: Group Leader, Biological Labeling and Scattering, ORNL
Jan 2018 – Oct 2020: Team Lead for Biology Laboratories, ORNL
April 2018 – present: Director of the Center for Structural Molecular Biology, ORNL
Oct 2017 – April 2021: Biological Materials and Biosystems Science Initiative Lead, ORNL
July 2018 – present: Faculty, Genome Science and Technology Program, University of Tennessee, Knoxville
Oct 2016 – present: Faculty, Bredesen Center for Interdisciplinary Research and Graduate Education, University of Tennessee, Knoxville
Nov 2013 – present: Senior R&D Staff, Neutron Scattering Division, ORNL
March 2013 – present: Institutional Biosafety Committee, ORNL
Oct 2009 – Oct 2011: ORNL SEED money committee member
Sept 2009 – Oct 2013: R&D Staff, ORNL, Oak Ridge, Tennessee
Feb 2005 – Aug 2009: R&D Associate, ORNL, Oak Ridge, Tennessee
Feb 2005 – present: Joint Faculty, Biochemistry & Cellular & Molecular Biology, University of Tennessee
March 2002 – Jan 2005: Research Assistant Professor, Biochemistry & Cellular & Molecular Biology, University of Tennessee

PROFESSIONAL MEMBERSHIPS

American Chemical Society since 2000
The Biochemical Society- 1992-2000

HONORS AND AWARDS

2019: Ten for Ten Scientific Ideas Award, 2019 Energy Frontier Research Center Principal Investigators Meeting
2014: Significant Event Award for attracting new funding, ORNL

2008: U.S. D.O.E. Office of Science Outstanding Mentor Award
2007: U.S. D.O.E. Office of Science Outstanding Mentor Award
1993: Graduate Student EU commission scholarship (completed 1996)
1992: Graduate Student Forbairt scholarship (completed 1995)

TEACHING EXPERIENCE

2018 – present Ph.D advisor: Viswanthan Gurumoorthy, B.Sc. Genome Science and Technology Program

2014 – 2019 Ph.D advisor: Riddhi Shah, M.Sc. Bredesen Center (co-advisor with Dr. Brian Davison, ORNL)

2004 – present Committee member for Masters and PhD candidates. Stacy Hutchens, Biomedical Engineering, UTK (MSc 2004); Stacy Hutchens, Biomedical Engineering UTK (PhD 2007); Ifeyinwa Iwuchukwu, Chemical and Biomolecular Engineering, UTK (PhD 2012); Monique Lemieux, Genome Science and Technology Program, UTK (MSc 2013); Rosemary Le, Chemical and Biomolecular Engineering, UTK (PhD 2014); Bradley Harris, Chemical and Biomolecular Engineering, UTK (PhD 2014); Kasey Estenson, Genome Science and Technology Program (GST), UTK (2013–2017); Sarah Williamson, Chemical and Biomolecular Engineering, UTK (2014 - present); Nathan Brady, GST, UTK (2016 – 2021), Shantanu Shukla GST, UTK (2015 – 2020); Anton Astner, Biosystems Engineering and Environmental Science, UTK.

2003: Taught a course on Advance Topics in Biochemistry: Advances in Recombinant DNA Technology (2003). This course was developed for undergraduate students to demonstrate and highlight the relationship between basic research and biotechnology.

1999-present: Mentor and supervisor to approximately 25 undergraduate students partaking in Department of Energy Programs such as ERULF, HERE, GLCA, and SULI programs.

1998: Taught a course on the mechanisms of action of electron transferring flavoproteins to final year undergraduate students at University College Dublin.

1992-1997: Tutor and demonstrator to all levels of undergraduate students.

REVIEWING ACTIVITIES

Journal articles: American Chemical Society Symposium Series; Applied Biochemistry and Biotechnology; Biochimica et Biophysica Acta; Environmental Science and Technology; Journal of Microelectromechanical Systems; Journal of the American Chemical Society; Biophysical Journal; Journal of Physical Chemistry Letters; Cellulose; Enzyme Research; Process Biochemistry; Biosensors; Acta Biomaterialia; ACS Sustainable Chemistry and Engineering

Proposals: National Institutes of Health, National Science Foundation; Office of Biological and Environmental Research, Department of Energy

PUBLICATIONS

1. W. Leite, K. L. Weiss, G. Phillips, Q. Zhang, S. Qian, S. E. Tsutakawa, L. Coates, and H. O' Neill (2021). Conformational dynamics in the interaction of SARS-CoV- papain like protease with human interferon-stimulated gene protein . Journal of Physical Chemistry Letters. accepted for publication
2. M. Wilamowski, M. Hammel, W. Leite, Q. Zhang, Y. Kim, K. Weiss, R.Jedrzejczak, D. J. Rosenberg, Y. Fan, J. Bierma, A. H. Sarker, S.E. Tsutakawa, S. V. Pingali, H. M. O'Neill, A. Joachimiak, G. L. Hura. Transient and stabilized complexation of Nsp7, Nsp8 and Nsp12 in the SARS-CoV-2 replication-transcription complex (2021). Biophysical Journal. Accepted for publication
3. Y. Yuan, H. Li, W. Leite, Q. Zhang, P. V. Bonnesen, J. L. Labbé, K. L. Weiss, S.V. Pingali, K. Hong, V. S. Urban, S. I. Salmon and H. O'Neill "Biosynthesis and characterization of deuterated chitosan in filamentous fungus and yeast" (2021) Carbohydrate Polymers, accepted

4. Kneller, D. W., Phillips, G., Weiss, K. L., Pant, S., Zhang, Q., O'Neill, H. M., Coates, L., Kovalevsky, A. (2020). Unusual zwitterionic catalytic site of SARS-CoV-2 main protease revealed by neutron crystallography. Journal of Biological Chemistry, 295, 17365-17373. https://doi.org/10.1074/jbc.AC120.016154
5. R. Shah, S. Bhagia, J. Keum, S. V. Pingali, A. J. Ragauskas, B. H. Davison, and H. O'Neill "Structural Insights into Low and High Recalcitrance Natural Poplar Variants using Neutron and X-ray scattering" ACS Sustainable Chem. Eng. 2020, https://doi.org/10.1021/acssuschemeng.0c05251
6. Zhu, Y; Plaza, N; Kojima, Y ; Yoshida, M ; Zhang, JW; Jellison, J; Pingali, SV; O'Neill, H ; Goodell, B Nanostructural Analysis of Enzymatic and Non-enzymatic Brown Rot Fungal Deconstruction of the Lignocellulose Cell Wall Frontiers in Microbiology Volume: 11, Article Number: 1389 DOI: 10.3389/fmicb.2020.01389
7. Astner A., Hayes D.G., Pingali S.V., O'Neill H.M., Littrell K.C., Evans B.R., Urban V.S., "Effects of soil particles and convective transport on dispersion and aggregation of nanoplastics via small-angle neutron scattering (SANS) and ultra SANS (USANS)", PLoS One, 15, e0235893 (2020).
8. Kneller, D.W., Phillips, G., O'Neill, H.M., Jedrzejczak, R., Stols, L., Langan, P., Joachimiak, A., Coates, L., Kovalevsky, A. "Structural plasticity of SARS-CoV-2 3CL Mpro active site cavity revealed by room temperature X-ray crystallography" Nature Communications, 11, 3202 (2020).
9. Pingali S.V., Smith M.D., Liu S., Rawal T., Pu Y., Shah R., Evans B.R., Urban V.S., Davison B., Cai C.M., Ragauskas A., O'Neill H.M., Smith J.C., Petridis L., "Deconstruction of biomass enabled by local demixing of cosolvents at cellulose and lignin surfaces", Proceedings of the National Academy of Sciences of the United States of America, 117, 29, 16776-16781 (2020).
10. Sherekar M., Han S., Ghirlando R., Messing S., Drew M., Rabara D., Waybright T., Juneja P., O'Neill H.M., Stanley C.B., Bhowmik D., Ramanathan A., Subramaniam S., Nissley D.V., Gillette W., McCormick F., Esposito D., "Biochemical and structural analyses reveal that the tumor suppressor neurofibromin (NF1) forms a high-affinity dimer", Journal of Biological Chemistry, 295, 1105-1119 (2020).
11. Shrestha, U. R.; Juneja, P.; Zhang, Q.; Gurumoorthy, V.; Borreguero, J. M.; Urban, V.; Cheng, X.; Pingali, S. V.; Smith, J. C.; O'Neill, H. M.; Petridis, L., Generation of the configurational ensemble of an intrinsically disordered protein from unbiased molecular dynamics simulation. *Proc Natl Acad Sci USA*, 116 (41), 20446 (2020).
12. Evans, B.; Pingali, S. V.; Bhagia, S.; O'Neill, H.; Ragauskas, A. J. "Structural Studies of Deuterium-Labeled Switchgrass Biomass" in "Understanding Lignocellulose: Synergistic Computational and Analytic Methods" ACS Symposium Series Vol. 1338, Chapter 2 pp 17-32, DOI: 10.1021/bk-2019-1338.ch002
13. Astner, A. F, Hayes, D. G., O'Neill, H., Evans, B. R., Pingali, S., Urban, V. S., Young, T. M. "Mechanical formation of micro- and nano-plastic materials for environmental studies in agricultural ecosystems" Science of the Total Environment Volume: 685 Pages: 1097-1106 DOI: 10.1016/j.scitotenv.2019.06.241
14. Rawal, TB; Ozcan, A; Liu, SH ; Pingali, SV; Akbilgic, O; Tetard, L; O'Neill, H; Santra, S; Petridis, L "Interaction of Zinc Oxide Nanoparticles with Water: Implications for Catalytic Activity" ACS Applied Nano Materials Volume: 2 Issue: 7 Pages: 4257-4266 DOI: 10.1021/acsanm.9b00714
15. Sharma, V. K.; Hayes, D. G.; Gupta, S.; Urban, V. S.; O'Neill, H. M.; Pingali, S. V.; Ohl, M.; Mamontov, E. "Incorporation of Melittin Enhances Interfacial Fluidity of Bicontinuous Microemulsions" Journal of Physical Chemistry C Volume: 123 Issue: 17 Pages: 11197-11206 DOI: 10.1021/acs.jpcc.9b00103
16. Ashkar, R; Bilheux, HZ; Bordallo, H; Briber, R; Callaway, DJE; Cheng, XL; Chu, XQ; Curtis, JE; Dadmun, M ; Fenimore, P; Fushman, D; Gabel, F; Gupta, K; Herberle, F; Heinrich, F; Hong, L ; Katsaras, J ; Kelman, Z ; Kharlampieva, E ; Kneller, GR ; Kovalevsky, A ; Krueger, S ; Langan, P; Lieberman, R ; Liu, Y ; Losche, M ; Lyman, E ; Mao, YM ; Marino, J ; Mattos, C ; Meilleur, F ; Moody, P ; Nickels, JD ; O'Dell, WB ; O'Neill, H ; Perez-Salas, U ; Peters, J ; Petridis, L ; Sokolov, AP ; Stanley, C ; Wagner, N ; Weinrich, M ; Weiss, K ; Wymore, T ; Zhang, Y ; Smith, JC

"Neutron scattering in the biological sciences: progress and prospects" Acta Crystallographica Section D-Structural Biology Volume: 74 Pages: 1129-1168 Part: 12 DOI:10.1107/S2059798318017503
17. Shah, R ; Huang, SX ; Pingali, SV ; Sawada, D ; Pu, YQ ; Rodriguez, M ; Ragauskas, AJ ; Kim, SH ; Evans, BR ; Davison, BH ; O'Neill, H "Hemicellulose-Cellulose Composites Reveal Differences in Cellulose Organization after Dilute Acid Pretreatment" Biomacromolecules Volume: 20 Issue: 2 Pages: 893-903 DOI: 10.1021/acs.biomac.8b01511
18. Liu, Z; Yang, CX ; Huang, J ; Ciampalini, G ; Li, J; Sakai, VG; Tyagi, M; O'Neill, H; Zhang, Q; Capaccioli, S; Ngai, KL ; Hong, L "Direct Experimental Characterization of Contributions from Self-Motion of Hydrogen and from Interatomic Motion of Heavy Atoms to Protein Anharmonicity" Journal of Physical Chemistry B Volume: 122 Issue: 43 Pages: 9956-9961 DOI: 10.1021/acs.jpcb.8b09355
19. B.R. Evans, M. Foston, H. O'Neill, D. Reeves, C. Rempe, K. McGrath, and A.J. Ragauskas "Production of Deuterated Biomass by Cultivation of the Duckweed Lemna minor in D_2O" Planta Volume: 249 Issue: 5 Pages: 1465-1475 DOI: 10.1007/s00425-019-03097-3
20. L. Stingaciu, H. O'Neill, M. Liberton, H.B. Pakrasi, VS. Urban "Influence of Chemically Disrupted Photosynthesis on Cyanobacterial Thylakoids Dynamics" Scientific Reports Volume: 9 Article Number: 5711 DOI: 10.1038/s41598-019-42024-0
21. Shrestha, U; Smith, S; Pingali, SV; Yang, H; Zahran, M; Breunig, L; Wilson, L; Kowalik, M; Kubicki, J; Cosgrove, D; O'Neill, H; Petridis, L "Arabinose Substitution Enhances Rigidity of Grass Arabinoxylans" Cellulose Volume: 26 Issue: 4 Pages: 2267-2278 DOI: 10.1007/s10570-018-2202-8
22. M. Raeeszadeh-Sarmazdeh, N Patel, S Cruise, L Owen, H O'Neill, ET. Boder "Stable domain identification of Cellulose Synthase using Yeast Surface Display" Biotechnology Journal, accepted (2018) Volume: 14 Issue: 4 Article Number: 1800353 DOI: 10.1002/biot.201800353
23. P. Phyo, T. Wang, S. Kiemle, H. O'Neill, S. V. Pingali, M. Hong, and D. Cosgrove (2018) "Gradients in wall mechanics and polysaccharides along growing Arabidopsis inflorescence stems" *Plant Physiology*, DOI: https://doi.org/10.1104/pp.17.01270
24. J.D. Kubicki, H. Yang, D. Sawada, H. O'Neill, D. Oehme1 and D. Cosgrove "The Shape of Native Plant Cellulose Microfibrils" Scientific Reports 8:13983 DOI:10.1038/s41598-018-32211-w (2018)
25. Hayes, DG; Pingali, SV; O'Neill, HM; Urban, VS; Ye, R "Observation of a structural gradient in Winsor-III microemulsion systems" Soft Matter Volume: 14 Issue: 25 Pages: 5270-5276 DOI: 10.1039/c8sm00322j
26. D. G. Hayes; R. Ye; R.N. Dunlap; D.B. Anunciado; S. V. Pingali; H. M. O'Neill; V. S Urban "Bicontinuous Microemulsions as a Biomembrane Mimetic System for Melittin" *BBA – Biomembranes,* Volume: 1860 Issue: 2 Pages: 624-632 (2018)
27. P. Phyo, T Wang, Y. Yang, Hugh O'Neill, and M. Hong "Direct Determination of Hydroxymethyl Conformations of Plant Cell Wall Cellulose Using 1H Polarization Transfer Solid-State NMR" Biomacromolecules, 19 (5), pp 1485–1497 DOI: 10.1021/acs.biomac.8b00039 (2018)
28. Vural, D; Gainaru, C; O'Neill, H; Pu, YQA; Smith, MD; Parks, JM; Pingali, SV; Mamontov,E; Davison, BH; Sokolov, AP; Ragauskas, AJ ; Smith, JC ; Petridis, L "Impact of hydration and temperature history on the structure and dynamics of lignin" Green Chemistry 20, 1602-1611 (2018)
29. Makarem, M ; Lee, CM ; Sawada, D ; O'Neill, HM ; Kim, SH "Distinguishing Surface versus Bulk Hydroxyl Groups of Cellulose Nanocrystals Using Vibrational Sum Frequency Generation Spectroscopy" J. Physical Chemistry Letters 9, 70-75 (2018)
30. Sawada, D; Kalluri, UC; O'Neill, H; Urban, V; Langan, P; Davison, B; Pingali, SV "Tension wood structure and morphology conducive for better enzymatic digestion" Biotechnology for Biofuels 11, 44 (2018)
31. Smith II, C; Wagle, D; O'Neill, H; Evans, B; Baker, S; Baker, G "Bacterial Cellulose Ionogels as Chemosensory Supports" ACS Applied Materials & Interfaces, 2017, 9 (43), pp 38042–38051
32. Hayes D.G., Ye R., Dunlap B.S., Cuneo M.J., Pingali S.V., O'Neill H.M., Urban V.S. (2017) Proteins extraction into the biocontinous microemulsion phase of a water/SDS/pentanol/dodecane

Winsor-III system: Effect on nanostructure and protein conformation. *Colloids Surf B Biointerfaces* (2017);160:144-153.
33. H. O'Neill, S. V. Pingali, L. Petridis, J. He, E. Mamontov, L. Hong, V. Urban, B. Evans, P. Langan, J. C. Smith, and B. H. Davison "Dynamics of water bound to crystalline cellulose" Scientific Reports, volume 7, Article number: 11840 (2017) doi:10.1038/s41598-017-12035-w
34. M.D. Gelenter; T. Wang; Shu-Yu Liao; H. O'Neill, Ph.D.; M. Hong "2H-13C Correlation Solid-State NMR for Investigating Dynamics and Water Accessibilities of Proteins and Carbohydrates" Journal of Biomolecular NMR, 68(4):257-270
35. Smith, CJ; Wagle, DV; O'Neill, HM; Evans, BR; Baker, SN; Baker, GA "Multi-Purpose Cellulosic Ionogels"in Ionic Liquids: Current State and Future Directions (Edited by:Shiflett, MB; Scurto, AM) ACS Symposium Series Volume: 1250 Pages: 143-155 (2017)
36. B. R. Evans, G. Bali, A. Ragauskas, R. Shah, C. Howard, H. M. O'Neill, F. Lavenhouse, D. Ramirez, K. Weston, K. Ramey, V. Cangemi, B. Kinney, C. Partee, T. Ware, B. Davison, "Allelopathic effects of exogenous phenylalanine: a comparison of four monocot species." Planta, (2017). http://dx.doi.org/10.1007/s00425-017-2720-x
37. Sharma, V. K.; Hayes, D. G.; Urban, V. S.; O'Neill, H. M.; Tyagi, M.; Mamontov, E., Nanoscopic dynamics of bicontinous microemulsions: effect of membrane associated protein. *Soft Matter* **2017,** *13* (28), 4871-4880.
38. Makarem, M.; Sawada, D.; O'Neill, H. M.; Lee, C. M.; Kafle, K.; Park, Y. B.; Mitta, A.; Kim, S. H., Dependence of Sum Frequency Generation (SFG) Spectral Features on the Mesoscale Arrangement of SFG-Active Crystalline Domains Interspersed in SFG-Inactive Matrix: A Case Study with Cellulose in Uniaxially Aligned Control Samples and Alkali-Treated Secondary Cell Walls of Plants. *J Phys Chem C* **2017,** *121* (18), 10249-10257.
39. Liu, Z.; Huang, J.; Tyagi, M.; O'Neill, H.; Zhang, Q.; Mamontov, E.; Jain, N.; Wang, Y. J.; Zhang, J.; Smith, J. C.; Hong, L., Dynamical Transition of Collective Motions in Dry Proteins. *Phys Rev Lett* **2017,** *119* (4).
40. Goodell, B.; Zhu, Y.; Kim, S.; Kafle, K.; Eastwood, D.; Daniel, G.; Jellison, J.; Yoshida, M.; Groom, L.; Pingali, S. V.; O'Neill, H., Modification of the nanostructure of lignocellulose cell walls via a non-enzymatic lignocellulose deconstruction system in brown rot wood-decay fungi. *Biotechnol Biofuels* **2017,** *10*.
41. Anunciado, D. B.; Nyugen, V. P.; Hurst, G. B.; Doktycz, M. J.; Urban, V.; Langan, P.; Mamontov, E.; O'Neill, H., In Vivo Protein Dynamics on the Nanometer Length Scale and Nanosecond Time Scale. *J Phys Chem Lett* **2017,** *8* (8), 1899-1904.
42. Pingali, SV; Urban, VS; Heller, WT; McGaughey, J; O'Neill, H; Foston, MB; Li, H; Wyman, CE; Myles, DA.; Langan, P; Ragauskas, A.; Davison, B.; Evans, B. R., Understanding Multiscale Structural Changes During Dilute Acid Pretreatment of Switchgrass and Poplar. *Acs Sustain Chem Eng* **2017,** *5* (1), 426-435.
43. Mamontov, E.; O'Neill, H., Microscopic relaxations in a protein sustained down to 160 K in a non-glass forming organic solvent. *Biochimica Et Biophysica Acta-General Subjects* **2017,** *1861* (1), 3513-3519.
44. Shrestha, U; Bhowmik, D; Van Delinder, K; Mamontov, E; O'Neill, H; Zhang, Q; Alatas, A; Chu, X.Q" Collective excitations in protein as a measure of balance between its softness and rigidity" J. Phys. Chem. B,2017,121, 923–930
45. S Perticaroli, G Ehlers, C B. Stanley, E Mamontov, H O'Neill, Q Zhang, X Cheng, D A. A. Myles, Jo Katsaras, J D. Nickels "Description of Hydration Water in Protein Solutions" *J. Am. Chem. Soc.*, 2017, 139 (3), pp 1098–1105
46. VG Vandavasi and H O' Neill "Heterologous Expression and Purification of Catalytic Domain of CESA1 from Arabidopsis "Bio-protocol 6(20): e1965. DOI: 10.21769/BioProtoc.1965
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48. Dhindsa GK, Bhowmik D, Goswami M, O'Neill HM, Mamontov E, Sumpter BG, Hong L, Ganesh P, Chu X-q. Enhanced Dynamics of Hydrated tRNA on Nanodiamond Surfaces: A Combined Neutron Scattering and MD Simulation Study. The Journal of Physical Chemistry B. 2016. *J. Phys. Chem. B*, 2016, 120 (38), pp 10059–10068
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50. Stingaciu L-R, O'Neill H, Liberton M, Urban VS, Pakrasi HB, Ohl M. Revealing the dynamics of thylakoid membranes in living cyanobacterial cells. Scientific reports. 2016;6.
51. Rai DK, Sharma VK, Anunciado D, O'Neill H, Mamontov E, Urban V, Heller WT, Qian S. Neutron Scattering Studies of the Interplay of Amyloid β Peptide (1–40) and An Anionic Lipid 1, 2-dimyristoyl-sn-glycero-3-phosphoglycerol. Scientific Reports. 2016;6.
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53. O'Neill H, Shah R, Evans BR, He J, Pingali SV, Chundawat SP, Jones AD, Langan P, Davison BH, Urban V. Chapter Six-Production of Bacterial Cellulose with Controlled Deuterium–Hydrogen Substitution for Neutron Scattering Studies. Methods in Enzymology. 2015;565:123-46.
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55. Anunciado D, Rai DK, Qian S, Urban V, O'Neill H. Small-angle neutron scattering reveals the assembly of alpha-synuclein in lipid membranes. Biochimica et Biophysica Acta (BBA)-Proteins and Proteomics. 2015;1854(12):1881-9.
56. Sharma VK, Mamontov E, Anunciado DB, O'Neill H, Urban V. Nanoscopic Dynamics of Phospholipid in Unilamellar Vesicles: Effect of Gel to Fluid Phase Transition. J Phys Chem B. 2015;119(12):4460-70.
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63. Heller WT, Urban VS, Lynn GW, Weiss KL, O'Neill HM, Pingali SV, et al. The Bio-SANS instrument at the High Flux Isotope Reactor of Oak Ridge National Laboratory. J Appl Crystallogr. 2014;47:1238-46.
64. Bodenheimer AM, Cuneo MJ, Swartz PD, He JH, O'Neill HM, Myles DAA, et al. Crystallization and preliminary X-ray diffraction analysis of Hypocrea jecorina Cel7A in two new crystal forms. Acta Crystallogr F. 2014;70:773-6.
65. Mamontov E, O'Neill H. Reentrant Condensation of Lysozyme: Implications for Studying Dynamics of Lysozyme in Aqueous Solutions of Lithium Chloride. Biopolymers. 2014;101(6):624-9.
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small-angle neutron scattering and molecular dynamics simulation. Arch Biochem Biophys. 2014;550:50-7.
67. Wang H, Gurau G, Pingali SV, O'Neill HM, Evans BR, Urban VS, et al. Physical Insight into Switchgrass Dissolution in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate. Acs Sustain Chem Eng. 2014;2(5):1264-9.
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BOOK CHAPTERS

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5. Barbara R. Evans, Jane Y. Howe, Hugh O'Neill, and Madhavi Martin "Biopatterned paper containing metallic nanoparticles for manufacture of composite materials" (2007), Invention disclosure 05-324
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TECHNICAL REPORTS AND PROCEEDINGS PAPERS

1. Contributing author to "First Experiments: New Science Opportunities at the Spallation Neutron Source Second Target Station", December 2019 (https://neutrons.ornl.gov/sts/documents)
2. Contributing Author to workshop report entitled "Understanding Complexity in Biological and Environmental Systems Through Neutron Science" March, 2019
3. Contributing Author to workshop report entitled "Workshop to Identify Opportunities Biological and Environmental Research Uniquely Enabled by the APS Upgrade" August 28-29, 2018 (http://www.osti.gov/scitech/)
4. Contributing author "Technologies for Characterizing Molecular and Cellular Systems Relevant to Bioenergy and Environment Workshop" Report from workshop convened by U.S. Department of Energy Office of Science Office of Biological and Environmental Research September 21–23, 2016
5. Contributing author "How Light and Neutron Facilities Can Enable Biological Systems Science Relevant to DOE's Biological and Environmental Research " Report from the Workshop Convened at SLAC National Accelerator Laboratory Menlo Park, California August 25, 2016
6. Qian S., Pingali S.V., Weiss K., Urban V.S., O'Neill H.M., Langan P., (2016) "Neutron Scattering for Biological Research: Progress at the Bio-SANS Beam Line", TechConnect Briefs: Advanced Materials: Chapter 1 Nanoscale Materials Characterization ISBN: 978-0-9975-1170-3
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10. Xiang Yu, Yugang Li, Hugh M. O'Neill, S. Michael Kilbey II, Jimmy W. Mays, Phillip F. Britt, and Kunlun Hong "Synthesis and Characterization of Block Copolymers with Polythiophene Segments by

the Combination of Atom Transfer Radical Polymerization and Kumada Catalyst-Transfer Polycondensation" (2011) *American Chemical society PMSE Division Preprints*

11. Hugh O'Neill, Mateus B. Cardoso, Xiang Yu, Angela Pack, Dmitriy Smolensky, Qiu Zhang, William T. Heller, Kunlun Hong (2011) "Development of biohybrid solar energy conversion systems" *American Chemical society Fuel Chemistry Division Preprints*
12. Hugh O'Neill, Xu Liu, Erin Lauer, Xiang Yu, Kunlun Hong "Development of a biohybrid micellar system for solar hydrogen production" (2010) *American Chemical society Fuel Chemistry Division Preprints*
13. Mateus B. Cardoso, Dmitriy Smolensky, Kunlun Hong, William T. Heller, and Hugh O'Neill "Supramolecular Assembly of Artificial Photoconversion Systems", (2010) *American Chemical society PMSE Division Preprints*
14. Mateus B. Cardoso, Dmitriy Smolensky, William T. Heller, Hugh O'Neill (2010) "Investigation of detergent effects on the solution structure of spinach Light Harvesting Complex II". *J. Phys. Conf. Series* 251: 012041
15. Latasha Garrett and Hugh O'Neill (2007) "The effect of surface chemistry on the properties of proteins confined in nanoporous materials" *Journal of Undergraduate Research*, 7, 15-21
16. Hugh O'Neill, Barbara R. Evans, Ida Lee and Elias Greenbaum (2005) "Photovoltaic properties of Spinach Photosystem I reaction centers in solution" *Proceedings of the International Association of Nanotechnology*
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23. Hugh O'Neill and Jonathan Woodward (2000) "Construction of a bio-hydrogen fuel cell that utilizes environmental sources of carbohydrates" Report for Energy Harvesting/Biofuel Cells, Defense Advanced Research Projects Agency.

INVITED PRESENTATIONS (since 2010)

1. "COVID-19 research at Neutron Sources", American Physical Society, Accelerators for Society, April 18, 2021
2. "Opportunities for characterizing molecular to mesoscale biological processes using neutrons" at The Center for Biomolecular Structure lecture series, NSLSII, Brookhaven National Lab, February 17, 2021.
3. "Bio-Deuteration at ORNL", DUENET Meeting, November 2, 2020
4. "Biological Applications of Neutron Scattering" presented at the Advanced Light Source Biosciences Workshop Februrary 13th, 2019

5. “Hemicellulose-cellulose composites reveal differences in cellulose organization after dilute acid pretreatment” Presented at the American Chemical Society Meeting Mar 31-APR 04, 2019 Orlando, FL
6. “Fundamental insights into biomass deconstruction using neutron scattering” presented at the 2nd CRC-CABLE Bioeconomy in East Tennessee Symposium
7. "Opportunities for characterizing molecular to mesoscale biological processes using neutrons" EMSL Integration 2018 Molecular Biological and Environmental Science August 6-8, 2018 [plenary talk]
8. "Neutron scattering Biology Program: From Atoms to Cells" Opportunities in Biological and Environmental Research Uniquely Enabled by the APS Upgrade, Advanced Photon Source, ANL, August 28-29, 2018
9. "Combining deuterium-labeling and neutron scattering to gain molecular-level insights relevant to biomass deconstruction" 256th American Chemical Society National Meeting Boston, August 19-23, 2018
10. "Opportunities for characterizing molecular to mesoscale biological processes using neutrons" Stanford Synchrotron Radiation Lightsource (SSRL/SLAC National Accelerator Laboratory (SLAC) October 25, 2017
11. "Domain organization in CESA proteins of the plant cellulose synthesis complex" 6th International Conference on Plant Cell Wall Biology, Dalian, China, July 16 – 20, 2017
12. "Organization of domains in CESA proteins of the plant cellulose synthesis complex" 253rd ACS National Meeting in San Francisco, California, April 2-6, 2017
13. "Investigations of Plant Cell Wall Synthesis and Deconstruction" Department of Biological Sciences, Purdue University, April 18, 2017
14. “Structural studies of the cellulose synthesis complex” Biochemistry and Cellular and Molecular Biology Department, University of Tennessee, Knoxville, February 15, 2017
15. “Characterizing plant and microbial structural transformations for bioconversion using neutrons” 2017 Genomic Sciences Program Annual Principal Investigator (PI) Meeting February 5-8, 2017
16. “Structural Studies of Recombinant Plant CESA Domains of the Plant Cellulose Synthesis Complex “ 5th Biennial Physical Biosciences Research Meeting, Gaithersburg, MD October 16-19, 2016
17. "Neutron technologies for characterizing molecular to mesoscale biological processes" at Technologies for Characterizing Molecular and Cellular Systems Relevant to Bioenergy and Environment” held September 21-23, 2016, in Rockville, Maryland
18. “Neutrons in biology” at the FICUS coordination meeting Joint Genome Institute (JGI) July 11, 2016
19. “What neutron scattering can tell us about biomass pretreatment” annual BESC Characterization Workshop January 7th and 8th, 2016 at the Mission Inn in Riverside, CA.
20. “Lignocellulose Biofuels Research at ORNL” 2015 International Chemical Congress of the Pacific Basin Societies, Honolulu, Hawaii, December 15 – 20, 2015
21. “Small-angle neutron scattering reveals the assembly of alpha-synuclein in lipid membranes” presented at the NINDS sponsored SFN satellite meeting entitled “How can understanding protein structure help us unravel the mysteries of neurodegenerative disease? Chicago, Oct 18,2015
22. “Applications of Neutron Scattering in Studies of Complex Biological Systems” Genomic Science Contractors-Grantees Meeting XIII/USDA-DOE Plant Feedstock Genomics for Bioenergy Meeting at Washington DC (Tyson’s Corner, Virginia) February, 2014
23. “The Bio-deuteration Laboratory at Oak Ridge National Laboratory” Frontiers in Neutron Biology, ORNL April 16-18, 2013
24. “Investigation of water dynamics in a model cellulosic system” CELL: Division of 245th American Chemical Society Meeting, New Orleans, April 7 - 11, 2013
25. “Development of Biohybrid Solar Energy Conversion Systems Based on Plant Light Harvesting Complex II” University of Tennessee STAIR Seminar March 19, 2013
26. **“**Investigation of Structural Changes in Cel7A Cellulase when Bound to Cellulose Substrates” Frontiers in Biorefining 2012 Oct 30 – Nov 2, St. Simons Island, GA

27. “Biohybrid Photoconversion systems” at the Symposium of the China-US 2011 Joint Center for Ecosystem and Environmental Change, at Purdue University, to present at the workshop entitled "Barriers to Sustainable Photosynthetic Production of Biofuels and Bioenergy." Sept 29th 2011
28. “Development of Biohybrid Photoconversion Systems Based on Plant Light Harvesting Complex II” 2012 Annual Meeting of the American Crystallographic Association, Boston, Massachusetts July 28 to August 1
29. “Development of Biohybrid Photoconversion Systems Based on Plant Light Harvesting Complex II” Department of Chemistry, University of Missouri at Columbia Sept 2012
30. “Studies on Natural Light Harvesting Antennae: *Towards development of artificial photosynthetic systems*” Biochemistry and Cellular and Molecular Biology Department, University of Tennessee, Knoxville. Invited presentation Oct 2010

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GRADUATE AND POST-DOCTORAL ADVISORS

Professor Stephen Mayhew, University College Dublin, retired.
Dr. Jonathan Woodward, Oak Ridge National Laboratory, retired

FUNDING

Current

1. DOE BER ERKPA14 9/01/20-09/30/22
   A multimodal small-angle neutron scattering instrument for studies of flexible and dynamic biological assemblies
   The goal of this project is to develop a conceptual design of a SANS instrument optimized for characterization of biological systems for the Second Target Station at ORNL's Spallation Neutron Source
   Role: PI

2. DOE BER ERKP291 10/01/18-09/30/21
   Center for Structural Molecular Biology
   The center supports and develops the user access and science research program of the Bio-SANS instrument at the High Flux Isotope Reactor and the Bio-Deuteration Laboratory located at the Spallation Neutron Source.
   Role: PI, Director
3. DOE BER ERKP300 10/01/19-08/31/20
   A multimodal small-angle neutron scattering instrument for studies of flexible and dynamic biological assemblies
   The goal of this project is to develop a conceptual design of a SANS instrument optimized for characterization of biological systems for the Second Target Station at ORNL's Spallation Neutron Source
   Role: PI
4. DOE BES ERKCSE5 08/01/18-07/31/21
   Center for Lignocellulose Structure and Formation, a DOE Energy Frontier Research Center [Penn State Lead Institution]
   The goal of this project is to understand the molecular basis for how the plant cell wall is synthesized and assembled.
   Role: ORNL PI
5. LDRD Director's R&D Fund, Oak Ridge National Laboratory (8858) 10/01/17-09/30/20
   Obtaining atomistic insights into flexible biomolecular systems by data-driven integration of cryo-electron microscopy, neutron scattering and molecular simulations
   Role: PI
6. DOE BER ERKP752 10/01/18-09/30/21
   Neutron Imaging and Simulation of Lignocellulose Deconstruction
   The goal of this project is a multitscale analysis of lignocellulose deconstruction using neutron scattering and computational simulation techniques.
   Role: Co-PI- Task lead

Completed projects (since 2010)

1. LDRD Director's R&D Fund, Oak Ridge National Laboratory (8272) 10/01/16-09/30/19
   Integrating Small-Angle Neutron Scattering with Molecular Simulation to Determine Structural Ensembles of Complex Biological Systems
   Role: Co-PI
2. DOE BES ERKCC69 08/01/014-07/31/18
   The Photosynthetic Antenna Research Center, a DOE Energy Frontier Research Center

The goal of this center is the development of novel approaches to the capture of solar energy through a fundamental understanding of natural photosynthetic processes.
Role: Research Affiliate

3. DOE BER 3ERKP851 05/01/14- 05/01/17
Advanced Biosystems Imaging Integrates neutron sciences, nanofabrication and high speed computation to study how observable biological processes, carried out over wide ranging temporal and spatial scales arise from molecular scale events.
Role: Co-PI
4. LDRD Director's R&D Fund, Oak Ridge National Laboratory 10/01/14-09/30/17
Increasing advanced biofuels production from terpenes in *Eucalyptus* leaves
The goal of this project is to study the properties of microemulsion systems optimized for biocatalytic conversion.
Role: Co-PI
5. LDRD Director's R&D Fund, Oak Ridge National Laboratory 10/01/12-09/30/15
Structural Biology of Metabolic and Signaling Pathways in Plants
The goal of this project is to determine the structure of the cellulose synthase complex using a combination of protein crystallography, small-angle scattering and computation.
Role: PI
6. LDRD Director's R&D Fund, Oak Ridge National Laboratory 10/01/12-09/30/14
Developing Grazing Incident Small-Angle Neutron Scattering for Studying the Interplay between Amyloid-beta Peptide and Cholesterol in Lipid Bilayers
The goal of this project is to develop grazing incidence SANS to investigate the interaction of amyloidogenic proteins and lipid membranes.
Role: Co-PI
7. LDRD Director's R&D Fund, Oak Ridge National Laboratory 10/01/12-09/30/14
Meso-scale Liquid Confinement Systems for Enhanced Bioseparations and Bioconversion Strategies
The goal of this project is study the properties of microemulsion systems optimized for biocatalytic conversion.
Role: Co-PI
8. LDRD 5079 Director's R&D Fund, Oak Ridge National Laboratory 10/01/08-09/30/11
Supra-Macromolecular Assembly of Artificial Photoconversion Units
Role: PI,
9. SERDP (Strategic Environmental Research Program (SERDP)) 10/01/09-09/30/10
Directed Biosynthesis of Oriented Crystalline Cellulose for Advanced Composite Fibers
Role: PI