Hugh M O neill

List of Publications by Citations

133 papers	4,091 citations	35 h-index	59 g-index
140 ext. papers	4,906 ext. citations	6.1 avg, IF	5.5 L-index

#	Paper	IF	Citations
133	Biomimetic synthesis of calcium-deficient hydroxyapatite in a natural hydrogel. *Biomaterials*, **2006**, 27, 4661-70	15.6	279
132	Structural plasticity of SARS-CoV-2 3CL M active site cavity revealed by room temperature X-ray crystallography. *Nature Communications*, **2020**, 11, 3202	17.4	185
131	Palladium-bacterial cellulose membranes for fuel cells. *Biosensors and Bioelectronics*, **2003**, 18, 917-23	11.8	181
130	Common processes drive the thermochemical pretreatment of lignocellulosic biomass. *Green Chemistry*, **2014**, 16, 63-68	10	159
129	High photo-electrochemical activity of thylakoid–carbon nanotube composites for photosynthetic energy conversion. *Energy and Environmental Science*, **2013**, 6, 1891	35.4	146
128	Self-organized photosynthetic nanoparticle for cell-free hydrogen production. *Nature Nanotechnology*, **2010**, 5, 73-9	28.7	146
127	Breakdown of cell wall nanostructure in dilute acid pretreated biomass. *Biomacromolecules*, **2010**, 11, 2329-35	6.9	126
126	Comparative Structural and Computational Analysis Supports Eighteen Cellulose Synthases in the Plant Cellulose Synthesis Complex. *Scientific Reports*, **2016**, 6, 28696	4.9	104
125	Dynamics of protein and its hydration water: neutron scattering studies on fully deuterated GFP. *Biophysical Journal*, **2012**, 103, 1566-75	2.9	101
124	Effect of lignin content on changes occurring in poplar cellulose ultrastructure during dilute acid pretreatment. *Biotechnology for Biofuels*, **2014**, 7, 150	7.8	94
123	A microbial fuel cell operating at low pH using the acidophile Acidiphilium cryptum. *Biotechnology Letters*, **2008**, 30, 1367-72	3	80
122	A Structural Study of CESA1 Catalytic Domain of Arabidopsis Cellulose Synthesis Complex: Evidence for CESA Trimers. *Plant Physiology*, **2016**, 170, 123-35	6.6	78
121	Organization and flexibility of cyanobacterial thylakoid membranes examined by neutron scattering. *Journal of Biological Chemistry*, **2013**, 288, 3632-40	5.4	73
120	The Bio-SANS instrument at the High Flux Isotope Reactor of Oak Ridge National Laboratory. *Journal of Applied Crystallography*, **2014**, 47, 1238-1246	3.8	67
119	Characterization of the influence of the ionic liquid 1-butyl-3-methylimidazolium chloride on the structure and thermal stability of green fluorescent protein. *Journal of Physical Chemistry B*, **2010**, 114, 13866-71	3.4	65
118	Self-similar multiscale structure of lignin revealed by neutron scattering and molecular dynamics simulation. *Physical Review E*, **2011**, 83, 061911	2.4	61
117	Malleability of the SARS-CoV-2 3CL M Active-Site Cavity Facilitates Binding of Clinical Antivirals. *Structure*, **2020**, 28, 1313-1320.e3	5.2	61

116	Gradients in Wall Mechanics and Polysaccharides along Growing Inflorescence Stems. *Plant Physiology*, **2017**, 175, 1593-1607	6.6	57
115	Dynamics of water bound to crystalline cellulose. *Scientific Reports*, **2017**, 7, 11840	4.9	56
114	Description of Hydration Water in Protein (Green Fluorescent Protein) Solution. *Journal of the American Chemical Society*, **2017**, 139, 1098-1105	16.4	53
113	Modification of the nanostructure of lignocellulose cell walls via a non-enzymatic lignocellulose deconstruction system in brown rot wood-decay fungi. *Biotechnology for Biofuels*, **2017**, 10, 179	7.8	52
112	Secondary structure and rigidity in model proteins. *Soft Matter*, **2013**, 9, 9548-56	3.6	50
111	Unusual zwitterionic catalytic site of SARS-CoV-2 main protease revealed by neutron crystallography. *Journal of Biological Chemistry*, **2020**, 295, 17365-17373	5.4	50
110	Effect of antimicrobial peptide on the dynamics of phosphocholine membrane: role of cholesterol and physical state of bilayer. *Soft Matter*, **2015**, 11, 6755-67	3.6	48
109	Enhanced Photocatalytic Hydrogen Evolution by Covalent Attachment of Plastocyanin to Photosystem I. *Nano Letters*, **2004**, 4, 1815-1819	11.5	47
108	The Shape of Native Plant Cellulose Microfibrils. *Scientific Reports*, **2018**, 8, 13983	4.9	47
107	Mechanical formation of micro- and nano-plastic materials for environmental studies in agricultural ecosystems. *Science of the Total Environment*, **2019**, 685, 1097-1106	10.2	46
106	Nanoscopic dynamics of phospholipid in unilamellar vesicles: effect of gel to fluid phase transition. *Journal of Physical Chemistry B*, **2015**, 119, 4460-70	3.4	45
105	Structural coarsening of aspen wood by hydrothermal pretreatment monitored by small- and wide-angle scattering of X-rays and neutrons on oriented specimens. *Cellulose*, **2014**, 21, 1015-1024	5.5	41
104	The effect of deuteration on the structure of bacterial cellulose. *Carbohydrate Research*, **2013**, 374, 82-82.9		40
103	Elastic and conformational softness of a globular protein. *Physical Review Letters*, **2013**, 110, 028104	7.4	40
102	Generation of the configurational ensemble of an intrinsically disordered protein from unbiased molecular dynamics simulation. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 20446-20452	11.5	38
101	Comparison of changes in cellulose ultrastructure during different pretreatments of poplar. *Cellulose*, **2014**, 21, 2419-2431	5.5	37
100	Hydration control of the mechanical and dynamical properties of cellulose. *Biomacromolecules*, **2014**, 15, 4152-9	6.9	36
99	A resorbable calcium-deficient hydroxyapatite hydrogel composite for osseous regeneration. *Cellulose*, **2009**, 16, 887-898	5.5	36

98	Mean-squared atomic displacements in hydrated lysozyme, native and denatured. *Journal of Biological Physics*, **2010**, 36, 291-7	1.6	34
97	Morphological changes in the cellulose and lignin components of biomass occur at different stages during steam pretreatment. *Cellulose*, **2014**, 21, 873-878	5.5	31
96	Characterization of sol-gel-encapsulated proteins using small-angle neutron scattering. *ACS Applied Materials & Interfaces*, **2009**, 1, 2262-8	9.5	31
95	Insight into the structure of light-harvesting complex II and its stabilization in detergent solution. *Journal of Physical Chemistry B*, **2009**, 113, 16377-83	3.4	31
94	Protein Localization in Silica Nanospheres Derived via Biomimetic Mineralization. *Advanced Functional Materials*, **2010**, 20, 3031-3038	15.6	31
93	Neutron scattering in the biological sciences: progress and prospects. *Acta Crystallographica Section D: Structural Biology*, **2018**, 74, 1129-1168	5.5	31
92	Direct Determination of Hydroxymethyl Conformations of Plant Cell Wall Cellulose Using H Polarization Transfer Solid-State NMR. *Biomacromolecules*, **2018**, 19, 1485-1497	6.9	30
91	Revealing the Dynamics of Thylakoid Membranes in Living Cyanobacterial Cells. *Scientific Reports*, **2016**, 6, 19627	4.9	28
90	Controlled incorporation of deuterium into bacterial cellulose. *Cellulose*, **2014**, 21, 927-936	5.5	28
89	Small angle neutron scattering reveals pH-dependent conformational changes in Trichoderma reesei cellobiohydrolase I: implications for enzymatic activity. *Journal of Biological Chemistry*, **2011**, 286, 32801-9	5.4	28
88	Room-temperature X-ray crystallography reveals the oxidation and reactivity of cysteine residues in SARS-CoV-2 3CL M: insights into enzyme mechanism and drug design. *IUCrJ*, **2020**, 7,	4.7	27
87	SANS study of cellulose extracted from switchgrass. *Acta Crystallographica Section D: Biological Crystallography*, **2010**, 66, 1189-93		25
86	The application and use of chemical space mapping to interpret crystallization screening results. *Acta Crystallographica Section D: Biological Crystallography*, **2008**, 64, 1240-9		24
85	Cloning and analysis of the genes for a novel electron-transferring flavoprotein from Megasphaera elsdenii. Expression and characterization of the recombinant protein. *Journal of Biological Chemistry*, **1998**, 273, 21015-24	5.4	24
84	Understanding Multiscale Structural Changes During Dilute Acid Pretreatment of Switchgrass and Poplar. *ACS Sustainable Chemistry and Engineering*, **2017**, 5, 426-435	8.3	23
83	Bacterial Cellulose Ionogels as Chemosensory Supports. *ACS Applied Materials & Interfaces*, **2017**, 9, 38042-38051	9.5	23
82	Spectroscopy and Photochemistry of Spinach Photosystem I Entrapped and Stabilized in a Hybrid Organosilicate Glass. *Chemistry of Materials*, **2005**, 17, 2654-2661	9.6	23
81	Distinguishing Surface versus Bulk Hydroxyl Groups of Cellulose Nanocrystals Using Vibrational Sum Frequency Generation Spectroscopy. *Journal of Physical Chemistry Letters*, **2018**, 9, 70-75	6.4	23

80	In Vivo Protein Dynamics on the Nanometer Length Scale and Nanosecond Time Scale. *Journal of Physical Chemistry Letters*, **2017**, 8, 1899-1904	6.4	22
79	Apparent Decoupling of the Dynamics of a Protein from the Dynamics of its Aqueous Solvent. *Journal of Physical Chemistry Letters*, **2012**, 3, 380-5	6.4	22
78	Dynamical Transition of Collective Motions in Dry Proteins. *Physical Review Letters*, **2017**, 119, 048101	7.4	21
77	Probing the consequences of antenna modification in cyanobacteria. *Photosynthesis Research*, **2013**, 118, 17-24	3.7	20
76	Coherent neutron scattering and collective dynamics in the protein, GFP. *Biophysical Journal*, **2013**, 105, 2182-7	2.9	20
75	Protein extraction into the bicontinuous microemulsion phase of a Water/SDS/pentanol/dodecane winsor-III system: Effect on nanostructure and protein conformation. *Colloids and Surfaces B: Biointerfaces*, **2017**, 160, 144-153	6	20
74	Role of methyl groups in dynamics and evolution of biomolecules. *Journal of Biological Physics*, **2012**, 38, 497-505	1.6	20
73	Neutron Scattering Studies of the Interplay of Amyloid Peptide(1-40) and An Anionic Lipid 1,2-dimyristoyl-sn-glycero-3-phosphoglycerol. *Scientific Reports*, **2016**, 6, 30983	4.9	20
72	Impact of hydration and temperature history on the structure and dynamics of lignin. *Green Chemistry*, **2018**, 20, 1602-1611	10	19
71	Analysis of the solution structure of Thermosynechococcus elongatus photosystem I in n-dodecyl-D-maltoside using small-angle neutron scattering and molecular dynamics simulation. *Archives of Biochemistry and Biophysics*, **2014**, 550-551, 50-7	4.1	19
70	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. *Journal of Physical Chemistry C*, **2017**, 121, 10249-10257	3.8	18
69	Physical Insight into Switchgrass Dissolution in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate. *ACS Sustainable Chemistry and Engineering*, **2014**, 2, 1264-1269	8.3	18
68	Excited-state dynamics of water-soluble polythiophene derivatives: temperature and side-chain length effects. *Journal of Physical Chemistry B*, **2012**, 116, 14451-60	3.4	18
67	Ammonia-salt solvent promotes cellulosic biomass deconstruction under ambient pretreatment conditions to enable rapid soluble sugar production at ultra-low enzyme loadings. *Green Chemistry*, **2020**, 22, 204-218	10	18
66	Tension wood structure and morphology conducive for better enzymatic digestion. *Biotechnology for Biofuels*, **2018**, 11, 44	7.8	17
65	Deuterium incorporation in biomass cell wall components by NMR analysis. *Analyst, The*, **2012**, 137, 1090-3	5	17
64	Temperature Dependence of Logarithmic-like Relaxational Dynamics of Hydrated tRNA. *Journal of Physical Chemistry Letters*, **2013**, 4, 936-42	6.4	17
63	Arabinose substitution effect on xylan rigidity and self-aggregation. *Cellulose*, **2019**, 26, 2267-2278	5.5	17

62	Nanoscopic dynamics of bicontinous microemulsions: effect of membrane associated protein. *Soft Matter*, **2017**, 13, 4871-4880	3.6	16
61	Supramolecular assembly of biohybrid photoconversion systems. *Energy and Environmental Science*, **2011**, 4, 181-188	35.4	16
60	Small-angle X-ray scattering study of photosystem I-detergent complexes: implications for membrane protein crystallization. *Journal of Physical Chemistry B*, **2007**, 111, 4211-9	3.4	16
59	Effect of D2O on growth properties and chemical structure of annual ryegrass (Lolium multiflorum). *Journal of Agricultural and Food Chemistry*, **2014**, 62, 2595-604	5.7	15
58	Effect of protein incorporation on the nanostructure of the bicontinuous microemulsion phase of Winsor-III systems: a small-angle neutron scattering study. *Langmuir*, **2015**, 31, 1901-10	4	15
57	Neutron Technologies for Bioenergy Research. *Industrial Biotechnology*, **2012**, 8, 209-216	1.3	15
56	Properties of carbohydrate-metabolizing enzymes immobilized in sol-gel beads: stabilization of invertase and □glucosidase by Blue Dextran**. *Biotechnology Letters*, **2002**, 24, 783-790	3	15
55	Laser-induced breakdown spectroscopy used to detect palladium and silver metal dispersed in bacterial cellulose membranes. *Applied Optics*, **2003**, 42, 6174-8	1.7	15
54	Interaction of Zinc Oxide Nanoparticles with Water: Implications for Catalytic Activity. *ACS Applied Nano Materials*, **2019**, 2, 4257-4266	5.6	14
53	Small-angle neutron scattering reveals the assembly of alpha-synuclein in lipid membranes. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2015**, 1854, 1881-1889	4	14
52	Biochemical and structural analyses reveal that the tumor suppressor neurofibromin (NF1) forms a high-affinity dimer. *Journal of Biological Chemistry*, **2020**, 295, 1105-1119	5.4	14
51	Nanostructural Analysis of Enzymatic and Non-enzymatic Brown Rot Fungal Deconstruction of the Lignocellulose Cell Wall. *Frontiers in Microbiology*, **2020**, 11, 1389	5.7	13
50	Enhanced Dynamics of Hydrated tRNA on Nanodiamond Surfaces: A Combined Neutron Scattering and MD Simulation Study. *Journal of Physical Chemistry B*, **2016**, 120, 10059-10068	3.4	13
49	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*, **2020**, 117, 16776-16781	11.5	13
48	Hemicellulose-Cellulose Composites Reveal Differences in Cellulose Organization after Dilute Acid Pretreatment. *Biomacromolecules*, **2019**, 20, 893-903	6.9	13
47	Production of deuterated switchgrass by hydroponic cultivation. *Planta*, **2015**, 242, 215-22	4.7	12
46	H-C correlation solid-state NMR for investigating dynamics and water accessibilities of proteins and carbohydrates. *Journal of Biomolecular NMR*, **2017**, 68, 257-270	3	11
45	Sol□gel entrapped light harvesting antennas: immobilization and stabilization of chlorosomes for energy harvesting. *Journal of Materials Chemistry*, **2012**, 22, 22582		11

44	Bicontinuous microemulsions as a biomembrane mimetic system for melittin. *Biochimica Et Biophysica Acta - Biomembranes*, **2018**, 1860, 624-632	3.8	11
43	Transient and stabilized complexes of Nsp7, Nsp8, and Nsp12 in SARS-CoV-2 replication. *Biophysical Journal*, **2021**, 120, 3152-3165	2.9	11
42	Biochemical and structural analyses reveal that the tumor suppressor neurofibromin (NF1) forms a high-affinity dimer. *Journal of Biological Chemistry*, **2020**, 295, 1105-1119	5.4	10
41	Combined Small-Angle Neutron Scattering, Diffusion NMR, and Molecular Dynamics Study of a Eutectogel: Illuminating the Dynamical Behavior of Glyceline Confined in Bacterial Cellulose Gels. *Journal of Physical Chemistry B*, **2020**, 124, 7647-7658	3.4	10
40	Production of bacterial cellulose with controlled deuterium-hydrogen substitution for neutron scattering studies. *Methods in Enzymology*, **2015**, 565, 123-46	1.7	9
39	Folding propensity of intrinsically disordered proteins by osmotic stress. *Molecular BioSystems*, **2016**, 12, 3695-3701		9
38	Small Angle Neutron Scattering Shows Nanoscale PMMA Distribution in Transparent Wood Biocomposites. *Nano Letters*, **2021**, 21, 2883-2890	11.5	8
37	Influence of Chemically Disrupted Photosynthesis on Cyanobacterial Thylakoid Dynamics in Synechocystis sp. PCC 6803. *Scientific Reports*, **2019**, 9, 5711	4.9	7
36	Localized entrapment of green fluorescent protein within nanostructured polymer films. *Soft Matter*, **2011**, 7, 11453	3.6	7
35	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*, **2020**, 15, e0235893	3.7	7
34	Incorporation of Melittin Enhances Interfacial Fluidity of Bicontinuous Microemulsions. *Journal of Physical Chemistry C*, **2019**, 123, 11197-11206	3.8	6
33	Cellulose-lignin composite fibres as precursors for carbon fibres. Part 1 - Manufacturing and properties of precursor fibres. *Carbohydrate Polymers*, **2021**, 252, 117133	10.3	6
32	Cellulose synthase interactive1- and microtubule-dependent cell wall architecture is required for acid growth in Arabidopsis hypocotyls. *Journal of Experimental Botany*, **2020**, 71, 2982-2994	7	5
31	Conformational Dynamics in the Interaction of SARS-CoV-2 Papain-like Protease with Human Interferon-Stimulated Gene 15 Protein. *Journal of Physical Chemistry Letters*, **2021**, 12, 5608-5615	6.4	5
30	Characterization of Morphology and Active Agent Mobility within Hybrid Silica Sol□Gel Composites. *Journal of Physical Chemistry C*, **2012**, 116, 13972-13979	3.8	4
29	Sunlight Energy Conversion Via Organics **2011**, 675-715		4
28	Effect of surface attachment on synthesis of bacterial cellulose. *Applied Biochemistry and Biotechnology*, **2005**, 121-124, 439-50	3.2	4
27	Potent and Selective Covalent Inhibitors of the Papain-like Protease from SARS-CoV-2 **2021**,		4

26	Biosynthesis and characterization of deuterated chitosan in filamentous fungus and yeast. *Carbohydrate Polymers*, **2021**, 257, 117637	10.3	4
25	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*, **2018**, 122, 9956-9961	3.4	4
24	Observation of a structural gradient in Winsor-III microemulsion systems. *Soft Matter*, **2018**, 14, 5270-5276	3.6	4
23	Multi-Purpose Cellulosic Ionogels. *ACS Symposium Series*, **2017**, 143-155	0.4	3
22	Production of deuterated biomass by cultivation of Lemna minor (duckweed) in DO. *Planta*, **2019**, 249, 1465-1475	4.7	3
21	Allelopathic effects of exogenous phenylalanine: a comparison of four monocot species. *Planta*, **2017**, 246, 673-685	4.7	3
20	Metabolic prosthesis for oxygenation of ischemic tissue. *IEEE Transactions on Biomedical Engineering*, **2009**, 56, 528-31	5	3
19	Cloning of electron-transferring flavoprotein from Megasphaera elsdenii. *Biochemical Society Transactions*, **1995**, 23, 379S	5.1	3
18	Structural Insights into Low and High Recalcitrance Natural Poplar Variants Using Neutron and X-ray Scattering. *ACS Sustainable Chemistry and Engineering*, **2020**, 8, 13838-13849	8.3	3
17	Identifying Stable Fragments of Arabidopsis thaliana Cellulose Synthase Subunit 3 by Yeast Display. *Biotechnology Journal*, **2019**, 14, e1800353	5.6	3
16	Collective Excitations in Protein as a Measure of Balance Between its Softness and Rigidity. *Journal of Physical Chemistry B*, **2017**, 121, 923-930	3.4	2
15	Reentrant condensation of lysozyme: Implications for studying dynamics of lysozyme in aqueous solutions of lithium chloride. *Biopolymers*, **2014**, 101, 624-9	2.2	2
14	Crystallization and preliminary X-ray diffraction analysis of Hypocrea jecorina Cel7A in two new crystal forms. *Acta Crystallographica Section F, Structural Biology Communications*, **2014**, 70, 773-6	1.1	2
13	Development of Bacterial Cellulose Nanocomposites. *Materials Research Society Symposia Proceedings*, **2011**, 1312, 1		2
12	Oligomerization state and pigment binding strength of the peridinin-Chl a-protein. *FEBS Letters*, **2015**, 589, 2713-9	3.8	1
11	Investigation of detergent effects on the solution structure of spinach Light Harvesting Complex II. *Journal of Physics: Conference Series*, **2010**, 251, 012041	0.3	1
10	Fed-batch production of deuterated protein in Escherichia coli for neutron scattering experimentation. *Methods in Enzymology*, **2021**, 659, 219-240	1.7	1
9	Protonation states in SARS-CoV-2 main protease mapped by neutron crystallography		1

8	Melittin exerts opposing effects on short- and long-range dynamics in bicontinuous microemulsions. *Journal of Colloid and Interface Science*, **2021**, 590, 94-102	9.3	1
7	Structural Studies of Deuterium-Labeled Switchgrass Biomass. *ACS Symposium Series*, **2019**, 17-32	0.4	1
6	Structural Reorganization of Noncellulosic Polymers Observed In Situ during Dilute Acid Pretreatment by Small-Angle Neutron Scattering. *ACS Sustainable Chemistry and Engineering*, **2022**, 10, 314-322	8.3	1
5	Incorporation of Membrane Proteins Into Bicontinuous Microemulsions Through Winsor-III System-Based Extraction. *Journal of Surfactants and Detergents*, **2021**, 24, 649-660	1.9	0
4	The Nicotinamide Cofactors: Applications in Biotechnology. *ACS Symposium Series*, **2001**, 103-130	0.4	
3	Electron-transferring flavoprotein from Megasphaera elsdenii; gene organisation and structural information. *Biochemical Society Transactions*, **1998**, 26, S214	5.1	
2	Effect of Surface Attachment on Synthesis of Bacterial Cellulose **2005**, 439-450		
1	Investigating the structural flexibility of intrinsically disordered proteins. *FASEB Journal*, **2010**, 24, 684.8	0.9	