

Pamela S Whitfield

List of Publications by Year in descending order

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75
papers

2,570
citations

201674

27
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189892

50
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79
all docs

79
docs citations

79
times ranked

4326
citing authors

#	ARTICLE	IF	CITATIONS
1	The Certification of Standard Reference Material 1979: Powder Diffraction Line Profile Standard for Crystallite Size Analysis. <i>Journal of Research of the National Institute of Standards and Technology</i> , 2020, 125, .	1.2	2
2	In situ measurements of reactions in a glass-forming batch by X-ray and neutron diffraction. <i>Journal of the American Ceramic Society</i> , 2019, 102, 1495-1506.	3.8	9
3	Metastable $\text{Li}_{1+x}\text{Mn}_2\text{O}_4$ ($0 \leq x \leq 1$) Spinel Phases Revealed by in Operando Neutron Diffraction and First-Principles Calculations. <i>Chemistry of Materials</i> , 2019, 31, 124-134.	6.7	28
4	POWGEN: rebuild of a third-generation powder diffractometer at the Spallation Neutron Source. <i>Journal of Applied Crystallography</i> , 2019, 52, 1189-1201.	4.5	57
5	Structure Evolution and Reactivity of the $\text{Sc}_{2-x}\text{V}_x\text{O}_{3+x}$ ($0 \leq x \leq 2.0$) System. <i>Inorganic Chemistry</i> , 2018, 57, 5607-5614.		3
6	Intrinsic point defects in off-stoichiometric $\text{Cu}_2\text{ZnSnSe}_4$: A neutron diffraction study. <i>Journal of Applied Physics</i> , 2018, 123, .	2.5	39
7	Structure, Phase Composition, and Thermoelectric Properties of $\text{Yb}_x\text{Co}_4\text{Sb}_{12}$ and Their Dependence on Synthesis Method. <i>ACS Applied Energy Materials</i> , 2018, 1, 113-122.	5.1	18
8	Structural Competition and Reactivity of Rare-Earth Oxide Phases in $\text{Y}_x\text{Pr}_{2-x}\text{O}_3$ ($0.05 \leq x \leq 0.80$). <i>Inorganic Chemistry</i> , 2018, 57, 14106-14115.	4.0	6
9	Certification of Standard Reference Material 1879b respirable cristobalite. <i>Powder Diffraction</i> , 2018, 33, 202-208.	0.2	1
10	Event-based processing of neutron scattering data at the Spallation Neutron Source. <i>Journal of Applied Crystallography</i> , 2018, 51, 616-629.	4.5	35
11	Role of lattice distortion and A site cation in the phase transitions of methylammonium lead halide perovskites. <i>Physical Review Materials</i> , 2018, 2, .	2.4	20
12	<i>In Situ</i> Neutron Diffraction Studies of the Ion Exchange Synthesis Mechanism of $\text{Li}_2\text{Mg}_2\text{P}_3\text{O}_9\text{N}$: Evidence for a Hidden Phase Transition. <i>Journal of the American Chemical Society</i> , 2017, 139, 9192-9202.	13.7	19
13	Controlling superstructural ordering in the clathrate-I $\text{Ba}_8\text{M}_{16}\text{P}_{30}$ ($\text{M} = \text{Cu}, \text{Zn}$) through the formation of metal-metal bonds. <i>Chemical Science</i> , 2017, 8, 3650-3659.	7.4	21
14	Enhanced Photoluminescence Emission and Thermal Stability from Introduced Cation Disorder in Phosphors. <i>Journal of the American Chemical Society</i> , 2017, 139, 11766-11770.	13.7	190
15	Combinatorial appraisal of transition states for <i>in situ</i> pair distribution function analysis. <i>Journal of Applied Crystallography</i> , 2017, 50, 1744-1753.	4.5	18
16	Certification of standard reference material 1878b respirable α -quartz. CORRIGENDUM. <i>Powder Diffraction</i> , 2016, 31, 304-304.	0.2	0
17	Asymmetric band flipping for time-of-flight neutron diffraction data. <i>Journal of Applied Crystallography</i> , 2016, 49, 1806-1809.	4.5	0
18	Certification of standard reference material 1878b respirable α -quartz. <i>Powder Diffraction</i> , 2016, 31, 211-215.	0.2	3

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19	Oxygen Storage Properties of La _{1-x} Sr _x FeO _{3-δ} for Chemical-Looping Reactions—An In Situ Neutron and Synchrotron X-ray Study. Chemistry of Materials, 2016, 28, 3951-3960.	6.7	57
20	Lattice dynamics and the nature of structural transitions in organolead halide perovskites. Physical Review B, 2016, 94, .	3.2	46
21	Synthesis of a Ferrolite: A Zeolitic Al ^{III} Framework. Angewandte Chemie - International Edition, 2016, 55, 13195-13199.	13.8	7
22	Anisotropic Exchange within Decoupled Tetrahedra in the Quantum Breathing Pyrochlore $Ba_3Mn_2O_{13}$. Physical Review Letters, 2016, 116, 257204.	7.8	55
23	Structures, Phase Transitions and Tricritical Behavior of the Hybrid Perovskite Methyl Ammonium Lead Iodide. Scientific Reports, 2016, 6, 35685.	3.3	440
24	Quantitative phase analysis of challenging samples using neutron powder diffraction. Sample #4 from the CPD QPA round robin revisited. Powder Diffraction, 2016, 31, 192-197.	0.2	4
25	Solvothermal Synthesis and Surface Chemistry To Control the Size and Morphology of Nanoquartz. Crystal Growth and Design, 2015, 15, 5327-5331.	3.0	10
26	Diffraction studies from minerals to organics: lessons learned from materials analyses. Powder Diffraction, 2014, 29, S2-S7.	0.2	1
27	Ionic Conduction in Cubic Na ₃ TiP ₃ O ₉ N, a Secondary Na-Ion Battery Cathode with Extremely Low Volume Change. Chemistry of Materials, 2014, 26, 3295-3305.	6.7	68
28	Contribution to the crystallography of hydrotalcites: the crystal structures of woodallite and takovite. Journal of Geosciences (Czech Republic), 2013, , 273-279.	0.6	10
29	Crystalline domain size and faulting in the new NIST SRM 1979 zinc oxide. Powder Diffraction, 2013, 28, S22-S32.	0.2	9
30	Laboratory X-ray Powder Diffraction. NATO Science for Peace and Security Series B: Physics and Biophysics, 2012, , 53-63.	0.3	0
31	Novel Pn Polymorph for Li ₂ MnSiO ₄ and Its Electrochemical Activity As a Cathode Material in Li-Ion Batteries. Chemistry of Materials, 2011, 23, 5446-5456.	6.7	85
32	Fluorocronite, the natural analogue of PbF_2 , from the Sakha Republic, Russian Federation. European Journal of Mineralogy, 2011, 23, 695-700.	1.3	5
33	The crystal structure of stichtite, re-examination of barbertonite, and the nature of polytypism in MgCr hydrotalcites. American Mineralogist, 2011, 96, 179-187.	1.9	30
34	Novel PnLi ₂ MnSiO ₄ : synthesis, DFT-aided characterization and charge/discharge. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C489-C490.	0.3	0
35	300 barin situgas pressure cell for powder diffractometers. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C247-C247.	0.3	0
36	In-situ XRD study of the succinonitrile—lithium bis(trifluoromethylsulfonyl)imide (LiTFSI) phase diagram. Solid State Ionics, 2010, 181, 740-744.	2.7	18

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37	Carbon dioxide-induced crystallization in poly(L-lactic acid) and its effect on foam morphologies. <i>Polymer International</i> , 2010, 59, 1709-1718.	3.1	65
38	Supramolecular Chromotropism of the Crystalline Phases of 4,5,6,7-Tetrafluorobenzo-2,1,3-telluradiazole. <i>Journal of the American Chemical Society</i> , 2010, 132, 17265-17270.	13.7	69
39	Crystal structure of the mineral strontiodresserite from laboratory powder diffraction data. <i>Powder Diffraction</i> , 2010, 25, 322-328.	0.2	6
40	Problem Solving with the TOPAS Macro Language: Corrections and Constraints in Simulated Annealing and Rietveld Refinement. <i>Materials Science Forum</i> , 2010, 651, 11-25.	0.3	9
41	Mineralogical adventures of a powder diffractionist. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2010, 66, s45-s46.	0.3	0
42	Phase Identification and Quantitative Methods. , 2009, , 226-260.		3
43	Spherical harmonics preferential orientation corrections and structure solution from powder diffraction data – a possible avenue of last resort. <i>Journal of Applied Crystallography</i> , 2009, 42, 134-136.	4.5	16
44	In situ laboratory X-ray powder diffraction study of wollastonite carbonation using a high-pressure stage. <i>Applied Geochemistry</i> , 2009, 24, 1635-1639.	3.0	13
45	The effects of particle statistics on Rietveld analysis of cement. <i>Zeitschrift für Kristallographie, Supplement</i> , 2009, 2009, 53-59.	0.5	5
46	Modified design and use of a high-pressure environmental stage for laboratory X-ray powder diffractometers. <i>Journal of Applied Crystallography</i> , 2008, 41, 350-355.	4.5	4
47	Angastonite, CaMgAl ₂ (PO ₄) ₂ (OH)4·7H ₂ O: a new phosphate mineral from Angaston, South Australia. <i>Mineralogical Magazine</i> , 2008, 72, 1011-1020.	1.4	6
48	Ab initio structure determination of the low-temperature phase of succinonitrile from laboratory X-ray powder diffraction data – Coping with potential poor powder quality using DFT ab initio methods. <i>Powder Diffraction</i> , 2008, 23, 292-299.	0.2	15
49	Jadarite, LiNaSiB ₃ O ₇ (OH), a new mineral species from the Jadar Basin, Serbia. <i>European Journal of Mineralogy</i> , 2007, 19, 575-580.	1.3	35
50	Investigation of Li salt doped succinonitrile as potential solid electrolytes for lithium batteries. <i>Journal of Power Sources</i> , 2007, 174, 883-888.	7.8	82
51	Least-squares thermal expansion tensor of vanadate and arsenate triclinic apatites derived from laboratory X-ray powder diffraction cell data. <i>Journal of Applied Crystallography</i> , 2007, 40, 1019-1026.	4.5	2
52	Ab initio constrained crystal-chemical Rietveld refinement of Ca ₁₀ (V x P)O ₄ (OH)F ₂ apatites. <i>Acta Crystallographica Section B: Structural Science</i> , 2007, 63, 37-48.	1.8	20
53	Triclinic apatites. <i>Acta Crystallographica Section B: Structural Science</i> , 2007, 63, 251-256.	1.8	40
54	LiNaSiB ₃ O ₇ (OH) – novel structure of the new borosilicate mineral jadarite determined from laboratory powder diffraction data. <i>Acta Crystallographica Section B: Structural Science</i> , 2007, 63, 396-401.	1.8	13

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55	Diffraction analysis of the lithium battery cathode material $\text{Li}_{1.2}\text{Mn}_{0.4}\text{Ni}_{0.3}\text{Co}_{0.1}\text{O}_2$. Zeitschrift für Kristallographie, Supplement, 2007, 2007, 483-488.	0.5	9
56	Layered Open Pore Poly(l-lactic acid) Nanomorphology. Biomacromolecules, 2006, 7, 2937-2941.	5.4	56
57	Quantitative Rietveld analysis of hydrated cementitious systems. Powder Diffraction, 2006, 21, 111-113.	0.2	21
58	Geometrical parameterization of the crystal chemistry of P63/mapatite. II. Precision, accuracy and numerical stability of the crystal-chemical Rietveld refinement. Journal of Applied Crystallography, 2006, 39, 369-375.	4.5	14
59	SVDdiagnostic, a program to diagnose numerical conditioning of Rietveld refinements. Journal of Applied Crystallography, 2006, 39, 458-465.	4.5	8
60	Electrical and thermal properties of $\text{La}_{0.7}\text{Sr}_{0.3}\text{Ga}_{0.6}\text{Fe}_{0.4}\text{O}_3$ ceramics. Ceramics International, 2006, 32, 339-344.	4.8	4
61	Structure, stability and electrical properties of the $\text{La}_{(2-x)}\text{Sr}_x\text{MnO}_4$ solid solution series. Solid State Ionics, 2006, 177, 1849-1853.	2.7	50
62	Effects of synthesis on electrochemical, structural and physical properties of solution phases of Li_2MnO_3 - $\text{LiNi}_{1-x}\text{Co}_x\text{O}_2$. Journal of Power Sources, 2005, 146, 617-621.	7.8	44
63	Oxygen transport in the LaNiCoO system. Solid State Ionics, 2005, 176, 1895-1901.	2.7	115
64	Investigation of possible superstructure and cation disorder in the lithium battery cathode material LiMnNiCoO using neutron and anomalous dispersion powder diffraction. Solid State Ionics, 2005, 176, 463-471.	2.7	98
65	Geometrical parameterization of the crystal chemistry of P63/m apatites: comparison with experimental data and ab initio results. Acta Crystallographica Section B: Structural Science, 2005, 61, 635-655.	1.8	38
66	Stability and Reactivity of LSGM Electrolytes With Nickel-Based Ceramic Cathodes. Journal of Fuel Cell Science and Technology, 2005, 2, 34-37.	0.8	18
67	Structural and sintering characteristics of the $\text{La}_2\text{Ni}_{1-x}\text{Co}_x\text{O}_4$ series. Ceramics International, 2004, 30, 1635-1639.	4.8	51
68	X-RAY DIFFRACTION ANALYSIS OF NANOPARTICLES: RECENT DEVELOPMENTS, POTENTIAL PROBLEMS AND SOME SOLUTIONS. International Journal of Nanoscience, 2004, 03, 757-763.	0.7	27
69	Quantitative Rietveld analysis of the amorphous content in cements and clinkers. Journal of Materials Science, 2003, 38, 4415-4421.	3.7	68
70	Pulsed laser deposition, characterization and thermochemical stability of $\text{SrFe}_y\text{Co}_{1-y}\text{O}_x$ thin films. Thin Solid Films, 2003, 426, 221-231.	1.8	11
71	Use of double Göbel mirrors with high-temperature stages for powder diffraction – a strategy to avoid severe intensity fade. Journal of Applied Crystallography, 2003, 36, 926-930.	4.5	2
72	In Situ X-Ray Absorption Study of a Layered Manganese-Chromium Oxide-Based Cathode Material. Journal of the Electrochemical Society, 2002, 149, A176.	2.9	135

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73	Sucrose synthesis of nanoparticulate alumina. Journal of Materials Science Letters, 2002, 21, 1773-1775.	0.5	10
74	Microwave Synthesis of $\text{Li}_{1.025}\text{Mn}_{1.975}\text{O}_4$ and $\text{Li}_{1+x}\text{Mn}_{2-x}\text{O}_4\text{F}_y$ ($x=0.05, 0.15; y=0.05, 0.1$). Journal of the Electrochemical Society, 2000, 147, 4476-4482.	2.9	52
75	Remote visual monitoring during time resolved in situ neutron diffraction study of recrystallization of melt-cast $\text{Bi}_{1.6}\text{Pb}_{0.4}\text{Sr}_2\text{Ca}_3\text{Cu}_4\text{O}_y$ by passage of dc current. Review of Scientific Instruments, 1998, 69, 2475-2479.	1.3	1