Pamela S Whitfield

List of Publications by Year
in descending order

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75 papers	2,570 citations	201674 27 h-index	189892 50 g-index
79 all docs	79 docs citations	79 times ranked	4326 citing authors

#	Article	IF	Citations
1	Structures, Phase Transitions and Tricritical Behavior of the Hybrid Perovskite Methyl Ammonium Lead Iodide. Scientific Reports, 2016, 6, 35685.	3.3	440
2	Enhanced Photoluminescence Emission and Thermal Stability from Introduced Cation Disorder in Phosphors. Journal of the American Chemical Society, 2017, 139, 11766-11770.	13.7	190
3	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
4	Oxygen transport in the LaNiCoO system. Solid State Ionics, 2005, 176, 1895-1901.	2.7	115
5	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
6	Novel Pn Polymorph for Li₂MnSiO₄ and Its Electrochemical Activity As a Cathode Material in Li-Ion Batteries. Chemistry of Materials, 2011, 23, 5446-5456.	6.7	85
7	Investigation of Li salt doped succinonitrile as potential solid electrolytes for lithium batteries. Journal of Power Sources, 2007, 174, 883-888.	7.8	82
8	Supramolecular Chromotropism of the Crystalline Phases of 4,5,6,7-Tetrafluorobenzo-2,1,3-telluradiazole. Journal of the American Chemical Society, 2010, 132, 17265-17270.	13.7	69
9	Quantitative Rietveld analysis of the amorphous content in cements and clinkers. Journal of Materials Science, 2003, 38, 4415-4421.	3.7	68
10	Ionic Conduction in Cubic Na₃TiP₃O₉N, a Secondary Na-Ion Battery Cathode with Extremely Low Volume Change. Chemistry of Materials, 2014, 26, 3295-3305.	6.7	68
11	Carbon dioxideâ€induced crystallization in poly(<scp>L</scp>â€lactic acid) and its effect on foam morphologies. Polymer International, 2010, 59, 1709-1718.	3.1	65
12	Oxygen Storage Properties of La_{1â€“x}Sr_xFeO_{3â^'Î´} for Chemical-Looping Reactionsâ€”An In Situ Neutron and Synchrotron X-ray Study. Chemistry of Materials, 2016, 28, 3951-3960.	6.7	57
13	POWGEN: rebuild of a third-generation powder diffractometer at the Spallation Neutron Source. Journal of Applied Crystallography, 2019, 52, 1189-1201.	4.5	57
14	Layered Open Pore Poly(l-lactic acid) Nanomorphology. Biomacromolecules, 2006, 7, 2937-2941.	5.4	56
15	Anisotropic Exchange within Decoupled Tetrahedra in the Quantum Breathing Pyrochlore<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Ba</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow><mml:mathvariant="nor. Physical Review Letters, 2016, 116, 257204.	7.8	55
16	Microwave Synthesis of Li[sub 1.025]Mn[sub 1.975]O[sub 4] and Li[sub 1+x]Mn[sub 2â^'x]O[sub 4â^'y]F[sub y]â€‰(xâ€‰=â€‰0.05,â€‰0.15;â€‰yâ€‰=â€‰0.05,â€‰0.1). Journal of the Electrochemical Society, 2000, 147, 4476.	2.9	52
17	Structural and sintering characteristics of the La2Ni1â^'xCoxO4+Î´ series. Ceramics International, 2004, 30, 1635-1639.	4.8	51
18	Structure, stability and electrical properties of the La(2â^'x)SrxMnO4Â±Î´ solid solution series. Solid State Ionics, 2006, 177, 1849-1853.	2.7	50

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19	Lattice dynamics and the nature of structural transitions in organolead halide perovskites. Physical Review B, 2016, 94, .	3.2	46
20	Effects of synthesis on electrochemical, structural and physical properties of solution phases of Li2MnO3â€“LiNi1â^'xCoxO2. Journal of Power Sources, 2005, 146, 617-621.	7.8	44
21	Triclinic apatites. Acta Crystallographica Section B: Structural Science, 2007, 63, 251-256.	1.8	40
22	Intrinsic point defects in off-stoichiometric Cu2ZnSnSe4: A neutron diffraction study. Journal of Applied Physics, 2018, 123, .	2.5	39
23	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
24	Jadarite, LiNaSiB3O7(OH), a new mineral species from the Jadar Basin, Serbia. European Journal of Mineralogy, 2007, 19, 575-580.	1.3	35
25	Event-based processing of neutron scattering data at the Spallation Neutron Source. Journal of Applied Crystallography, 2018, 51, 616-629.	4.5	35
26	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
27	Metastable Li_{1+Î´}Mn₂O₄ (0 â‰¤ Î´ â‰¤ 1) Spinel Phases Revealed by in Operando Neutron Diffraction and First-Principles Calculations. Chemistry of Materials, 2019, 31, 124-134.	6.7	28
28	X-RAY DIFFRACTION ANALYSIS OF NANOPARTICLES: RECENT DEVELOPMENTS, POTENTIAL PROBLEMS AND SOME SOLUTIONS. International Journal of Nanoscience, 2004, 03, 757-763.	0.7	27
29	Quantitative Rietveld analysis of hydrated cementitious systems. Powder Diffraction, 2006, 21, 111-113.	0.2	21
30	Controlling superstructural ordering in the clathrate-I Ba8M16P30(M = Cu, Zn) through the formation of metalâ€“metal bonds. Chemical Science, 2017, 8, 3650-3659.	7.4	21
31	Ab initio constrained crystal-chemical Rietveld refinement of Ca10(V x P1â€…â^'â€…x O4)6F2 apatites. Acta Crystallographica Section B: Structural Science, 2007, 63, 37-48.	1.8	20
32	Role of lattice distortion and A site cation in the phase transitions of methylammonium lead halide perovskites. Physical Review Materials, 2018, 2, .	2.4	20
33	In Situ Neutron Diffraction Studies of the Ion Exchange Synthesis Mechanism of Li₂Mg₂P₃O₉N: Evidence for a Hidden Phase Transition. Journal of the American Chemical Society, 2017, 139, 9192-9202.	13.7	19
34	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
35	In-situ XRD study of the succinonitrileâ€“lithium bis(trifluoromethylsulfonyl)imide (LiTFSI) phase diagram. Solid State Ionics, 2010, 181, 740-744.	2.7	18
36	Combinatorial appraisal of transition states for in situ pair distribution function analysis. Journal of Applied Crystallography, 2017, 50, 1744-1753.	4.5	18

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37	Structure, Phase Composition, and Thermoelectric Properties of Yb_xCo₄Sb₁₂ and Their Dependence on Synthesis Method. ACS Applied Energy Materials, 2018, 1, 113-122.	5.1	18
38	Spherical harmonics preferential orientation corrections and structure solution from powder diffraction data â€“ a possible avenue of last resort. Journal of Applied Crystallography, 2009, 42, 134-136.	4.5	16
39	Ab initio structure determination of the low-temperature phase of succinonitrile from laboratory X-ray powder diffraction dataâ€”Coping with potential poor powder quality using DFT ab initio methods. Powder Diffraction, 2008, 23, 292-299.	0.2	15
40	Geometrical parameterization of the crystal chemistry ofP63/mapatite. II. Precision, accuracy and numerical stability of the crystal-chemical Rietveld refinement. Journal of Applied Crystallography, 2006, 39, 369-375.	4.5	14
41	LiNaSiB3O7(OH) â€“ novel structure of the new borosilicate mineral jadarite determined from laboratory powder diffraction data. Acta Crystallographica Section B: Structural Science, 2007, 63, 396-401.	1.8	13
42	In situ laboratory X-ray powder diffraction study of wollastonite carbonation using a high-pressure stage. Applied Geochemistry, 2009, 24, 1635-1639.	3.0	13
43	Pulsed laser deposition, characterization and thermochemical stability of SrFeyCo1â^'yOx thin films. Thin Solid Films, 2003, 426, 221-231.	1.8	11
44	Sucrose synthesis of nanoparticulate alumina. Journal of Materials Science Letters, 2002, 21, 1773-1775.	0.5	10
45	Contribution to the crystallography of hydrotalcites: the crystal structures of woodallite and takovite. Journal of Geosciences (Czech Republic), 2013, , 273-279.	0.6	10
46	Solvothermal Synthesis and Surface Chemistry To Control the Size and Morphology of Nanoquartz. Crystal Growth and Design, 2015, 15, 5327-5331.	3.0	10
47	Problem Solving with the TOPAS Macro Language: Corrections and Constraints in Simulated Annealing and Rietveld Refinement. Materials Science Forum, 2010, 651, 11-25.	0.3	9
48	Crystalline domain size and faulting in the new NIST SRM 1979 zinc oxide. Powder Diffraction, 2013, 28, S22-S32.	0.2	9
49	In situ measurements of reactions in a glassâ€forming batch by Xâ€ray and neutron diffraction. Journal of the American Ceramic Society, 2019, 102, 1495-1506.	3.8	9
50	Diffraction analysis of the lithium battery cathode material Li1.2Mn0.4Ni0.3Co0.1O2. Zeitschrift FÃ¼r Kristallographie, Supplement, 2007, 2007, 483-488.	0.5	9
51	SVDdiagnostic, a program to diagnose numerical conditioning of Rietveld refinements. Journal of Applied Crystallography, 2006, 39, 458-465.	4.5	8
52	Synthesis of a Ferrolite: A Zeolitic Allâ€Iron Framework. Angewandte Chemie - International Edition, 2016, 55, 13195-13199.	13.8	7
53	Angastonite, CaMgAl2(PO4)2(OH)4Â·7H2O: a new phosphate mineral from Angaston, South Australia. Mineralogical Magazine, 2008, 72, 1011-1020.	1.4	6
54	Crystal structure of the mineral strontiodresserite from laboratory powder diffraction data. Powder Diffraction, 2010, 25, 322-328.	0.2	6

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55	Structural Competition and Reactivity of Rare-Earth Oxide Phases in Y_xPr_{2â€“x}O₃ (0.05 â‰¤ x â‰¤ 0.80). Inorganic Chemistry, 2018, 57, 14106-14115.	4.0	6
56	Fluorocronite, the natural analogue of Î²-PbF2, from the Sakha Republic, Russian Federation. European Journal of Mineralogy, 2011, 23, 695-700.	1.3	5
57	The effects of particle statistics on Rietveld analysis of cement. Zeitschrift FÃ¼r Kristallographie, Supplement, 2009, 2009, 53-59.	0.5	5
58	Electrical and thermal properties of La0.7Sr0.3Ga0.6Fe0.4O3 ceramics. Ceramics International, 2006, 32, 339-344.	4.8	4
59	Modified design and use of a high-pressure environmental stage for laboratory X-ray powder diffractometers. Journal of Applied Crystallography, 2008, 41, 350-355.	4.5	4
60	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
61	Phase Identification and Quantitative Methods. , 2009, , 226-260.		3
62	Certification of standard reference material 1878b respirable Î±-quartz. Powder Diffraction, 2016, 31, 211-215.	0.2	3
63	Structure Evolution and Reactivity of the Sc_(2â€“x)V_xO_{3+Î´} (0 â‰¤ x â‰¤ 2.0) System. Inorganic Chemistry, 2018, 57, 5607-5614.	4.0	3
64	Use of double GÃ¶bel mirrors with high-temperature stages for powder diffraction â€“ a strategy to avoid severe intensity fade. Journal of Applied Crystallography, 2003, 36, 926-930.	4.5	2
65	Least-squares thermal expansion tensor of vanadate and arsenate triclinic apatites derived from laboratory X-ray powder diffraction cell data. Journal of Applied Crystallography, 2007, 40, 1019-1026.	4.5	2
66	The Certification of Standard Reference Material 1979: Powder Diffraction Line Profile Standard for Crystallite Size Analysis. Journal of Research of the National Institute of Standards and Technology, 2020, 125, .	1.2	2
67	Remote visual monitoring during time resolved in situ neutron diffraction study of recrystallization of melt-cast Bi1.6Pb0.4Sr2Ca3Cu4Oy by passage of dc current. Review of Scientific Instruments, 1998, 69, 2475-2479.	1.3	1
68	Diffraction studies from minerals to organics: lessons learned from materials analyses. Powder Diffraction, 2014, 29, S2-S7.	0.2	1
69	Certification of Standard Reference Material 1879b respirable cristobalite. Powder Diffraction, 2018, 33, 202-208.	0.2	1
70	Certification of standard reference material 1878b respirable Î±-quartz â€“ CORRIGENDUM. Powder Diffraction, 2016, 31, 304-304.	0.2	0
71	Asymmetric band flipping for time-of-flight neutron diffraction data. Journal of Applied Crystallography, 2016, 49, 1806-1809.	4.5	0
72	Mineralogical adventures of a powder diffractionist. Acta Crystallographica Section A: Foundations and Advances, 2010, 66, s45-s46.	0.3	0

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73	NovelPnLi2MnSiO4: synthesis, DFT-aided characterization and charge/discharge. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C489-C490.	0.3	0
74	300 barin situgas pressure cell for powder diffractometers. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C247-C247.	0.3	0
75	Laboratory X-ray Powder Diffraction. NATO Science for Peace and Security Series B: Physics and Biophysics, 2012, , 53-63.	0.3	0