David S Wragg

List of Publications by Year
in descending order

83 papers	3,250 citations	136950 32 h-index	155660 55 g-index
88 all docs	88 docs citations	88 times ranked	4378 citing authors

#	Article	IF	Citations
1	Detailed Structure Analysis of Atomic Positions and Defects in Zirconium Metalâ€"Organic Frameworks. Crystal Growth and Design, 2014, 14, 5370-5372.	3.0	306
2	Microwave-assisted synthesis of anionic metalâ€"organic frameworks under ionothermal conditions. Chemical Communications, 2006, , 2021-2023.	4.1	227
3	Anion Control in the Ionothermal Synthesis of Coordination Polymers. Journal of the American Chemical Society, 2007, 129, 10334-10335.	13.7	203
4	Structural determination of a highly stable metal-organic framework with possible application to interim radioactive waste scavenging: Hf-UiO-66. Physical Review B, 2012, 86, .	3.2	196
5	Ionothermal Synthesis of Unusual Cholineâ€Templated Cobalt Aluminophosphates. Angewandte Chemie - International Edition, 2007, 46, 7839-7843.	13.8	131
6	Spatial dynamics of lithiation and lithium plating during high-rate operation of graphite electrodes. Energy and Environmental Science, 2020, 13, 2570-2584.	30.8	124
7	How Crystallite Size Controls the Reaction Path in Nonaqueous Metal Ion Batteries: The Example of Sodium Bismuth Alloying. Chemistry of Materials, 2016, 28, 2750-2756.	6.7	113
8	Pure Silica Zeolite-type Frameworks: A Structural Analysis. Chemistry of Materials, 2008, 20, 1561-1570.	6.7	88
9	A Straightforward Descriptor for the Deactivation of Zeolite Catalyst H-ZSM-5. ACS Catalysis, 2017, 7, 8235-8246.	11.2	77
10	SAPO-34 methanol-to-olefin catalysts under working conditions: A combined in situ powder X-ray diffraction, mass spectrometry and Raman study. Journal of Catalysis, 2009, 268, 290-296.	6.2	76
11	Watching the Methanolâ€toâ€Olefin Process with Timeâ€and Spaceâ€Resolved Highâ€Energy Operando Xâ€ray Diffraction. Angewandte Chemie - International Edition, 2012, 51, 7956-7959.	13.8	68
12	In operando Synchrotron XRD/XAS Investigation of Sodium Insertion into the Prussian Blue Analogue Cathode Material Na 1.32 Mn[Fe(CN) 6] 0.83 Â· z H 2 O. Electrochimica Acta, 2016, 200, 305-313.	5.2	65
13	In situ solid-state NMR and XRD studies of the ADOR process and the unusual structure of zeolite IPC-6. Nature Chemistry, 2017, 9, 1012-1018.	13.6	63
14	Pitfalls in metalâ€"organic framework crystallography: towards more accurate crystal structures. Chemical Society Reviews, 2017, 46, 4867-4876.	38.1	60
15	Azamacrocycle-Containing Gallium Phosphates:Â A New Class of Inorganicâ˘'Organic Hybrid Material. Journal of the American Chemical Society, 1998, 120, 6822-6823.	13.7	56
16	Direct observation of catalyst behaviour under real working conditions with X-ray diffraction: Comparing SAPO-18 and SAPO-34 methanol to olefin catalysts. Journal of Catalysis, 2011, 279, 397-402.	6.2	54
17	Chemical Structures of Specific Sodium Ion Battery Components Determined by Operando Pair Distribution Function and Xâ€ray Diffraction Computed Tomography. Angewandte Chemie - International Edition, 2017, 56, 11385-11389.	13.8	54
18	Waste products as alternative phosphorus fertilisers part I: inorganic P species affect fertilisation effects depending on soil pH. Nutrient Cycling in Agroecosystems, 2015, 103, 167-185.	2.2	52

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19	The ionothermal synthesis of metal organic frameworks, Ln(C9O6H3)((CH3NH)2CO)2, using deep eutectic solvents. Solid State Sciences, 2010, 12, 418-421.	3.2	50
20	Anionic Gallium Phosphate Double Four-Ring Units Containing Occluded Oxygen. Journal of the American Chemical Society, 2000, 122, 11246-11247.	13.7	48
21	Determination of Molybdenum Species Evolution during Nonâ€Oxidative Dehydroaromatization of Methane and its Implications for Catalytic Performance. ChemCatChem, 2019, 11, 473-480.	3.7	48
22	The synthesis of gallium phosphate frameworks with and without fluoride ions present: attempts to direct the synthesis of double four-ring containing materials. Journal of Materials Chemistry, 2001, 11, 1850-1857.	6.7	47
23	The role of added water in the ionothermal synthesis of microporous aluminium phosphates. Solid State Sciences, 2009, 11, 411-416.	3.2	47
24	Bismuth Vanadate and Molybdate: Stable Alloying Anodes for Sodium-Ion Batteries. Chemistry of Materials, 2017, 29, 2803-2810.	6.7	44
25	A novel non-centrosymmetric metallophosphate-borate compound via ionothermal synthesis. Dalton Transactions, 2009, , 5287.	3.3	42
26	The adsorption of methanol and water on SAPO-34: in situ and ex situ X-ray diffraction studies. Microporous and Mesoporous Materials, 2010, 134, 210-215.	4.4	40
27	In Situ Flow MAS NMR Spectroscopy and Synchrotron PDF Analyses of the Local Response of the BrÃ¸nsted Acidic Site in SAPOâ€34 during Hydration at Elevated Temperatures. ChemPhysChem, 2018, 19, 519-528.	2.1	40
28	Nanoporous Intergrowths: How Crystal Growth Dictates Phase Composition and Hierarchical Structure in the CHA/AEI System. Chemistry of Materials, 2015, 27, 4205-4215.	6.7	37
29	Probing ZnAPO-34 Self-Assembly Using Simultaneous Multiple in Situ Techniques. Journal of Physical Chemistry C, 2011, 115, 6331-6340.	3.1	35
30	Copper Phosphonatoethanesulfonates: Temperature Dependent in Situ Energy Dispersive X-ray Diffraction Study and Influence of the pH on the Crystal Structures. Inorganic Chemistry, 2012, 51, 12540-12547.	4.0	35
31	Intergrowth structure modelling in silicoaluminophosphate SAPO-18/34 family. Microporous and Mesoporous Materials, 2014, 195, 311-318.	4.4	35
32	In Situ Comparison of Ionothermal Kinetics Under Microwave And Conventional Heating. Journal of Physical Chemistry C, 2009, 113, 20553-20558.	3.1	33
33	Unit cell thick nanosheets of zeolite H-ZSM-5: Structure and activity. Topics in Catalysis, 2013, 56, 558-566.	2.8	33
34	Versatile electrochemical cell for Li/Na-ion batteries and high-throughput setup for combined <i>operando</i> X-ray diffraction and absorption spectroscopy. Journal of Applied Crystallography, 2016, 49, 1972-1981.	4.5	33
35	Deactivation of Zeolite Catalyst H-ZSM-5 during Conversion of Methanol to Gasoline: Operando Time- and Space-Resolved X-ray Diffraction. Journal of Physical Chemistry Letters, 2018, 9, 1324-1328.	4.6	33
36	Unit cell expansion upon coke formation in a SAPO-34 catalyst: A combined experimental and computational study. Microporous and Mesoporous Materials, 2013, 165, 1-5.	4.4	32

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37	A new calcium trimellitate coordination polymer with a chain-like structure. Solid State Sciences, 2007, 9, 455-458.	3.2	30
38	Time- and space-resolved high energy operando X-ray diffraction for monitoring the methanol to hydrocarbons reaction over H-ZSM-22 zeolite catalyst in different conditions. Surface Science, 2016, 648, 141-149.	1.9	30
39	Structural changes in SAPO-34 due to hydrothermal treatment. A NMR, XRD, and DRIFTS study. Microporous and Mesoporous Materials, 2016, 225, 421-431.	4.4	28
40	Ionothermal synthesis of inorganicâ€“organic hybrid materials containing perfluorinated aliphatic dicarboxylate ligands. Dalton Transactions, 2009, , 1131.	3.3	26
41	Biocidal properties study of silver nanoparticles used for application in green housing. International Nano Letters, 2016, 6, 191-197.	5.0	25
42	Ionothermal synthesis, structure and characterization of three-dimensional zinc phosphates. Dalton Transactions, 2009, , 6715.	3.3	21
43	A novel pyridine-templated open framework gallophosphate. Chemical Communications, 1999, , 2037-2038.	4.1	20
44	Combined XRD and Raman studies of coke types found in SAPO-34 after methanol and propene conversion. Microporous and Mesoporous Materials, 2013, 173, 166-174.	4.4	20
45	Synthesis of a (N,C,C) Au(<scp>iii</scp>) pincer complex <i>via</i> C_{sp3}â€“H bond activation: increasing catalyst robustness by rational catalyst design. Chemical Communications, 2018, 54, 11104-11107.	4.1	20
46	Ionothermal synthesis of two novel metal organophosphonates. Dalton Transactions, 2009, , 795-799.	3.3	19
47	Synthesis and structure determination from an extremely small single crystal of a new layered gallium phosphate. Journal of Physics and Chemistry of Solids, 2001, 62, 1493-1497.	4.0	18
48	Rock â€˜nâ€™ Roll With Gold: Synthesis, Structure, and Dynamics of a (bipyridine)AuCl3 Complex. Organometallics, 2012, 31, 7093-7100.	2.3	18
49	Understanding the (De)Sodiation Mechanisms in Naâ€Based Batteries through Operando Xâ€Ray Methods. Batteries and Supercaps, 2021, 4, 1039-1063.	4.7	18
50	Solvothermal aluminophosphate zeotype synthesis with ionic liquid precursors. Dalton Transactions, 2011, 40, 4926.	3.3	17
51	Cu-catalyzed <i>N</i>-3-Arylation of Hydantoins Using Diaryliodonium Salts. Organic Letters, 2020, 22, 2687-2691.	4.6	16
52	Factors Determining Microporous Material Stability in Water: The Curious Case of SAPO-37. Chemistry of Materials, 2020, 32, 1495-1505.	6.7	15
53	Insights into Crystal Structure and Diffusion of Biphasic Na₂Zn₂TeO₆. ACS Applied Materials & Interfaces, 2020, 12, 28188-28198.	8.0	14
54	The fast Z-scan method for studying working catalytic reactors with high energy X-ray diffraction: ZSM-5 in the methanol to gasoline process. Physical Chemistry Chemical Physics, 2013, 15, 8662-8671.	2.8	12

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55	Ionothermal synthesis and crystal structures of metal phosphate chains. Journal of Solid State Chemistry, 2010, 183, 1625-1631.	2.9	11
56	Syntheses, Crystal Structures, and Thermal Stabilities of Polymorphs of Cr(thd)3. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2010, 636, 2422-2432.	1.2	9
57	Characterization and evaluation of synthetic Dawsonites as CO2 sorbents. Fuel, 2019, 236, 747-754.	6.4	9
58	Operando XRD studies on Bi₂MoO₆ as anode material for Na-ion batteries. Nanotechnology, 2022, 33, 185402.	2.6	9
59	A phase transition from monoclinic<i>C</i>2 with<i>Z</i>â€² = 1 to triclinic<i>P</i>1 with<i>Z</i>â€² = 4 for the quasiracemate<scp>L</scp>-2-aminobutyric acidâ€"<scp>D</scp>-methionine (1/1). Acta Crystallographica Section C, Structural Chemistry, 2016, 72, 536-543.	0.5	8
60	Structural Elucidation, Aggregation, and Dynamic Behaviour of <i>N,N,N,N</i>â€Copper(I) Schiff Base Complexes in Solid and in Solution: A Combined NMR, Xâ€ray Spectroscopic and Crystallographic Investigation. European Journal of Inorganic Chemistry, 2021, 2021, 4762-4775.	2.0	8
61	Structure and Polymorphism of <i>M</i>(thd)₃ (<i>M</i> = Al, Cr, Mn, Fe, Co, Ga, and In). Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2013, 639, 770-778.	1.2	7
62	Synthesis and Characterization of Stable Gold(III) PNP Pincer Complexes. European Journal of Inorganic Chemistry, 2018, 2018, 3113-3117.	2.0	7
63	Substitution of transition metals into azamacrocycleâ€"gallophosphate inorganicâ€"organic hybrid materials. Journal of Materials Chemistry, 2001, 11, 513-517.	6.7	6
64	Two New Series of Coordination Polymers and Evaluation of Their Properties by Density Functional Theory. Crystal Growth and Design, 2016, 16, 339-346.	3.0	6
65	The Reactivity of Multidentate Schiff Base Ligands Derived from Biâ€and Terphenyl Polyamines towards M(II) (M=Ni, Cu, Zn, Cd) and M(III) (M=Co, Y, Lu). European Journal of Inorganic Chemistry, 2021, 2021, 1869-1889.	2.0	6
66	Cu-catalyzed C(sp²)â€"N-bond coupling of boronic acids and cyclic imides. Chemical Communications, 2021, 57, 11851-11854.	4.1	6
67	The role of CNT in surface defect passivation and UV emission intensification of ZnO nanoparticles. Nanomaterials and Nanotechnology, 2022, 12, 184798042210794.	3.0	6
68	SAPO-37 microporous catalysts: revealing the structural transformations during template removal. Journal of Lithic Studies, 2017, 3, 79-88.	0.5	5
69	Chemical Structures of Specific Sodium Ion Battery Components Determined by Operando Pair Distribution Function and Xâ€ray Diffraction Computed Tomography. Angewandte Chemie, 2017, 129, 11543-11547.	2.0	5
70	Synthesis and Evaluation of K-Promoted Co_{3-x}Mg_xAl-Oxides as Solid CO₂ Sorbents in the Sorption-Enhanced Waterâ˜Gas Shift (SEWGS) Reaction. Industrial & Engineering Chemistry Research, 2020, 59, 17837-17844.	3.7	5
71	Structural and magnetic characterization of the elusive Jahn-Teller active <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>NaCrF</mml:mi><mml:mn>3</mml:mn></mml:msub> Physical Review Materials, 2020, 4, .	2.4	5
72	Synthesis of substituted (N,C) and (N,C,C) Au(<scp>iii</scp>) complexes: the influence of sterics and electronics on cyclometalation reactions. Dalton Transactions, 2022, 51, 5082-5097.	3.3	5

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73	Understanding the Deactivation Phenomena of Small-Pore Mo/H-SSZ-13 during Methane Dehydroaromatisation. Molecules, 2020, 25, 5048.	3.8	4
74	Crystal structure of (N^C) cyclometalated Au^{III}diazide at 100â€…K. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1725-1727.	0.5	4
75	Thermogravimetric Analysis â€“ A Viable Method for Screening Novel Materials for the Sorbent Enhanced Water-gas Shift Process. Energy Procedia, 2017, 114, 2294-2303.	1.8	3
76	Canted antiferromagnetism in high-purity <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>NaFeF</mml:mi></mml:mrow><mml:mn>3< prepared by a novel wet-chemical synthesis method. Physical Review Materials, 2020, 4, .	2.4	3
77	Response to â€œComment on â€˜Unusual Photoluminescence of CaHfO3 and SrHfO3 Nanoparticlesâ€™â€ Advanced Functional Materials, 2012, 22, 1114-1115.	14.9	2
78	Synthesis and Properties of Ethyl, Propyl, and Butyl Hexa-alkyldisilanes and Tetrakis(tri-alkylsilyl)silanes. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2014, 640, 2956-2961.	1.2	2
79	The Mixedâ€Valence, Mixedâ€Ligand Complex Co₃(thd)₃(EtO)₄(<i>tert</i>â€BuCOO). Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2011, 637, 2175-2182.	1.2	1
80	Two new Cu(ii) and La(iii) 2D coordination polymers, synthesis and in situ structural analysis by X-ray diffraction. Dalton Transactions, 2016, 45, 12827-12834.	3.3	1
81	Ab initio structure solution and thermal stability evaluation of a new Ca(<scp>ii</scp>) 3D coordination polymer using synchrotron powder X-ray diffraction data. CrystEngComm, 2017, 19, 5857-5863.	2.6	1
82	Jahn-Teller active fluoroperovskites ACrF3 (A=Na+,K+) : Magnetic and thermo-optical properties. Physical Review Materials, 2021, 5, .	2.4	1
83	Understanding the (De)Sodiation Mechanisms in Naâ€Based Batteries through Operando Xâ€ray Methods. Batteries and Supercaps, 2021, 4, 1035-1035.	4.7	1