Wendy J Shaw

List of Publications by Year
in descending order

109 papers	6,816 citations	61945 43 h-index	62565 80 g-index
115 all docs	115 docs citations	115 times ranked	5357 citing authors

#	Article	IF	Citations
1	Nanoscaffold Mediates Hydrogen Release and the Reactivity of Ammonia Borane. Angewandte Chemie - International Edition, 2005, 44, 3578-3582.	7.2	751
2	High-capacity hydrogen storage in lithium and sodium amidoboranes. Nature Materials, 2008, 7, 138-141.	13.3	583
3	In situ solid state 11B MAS-NMR studies of the thermal decomposition of ammonia borane: mechanistic studies of the hydrogen release pathways from a solid state hydrogen storage material. Physical Chemistry Chemical Physics, 2007, 9, 1831.	1.3	356
4	Dynamic Ï€âˆ’Ï€ Stacked Molecular Assemblies Emit from Green to Red Colors. Nano Letters, 2003, 3, 455-458.	4.5	231
5	In Situ Multinuclear NMR Spectroscopic Studies of the Thermal Decomposition of Ammonia Borane in Solution. Angewandte Chemie - International Edition, 2008, 47, 7493-7496.	7.2	168
6	Structure and Dynamics of Hydrated Statherin on Hydroxyapatite As Determined by Solid-State NMR. Biochemistry, 2001, 40, 15451-15455.	1.2	166
7	Mechanistic Insights into Catalytic H₂ Oxidation by Ni Complexes Containing a Diphosphine Ligand with a Positioned Amine Base. Journal of the American Chemical Society, 2009, 131, 5935-5945.	6.6	161
8	Beyond the Active Site: The Impact of the Outer Coordination Sphere on Electrocatalysts for Hydrogen Production and Oxidation. Accounts of Chemical Research, 2014, 47, 2621-2630.	7.6	152
9	Moving Protons with Pendant Amines: Proton Mobility in a Nickel Catalyst for Oxidation of Hydrogen. Journal of the American Chemical Society, 2011, 133, 14301-14312.	6.6	151
10	The COOH Terminus of the Amelogenin, LRAP, Is Oriented Next to the Hydroxyapatite Surface. Journal of Biological Chemistry, 2004, 279, 40263-40266.	1.6	131
11	Minimal Proton Channel Enables H₂ Oxidation and Production with a Water-Soluble Nickel-Based Catalyst. Journal of the American Chemical Society, 2013, 135, 18490-18496.	6.6	131
12	Proton Delivery and Removal in [Ni(P^R₂N^{R^{â€²}}₂)₂]²⁺ Hydrogen Production and Oxidation Catalysts. Journal of the American Chemical Society, 2012, 134, 19409-19424.	6.6	122
13	Amino acid modified Ni catalyst exhibits reversible H ₂ oxidation/production over a broad pH range at elevated temperatures. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 16286-16291.	3.3	112
14	Lanthanide selective sorbents: self-assembled monolayers on mesoporous supports (SAMMS). Journal of Materials Chemistry, 2004, 14, 3356.	6.7	109
15	Chimeric Peptides of Statherin and Osteopontin That Bind Hydroxyapatite and Mediate Cell Adhesion. Journal of Biological Chemistry, 2000, 275, 16213-16218.	1.6	105
16	M<scp>olecular</scp> R<scp>ecognition at the</scp> P<scp>rotein-</scp>H<scp>ydroxyapatite</scp> I<scp>nterface</scp>. Critical Reviews in Oral Biology and Medicine, 2003, 14, 370-376.	4.4	104
17	[Ni(P^{Ph}₂N^{Bn}₂)₂(CH₃CN)]²⁺ as an Electrocatalyst for H₂ Production: Dependence on Acid Strength and Isomer Distribution. ACS Catalysis, 2011, 1, 777-785.	5.5	104
18	A modular, energy-based approach to the development of nickel containing molecular electrocatalysts for hydrogen production and oxidation. Biochimica Et Biophysica Acta - Bioenergetics, 2013, 1827, 1123-1139.	0.5	102

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19	Determination of Statherin N-Terminal Peptide Conformation on Hydroxyapatite Crystals. Journal of the American Chemical Society, 2000, 122, 1709-1716.	6.6	92
20	Carbonâ€Nanotubeâ€Supported Bioâ€Inspired Nickel Catalyst and Its Integration in Hybrid Hydrogen/Air Fuel Cells. Angewandte Chemie - International Edition, 2017, 56, 1845-1849.	7.2	87
21	Experimental determination of the effect of the ratio of B/Al on glass dissolution along the nepheline (NaAlSiO4)â€“malinkoite (NaBSiO4) join. Geochimica Et Cosmochimica Acta, 2010, 74, 2634-2654.	1.6	85
22	The nucleation and growth of calcium phosphate by amelogenin. Journal of Crystal Growth, 2007, 304, 407-415.	0.7	82
23	Arginineâ€Containing Ligands Enhance H₂ Oxidation Catalyst Performance. Angewandte Chemie - International Edition, 2014, 53, 6487-6491.	7.2	82
24	Spectroscopic Studies of Dehydrogenation of Ammonia Borane in Carbon Cryogel. Journal of Physical Chemistry B, 2007, 111, 14285-14289.	1.2	79
25	Acidic ionic liquid/water solution as both medium and proton source for electrocatalytic H ₂ evolution by [Ni(P ₂ N ₂) ₂] ²⁺ complexes. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 15634-15639.	3.3	78
26	Designing electrochemically reversible H2 oxidation and production catalysts. Nature Reviews Chemistry, 2018, 2, 244-252.	13.8	78
27	An experimental study of the dissolution rates of simulated aluminoborosilicate waste glasses as a function of pH and temperature under dilute conditions. Applied Geochemistry, 2008, 23, 2559-2573.	1.4	75
28	Incorporating Peptides in the Outer-Coordination Sphere of Bioinspired Electrocatalysts for Hydrogen Production. Inorganic Chemistry, 2011, 50, 4073-4085.	1.9	73
29	Molecular dynamics study of the proposed proton transport pathways in [FeFe]-hydrogenase. Biochimica Et Biophysica Acta - Bioenergetics, 2014, 1837, 131-138.	0.5	71
30	Interaction of lithium hydride and ammonia borane in THF. Chemical Communications, 2008, , 5595.	2.2	70
31	STRUCTURALSTUDIES OFBIOMATERIALSUSINGDOUBLE-QUANTUMSOLID-STATENMR SPECTROSCOPY. Annual Review of Physical Chemistry, 2003, 54, 531-571.	4.8	68
32	Thermodynamic Roles of Basic Amino Acids in Statherin Recognition of Hydroxyapatite. Biochemistry, 2007, 46, 4725-4733.	1.2	62
33	Direct Comparison of the Performance of a Bioâ€Inspired Synthetic Nickel Catalyst and a [NiFe]â€Hydrogenase, Both Covalently Attached to Electrodes. Angewandte Chemie - International Edition, 2015, 54, 12303-12307.	7.2	61
34	A Solid State NMR Study of Dynamics in a Hydrated Salivary Peptide Adsorbed to Hydroxyapatite. Journal of the American Chemical Society, 2000, 122, 7118-7119.	6.6	60
35	Experimentally determined dissolution kinetics of Na-rich borosilicate glass at far from equilibrium conditions: Implications for Transition State Theory. Geochimica Et Cosmochimica Acta, 2008, 72, 2767-2788.	1.6	59
36	Understanding and Design of Bidirectional and Reversible Catalysts of Multielectron, Multistep Reactions. Journal of the American Chemical Society, 2019, 141, 11269-11285.	6.6	51

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37	Electrocatalytic H₂ production with a turnover frequency >10⁷ s^{â^'1}: the medium provides an increase in rate but not overpotential. Energy and Environmental Science, 2014, 7, 4013-4017.	15.6	49
38	Achieving Reversible H₂/H⁺ Interconversion at Room Temperature with Enzyme-Inspired Molecular Complexes: A Mechanistic Study. ACS Catalysis, 2016, 6, 6037-6049.	5.5	49
39	Adsorption of Amelogenin onto Self-Assembled and Fluoroapatite Surfaces. Journal of Physical Chemistry B, 2009, 113, 1833-1842.	1.2	48
40	Characterization of a new phase of ammonia borane. Energy and Environmental Science, 2010, 3, 796.	15.6	48
41	Molecular Catalysts with Diphosphine Ligands Containing Pendant Amines. Chemical Reviews, 2022, 122, 12427-12474.	23.0	48
42	The Structure and Orientation of the C-Terminus of LRAP. Biophysical Journal, 2008, 94, 3247-3257.	0.2	47
43	The structure, dynamics, and energetics of protein adsorptionâ€"lessons learned from adsorption of statherin to hydroxyapatite. Magnetic Resonance in Chemistry, 2007, 45, S32-S47.	1.1	44
44	A Solution NMR Investigation into the Early Events of Amelogenin Nanosphere Self-Assembly Initiated with Sodium Chloride or Calcium Chloride. Biochemistry, 2008, 47, 13215-13222.	1.2	44
45	Partial High-Resolution Structure of Phosphorylated and Non-phosphorylated Leucine-Rich Amelogenin Protein Adsorbed to Hydroxyapatite. Journal of Physical Chemistry C, 2011, 115, 13775-13785.	1.5	42
46	Changes in the quaternary structure of amelogenin when adsorbed onto surfaces. Biopolymers, 2009, 91, 103-107.	1.2	41
47	The Outer-Coordination Sphere: Incorporating Amino Acids and Peptides as Ligands for Homogeneous Catalysts to Mimic Enzyme Function. Catalysis Reviews - Science and Engineering, 2012, 54, 489-550.	5.7	40
48	Synthesis of carbamoylphosphonate silanes for the selective sequestration of actinides. Chemical Communications, 2002, , 1374-1375.	2.2	39
49	Decomposition Pathway of Ammonia Borane on the Surface of Nano-BN. Journal of Physical Chemistry C, 2010, 114, 13935-13941.	1.5	39
50	The Role of a Dipeptide Outerâ€Coordination Sphere on H₂â€Production Catalysts: Influence on Catalytic Rates and Electron Transfer. Chemistry - A European Journal, 2013, 19, 1928-1941.	1.7	38
51	The Influence of the Second and Outer Coordination Spheres on Rh(diphosphine)₂ CO₂ Hydrogenation Catalysts. ACS Catalysis, 2014, 4, 3663-3670.	5.5	37
52	Conformational Dynamics and Proton Relay Positioning in Nickel Catalysts for Hydrogen Production and Oxidation. Organometallics, 2013, 32, 7034-7042.	1.1	36
53	Structure, Orientation, and Dynamics of the C-Terminal Hexapeptide of LRAP Determined Using Solid-State NMR. Journal of Physical Chemistry B, 2008, 112, 16975-16981.	1.2	35
54	Investigating the Role of the Outer-Coordination Sphere in [Ni(P^{Ph}₂N^{Ph-R}₂)₂]²⁺ Hydrogenase Mimics. Inorganic Chemistry, 2012, 51, 6592-6602.	1.9	35

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55	Controlling proton movement: electrocatalytic oxidation of hydrogen by a nickel(<scp>ii</scp>) complex containing proton relays in the second and outer coordination spheres. Dalton Transactions, 2014, 43, 2744-2754.	1.6	35
56	Dual properties of a hydrogen oxidation Ni-catalyst entrapped within a polymer promote self-defense against oxygen. Nature Communications, 2018, 9, 864.	5.8	35
57	Enzyme Design from the Bottom Up: An Active Nickel Electrocatalyst with a Structured Peptide Outer Coordination Sphere. Chemistry - A European Journal, 2014, 20, 1510-1514.	1.7	34
58	Incorporating Amino Acid Esters into Catalysts for Hydrogen Oxidation: Steric and Electronic Effects and the Role of Water as a Base. Organometallics, 2012, 31, 6719-6731.	1.1	33
59	Molecular Structure and Dynamics in the Low Temperature (Orthorhombic) Phase of NH3BH3. Journal of Physical Chemistry A, 2008, 112, 4277-4283.	1.1	32
60	Hydrogen Storage Properties of New Hydrogen-Rich BH3NH3-Metal Hydride (TiH2, ZrH2, MgH2, and/or) Tj ETQq0 0 0 rgBT /Overlock 10	1.5	32
61	A proton channel allows a hydrogen oxidation catalyst to operate at a moderate overpotential with water acting as a base. Chemical Communications, 2014, 50, 792-795.	2.2	32
62	Evaluating the role of acidic, basic, and polar amino acids and dipeptides on a molecular electrocatalyst for H₂ oxidation. Catalysis Science and Technology, 2017, 7, 1108-1121.	2.1	31
63	Single-Amino Acid Modifications Reveal Additional Controls on the Proton Pathway of [FeFe]-Hydrogenase. Biochemistry, 2016, 55, 3165-3173.	1.2	29
64	Neutron Reflectometry Studies of the Adsorbed Structure of the Amelogenin, LRAP. Journal of Physical Chemistry B, 2013, 117, 3098-3109.	1.2	28
65	Water-assisted proton delivery and removal in bio-inspired hydrogen production catalysts. Dalton Transactions, 2015, 44, 10969-10979.	1.6	28
66	A Nanotube-Supported Dicopper Complex Enhances Pt-free Molecular H2/Air Fuel Cells. Joule, 2019, 3, 2020-2029.	11.7	28
67	Solid-state NMR studies of proteins immobilized on inorganic surfaces. Solid State Nuclear Magnetic Resonance, 2015, 70, 1-14.	1.5	26
68	Optimizing conditions for utilization of an H₂ oxidation catalyst with outer coordination sphere functionalities. Dalton Transactions, 2016, 45, 9786-9793.	1.6	26
69	Mineral Association Changes the Secondary Structure and Dynamics of Murine Amelogenin. Journal of Dental Research, 2013, 92, 1000-1004.	2.5	25
70	Sequence-Defined Energetic Shifts Control the Disassembly Kinetics and Microstructure of Amelogenin Adsorbed onto Hydroxyapatite (100). Langmuir, 2015, 31, 10451-10460.	1.6	24
71	The leucine rich amelogenin protein (LRAP) adsorbs as monomers or dimers onto surfaces. Journal of Structural Biology, 2010, 169, 266-276.	1.3	21
72	Phosphorylation and Ionic Strength Alter the LRAPâ€"HAP Interface in the N-Terminus. Biochemistry, 2013, 52, 2196-2205.	1.2	21

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73	The Role of Solvent and the Outer Coordination Sphere on H2Oxidation Using [Ni(PCy2NPyz2)2]2+. European Journal of Inorganic Chemistry, 2015, 2015, 5218-5225.	1.0	20
74	The energetic basis for hydroxyapatite mineralization by amelogenin variants provides insights into the origin of <i>amelogenesis imperfecta</i>. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 13867-13872.	3.3	20
75	Chicken fat for catalysis: a scaffold is as important for molecular complexes for energy transformations as it is for enzymes in catalytic function. Sustainable Energy and Fuels, 2019, 3, 3260-3278.	2.5	19
76	A Positive Charge in the Outer Coordination Sphere of an Artificial Enzyme Increases CO₂ Hydrogenation. Organometallics, 2020, 39, 1532-1544.	1.1	19
77	Radical and Non-Radical Mechanisms for Alkane Oxidations by Hydrogen Peroxideâˆ’Trifluoroacetic Acid. Journal of Organic Chemistry, 2001, 66, 789-795.	1.7	18
78	1H, 13C, and 15N resonance assignments of murine amelogenin, an enamel biomineralization protein. Biomolecular NMR Assignments, 2008, 2, 89-91.	0.4	17
79	Photoswitching a molecular catalyst to regulate CO₂ hydrogenation. Dalton Transactions, 2015, 44, 14854-14864.	1.6	17
80	Carbonâ€Nanotubeâ€Supported Bioâ€Inspired Nickel Catalyst and Its Integration in Hybrid Hydrogen/Air Fuel Cells. Angewandte Chemie, 2017, 129, 1871-1875.	1.6	17
81	Electrocatalytic Oxidation of Formate with Nickel Diphosphine Dipeptide Complexes: Effect of Ligands Modified with Amino Acids. European Journal of Inorganic Chemistry, 2013, 2013, 5366-5371.	1.0	16
82	Controls of nature: Secondary, tertiary, and quaternary structure of the enamel protein amelogenin in solution and on hydroxyapatite. Journal of Structural Biology, 2020, 212, 107630.	1.3	16
83	The leucine-rich amelogenin protein (LRAP) is primarily monomeric and unstructured in physiological solution. Journal of Structural Biology, 2015, 190, 81-91.	1.3	15
84	Investigating the role of chain and linker length on the catalytic activity of an H₂ production catalyst containing a Î²-hairpin peptide. Journal of Coordination Chemistry, 2016, 69, 1730-1747.	0.8	15
85	Active Hydrogenation Catalyst with a Structured, Peptide-Based Outer-Coordination Sphere. ACS Catalysis, 2012, 2, 2114-2118.	5.5	14
86	A solution NMR investigation into the impaired self-assembly properties of two murine amelogenins containing the point mutations T21â†’I or P41â†’T. Archives of Biochemistry and Biophysics, 2013, 537, 217-224.	1.4	14
87	Synthesis and characterization of a recoverable rhodium catalyst with a stimulus sensitive polymer ligand. Inorganic Chemistry Communication, 2005, 8, 894-896.	1.8	13
88	A solution NMR investigation into the murine amelogenin splice-variant LRAP (Leucine-Rich Amelogenin) Tj ETQq0 0 0 rgBT /Overlock 10	1.1	13
89	Covalent Attachment of the Waterâ€insoluble Ni(P Cy 2 N Phe 2) 2 Electrocatalyst to Electrodes Showing Reversible Catalysis in Aqueous Solution. Electroanalysis, 2016, 28, 2452-2458.	1.5	12
90	Solid-State NMR Identification of Intermolecular Interactions in Amelogenin Bound to Hydroxyapatite. Biophysical Journal, 2018, 115, 1666-1672.	0.2	12

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91	The flexible structure of the K24S28 region of Leucine-Rich Amelogenin Protein (LRAP) bound to apatites as a function of surface type, calcium, mutation, and ionic strength. Frontiers in Physiology, 2014, 5, 254.	1.3	11
92	Evaluating the impacts of amino acids in the second and outer coordination spheres of Rh-bis(diphosphine) complexes for CO2 hydrogenation. Faraday Discussions, 2019, 215, 123-140.	1.6	11
93	Using Surface Amide Couplings to Assemble Photocathodes for Solar Fuel Production Applications. ACS Applied Materials & Interfaces, 2020, 12, 4501-4509.	4.0	11
94	Spectroscopic Studies of Tributylstannyl Radical. Rates of Formation, Termination, and Abstraction Determined by Transient Absorption Spectroscopy. Organometallics, 2004, 23, 2080-2086.	1.1	10
95	Mechanistic Investigation on the Formation and Dehydrogenation of Calcium Amidoborane Ammoniate. ChemSusChem, 2012, 5, 927-931.	3.6	10
96	Structural characterization of the model amphipathic peptide Ac-LKKLLKLLKKLLKL-NH₂ in aqueous solution and with 2,2,2-trifluoroethanol and 1,1,1,3,3,3-hexafluoroisopropanol. Canadian Journal of Chemistry, 2013, 91, 406-413.	0.6	10
97	Improved protocol to purify untagged amelogenin â€" Application to murine amelogenin containing the equivalent P70 â†' T point mutation observed in human amelogenesis imperfecta. Protein Expression and Purification, 2015, 105, 14-22.	0.6	10
98	Absolute Rate Constants for Reactions of Tributylstannyl Radicals with Bromoalkanes, Episulfides, and Î±-Halomethyl-Episulfides, -Cyclopropanes, and -Oxiranes:Â New Rate Expressions for Sulfur and Bromine Atom Abstraction. Journal of Organic Chemistry, 2004, 69, 1020-1027.	1.7	9
99	Structural evolution of a recoverable rhodium hydrogenation catalyst. Journal of Organometallic Chemistry, 2008, 693, 2111-2118.	0.8	8
100	Biologically inspired phosphino platinum complexes. Inorganic Chemistry Communication, 2012, 22, 65-67.	1.8	7
101	Identification of major matrix metalloproteinase-20 proteolytic processing products of murine amelogenin and tyrosine-rich amelogenin peptide using a nuclear magnetic resonance spectroscopy based method. Archives of Oral Biology, 2018, 93, 187-194.	0.8	7
102	Direkter Leistungsvergleich eines bioinspirierten synthetischen Niâ€Katalysators und einer [NiFe]â€Hydrogenase, beide kovalent an eine Elektrode gebunden. Angewandte Chemie, 2015, 127, 12478-12482.	1.6	6
103	Synthetic approaches to artificial photosynthesis: general discussion. Faraday Discussions, 2019, 215, 242-281.	1.6	5
104	Chemical Method for Evaluating Catalytic Turnover Frequencies (TOF) of Moderate to Slow H₂ Oxidation Electrocatalysts. Organometallics, 2019, 38, 1311-1316.	1.1	3
105	Introduction to (photo)electrocatalysis for renewable energy. Chemical Communications, 2021, 57, 1540-1542.	2.2	3
106	Secondary structure and dynamics study of the intrinsically disordered silicaâ€mineralizing peptide P₅S₃ during silicic acid condensation and silica decondensation. Proteins: Structure, Function and Bioinformatics, 2017, 85, 2111-2126.	1.5	2
107	A protein scaffold enables hydrogen evolution for a Ni-bisdiphosphine complex. Dalton Transactions, 2021, 50, 15754-15759.	1.6	2
108	High-capacity hydrogen storage in lithium and sodium amidoboranes. , 2010, , 276-279.		0

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109	Synthesis of Carbamoylphosphonate Silanes for the Selective Sequestration of Actinides.. ChemInform, 2002, 33, 187-187.	0.1	0