Paul Sherwood

List of Publications by Year
in descending order

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83	8,983	94269 37	54797 84
papers	citations	h-index	g-index

87	87	87	10386
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Band alignment of rutile and anatase TiO2. Nature Materials, 2013, 12, 798-801.	13.3	1,924
2	QUASI: A general purpose implementation of the QM/MM approach and its application to problems in catalysis. Computational and Theoretical Chemistry, 2003, 632, 1-28.	1.5	887
3	Understanding the Behavior of Halogens as Hydrogen Bond Acceptors. Crystal Growth and Design, 2001, 1, 277-290.	1.4	631
4	The GAMESS-UK electronic structure package: algorithms, developments and applications. Molecular Physics, 2005, 103, 719-747.	0.8	484
5	DL-FIND: An Open-Source Geometry Optimizer for Atomistic Simulations. Journal of Physical Chemistry A, 2009, 113, 11856-11865.	1.1	466
6	Supramolecular Chemistry of Halogens:â€‰ Complementary Features of Inorganic (Mâˆ’X) and Organic (Câˆ’Xâ€˜) Halogens Applied to Mâˆ’XÂ·Â·Xâ€˜âˆ’C Halogen Bond Formation. Journal of the American Chemical Society, 2005, 127, 5979-5989.	6.6	365
7	<scp>C</scp>hem<scp>S</scp>hellâ€”a modular software package for <scp>QM</scp>/<scp>MM</scp> simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 101-110.	6.2	351
8	Zeolite Structure and Reactivity by Combined Quantum-Chemicalâˆ’Classical Calculations. Journal of Physical Chemistry B, 1999, 103, 6133-6141.	1.2	343
9	Superlinearly converging dimer method for transition state search. Journal of Chemical Physics, 2008, 128, 014106.	1.2	282
10	Computer simulation of zeolite structure and reactivity using embedded cluster methods. Faraday Discussions, 1997, 106, 79-92.	1.6	190
11	Multiscale methods for macromolecular simulations. Current Opinion in Structural Biology, 2008, 18, 630-640.	2.6	175
12	Optimization of quantum mechanical molecular mechanical partitioning schemes: Gaussian delocalization of molecular mechanical charges and the double link atom method. Journal of Chemical Physics, 2002, 117, 10534-10547.	1.2	173
13	Designing Intermolecular Interactions between Halogenated Peripheries of Inorganic and Organic Molecules: Electrostatically Directed Mï£¿Xâ‹…â‹…â‹…Xâ€²ï£¿C Halogen Bonds. Angewandte Chemie - International Edition, 2006, 45, 435-440.	11.2	152
14	Point defects in ZnO. Faraday Discussions, 2007, 134, 267-282.	1.6	151
15	Hydrogen bonding and perhalometallate ions: A supramolecular synthetic strategy for new inorganic materials. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 4956-4961.	3.3	126
16	Quantum-chemical studies of alkene chemisorption in chabazite: A comparison of cluster and embedded-cluster models. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 3401-3408.	1.7	121
17	From CO2 to Methanol by Hybrid QM/MM Embedding This work was supported by EU Esprit IV project 25047. S.A.F. is grateful to ICI and Synetix for funding. K. Waugh, L. Whitmore, S. Cristol, and P. Sushko are thanked for their helpful insights. QM/MM=quantum mechanics/molecular mechanics.. Angewandte Chemie - International Edition, 2001, 40, 4437.	7.2	102
18	Exploring the quantum mechanical/molecular mechanical replica path method: a pathway optimization of the chorismate to prephenate Claisen rearrangement catalyzed by chorismate mutase. Theoretical Chemistry Accounts, 2003, 109, 140-148.	0.5	100

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19	Hybrid QM/MM embedding approach for the treatment of localized surface states in ionic materials. International Journal of Quantum Chemistry, 2004, 99, 695-712.	1.0	97
20	Identification and Characterization of Active Sites and Their Catalytic Processesâ€"the Cu/ZnO Methanol Catalyst. Topics in Catalysis, 2003, 24, 161-172.	1.3	87
21	Fluoride ligands exhibit marked departures from the hydrogen bond acceptor behavior of their heavier halogen congeners. New Journal of Chemistry, 1999, 23, 965-968.	1.4	85
22	Et3NH+Co(CO)4-: hydrogen-bonded adduct or simple ion pair? Single-crystal neutron diffraction study at 15 K. Organometallics, 1992, 11, 2339-2341.	1.1	81
23	A parallel second-order MÃ¸ller-Plesset gradient. Molecular Physics, 1997, 91, 431-438.	0.8	78
24	An embedded cluster study of the formation of water on interstellar dust grains. Physical Chemistry Chemical Physics, 2009, 11, 5431.	1.3	78
25	Adsorption of water and methanol on zeolite Bro/nsted acid sites: Anabinitio, embedded cluster study including electron correlation. Journal of Chemical Physics, 1996, 105, 3770-3776.	1.2	77
26	Chemistry of polynuclear metal complexes with bridging carbene or carbyne ligands. Part 79. Synthesis and reactions of the alkylidynemetal complexes [M(î€‡CR)(CO)2(Î·-C5H5)](R = C6H3Me2-2,6, M = Cr,) Tj ETQq0 0 0 rgBT /Ove [MoFe(Âµ-CC6H3Me2-2,6)(CO)5(Î·-C5H5)]. Journal of the Chemical Society Dalton Transactions, 1988, , 2453-2465.	1.1	61
27	Donor and acceptor characteristics of native point defects in GaN. Journal Physics D: Applied Physics, 2019, 52, 335104.	1.3	49
28	Embedded Cluster Model for the ab Initio Study of Broensted Acidity in Zeolites. The Journal of Physical Chemistry, 1994, 98, 8134-8139.	2.9	48
29	Exploiting QM/MM Capabilities in Geometry Optimization:â€‰ A Microiterative Approach Using Electrostatic Embedding. Journal of Chemical Theory and Computation, 2007, 3, 1064-1072.	2.3	48
30	Open-Source, Python-Based Redevelopment of the ChemShell Multiscale QM/MM Environment. Journal of Chemical Theory and Computation, 2019, 15, 1317-1328.	2.3	46
31	QM/MM modelling of the TS-1 catalyst using HPCx. Journal of Materials Chemistry, 2006, 16, 1919.	6.7	45
32	The Quixote project: Collaborative and Open Quantum Chemistry data management in the Internet age. Journal of Cheminformatics, 2011, 3, 38.	2.8	45
33	Acceleration of the GAMESSâ€UK electronic structure package on graphical processing units. Journal of Computational Chemistry, 2011, 32, 2313-2318.	1.5	43
34	Metal Cluster Support Interactions in the Cu/ZnO System:Â A QM/MM Study. Journal of Physical Chemistry B, 2003, 107, 7045-7057.	1.2	42
35	Structure, optical properties and defects in nitride (IIIâ€"V) nanoscale cage clusters. Physical Chemistry Chemical Physics, 2008, 10, 1944.	1.3	42
36	Embedded-cluster calculations in a numeric atomic orbital density-functional theory framework. Journal of Chemical Physics, 2014, 141, 024105.	1.2	38

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37	Chemistry of polynuclear metal complexes with bridging carbene or carbyne ligands. Part 56. Synthesis of ironâ€“molybdenum compounds; crystal structures of [FeMo(Âμ-CR)(CO)6(Î·-C5H5)] and [FeMo2(Âμ3-RC2R)(CO)6(Î·-C5H5)2](R = C6H4Me-4). Journal of the Chemical Society Dalton Transactions, 1987, , 1209-1214.	1.1	36
38	Assignment of the complex vibrational spectra of the hydrogenated ZnO polar surfaces using QM/MM embedding. Journal of Chemical Physics, 2003, 118, 317-320.	1.2	36
39	Tautomeric equilibria in 3- and 5-hydroxyisoxazole in the gas phase and in aqueous solution: a test of molecular dynamics and continuum models of solvation. Journal of the Chemical Society Perkin Transactions II, 1992, , 2151.	0.9	35
40	Adsorption energies of NH3 and NH4+ in zeolites. An embedded cluster model including electron correlation. Chemical Physics Letters, 1995, 234, 367-372.	1.2	34
41	Activation of Carbon Dioxide over Zinc Oxide by Localised Electrons. ChemPhysChem, 2012, 13, 3453-3456.	1.0	34
42	Transformations of Âμ-methylene-diruthenium complexes into tetranuclear metal clusters with Âμ4-methylidyne and Âμ4-carbido groups: X-ray crystal structures of [Ru2Pt2(Âμ-H)(Âμ4-CH)(Âμ-CO)(CO)2(PPri3)2(Î·-C5H5)2] and [Ru2Pt2(Âμ-H)2(Âμ4-C)(Âμ-CO)2(PPri3)2(Î·-C5H5)2]. Journal of the Chemical Society Chemical Communications, 1987, , 454-456.	2.0	27
43	Strengthening of Nâˆ’HÂ·Â·Â·Co Hydrogen Bonds upon Increasing the Basicity of the Hydrogen Bond Acceptor (Co). Organometallics, 1996, 15, 1441-1445.	1.1	27
44	The Removal of the Muffin-Tin Approximation and Use of Self-Consistent-Field Electron Densities for Calculating the K -Edge X-Ray Absorption Near-Edge Structure of Chlorine. Europhysics Letters, 1995, 29, 647-652.	0.7	25
45	Formation of Heteroatom Active Sites in Zeolites by Hydrolysis and Inversion. Angewandte Chemie - International Edition, 2006, 45, 1633-1638.	7.2	25
46	Chemistry of polynuclear metal complexes with bridging carbene or carbyne ligands. Part 88. Carbaboranetungsteniridium compounds; crystal structure of the complex [WIr(Âμ-CC6H4Me-4)(CO)2(PEt3)2(Î·5-C2B9H9Me2)]. Journal of the Chemical Society Dalton Transactions, 1989, , 1845-1854.	1.1	24
47	The Growth of Copper Clusters over ZnO:â€‰ the Competition between Planar and Polyhedral Clusters. Journal of Physical Chemistry C, 2008, 112, 7420-7430.	1.5	24
48	Chemistry of polynuclear metal complexes with bridging carbene or carbyne ligands. Part 64. Addition of methylene groups to ironâ€“molybdenum complexes; crystal structures of [FeMo(Âμ-CH2){Âμ-Ïƒ:Î·-C(C6H4Me-4)â€†CH2}(CO)5(Î·-C5H5)] and [FeMo{Âμ-C(C6H4Me-4)C(OMe)C(H)}(CO)5(Î·-C5H5)]. Journal of the Chemical Society Dalton Transactions, 1987, , 2201-2209.	1.1	23
49	Chemistry of polynuclear metal complexes with bridging carbene or carbyne ligands. Part 57. Reactions of ironâ€“molybdenum complexes with oxygen and sulphur; crystal structure of [FeMo(Âμ-Î·2-SCC6H4Me-4)(CO)5(Î·-C5H5)]. Journal of the Chemical Society Dalton Transactions, 1987, , 2215-2219.	1.1	22
50	Chemistry of polynuclear metal complexes with bridging carbene or carbyne ligands. Part 65. Reactions of the complexes [FeW(Âμ-CR)(CO)5(Î·-C5Me5)] and [Fe2W(Âμ3-CR)(Âμ-CO)(CO)8(Î·-C5Me5)](R =) Tj ETQq0 0 0 rgBT /Overl [FeW{Âμ-C(R)C(O)C(Me)C(Me)}(CO)5(Î·-C5Me5)]Â·CH2Cl2and [FeW{Âμ-C(R)C(Et)C(H)C(Me)C(Me)}(Âμ-CO)(CO)3(Î·-C5Me5)]. Journal of the Chemical Society Dalton Transactions, 1987, , 2211-2218.	1.1	21
51	Chemistry of polynuclear metal complexes with bridging carbene or carbyne ligands. Part 91. Steric implications in the reactions of the complexes [M(î€‡CR)(CO)2(Î·-C5H5)](M = Mo or W, R = C6H4Me-4,) Tj ETQq1 1 0.784314 rgBT /O Society Dalton Transactions, 1989, , 1871-1878.	1.1	21
52	On the performance of molecular dynamics applications on current high-end systems. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2005, 363, 1987-1998.	1.6	21
53	The ribosome catalyzes peptide bond formation by providing high ionic strength. Molecular Physics, 2010, 108, 293-306.	0.8	21
54	Characterization of hydrogen dissociation over aluminium-doped zinc oxide using an efficient massively parallel framework for QM/MM calculations. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2011, 467, 1900-1924.	1.0	21

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55	Ruthenium-platinum carbonyl cluster complexes with bridging methylene, methylidyne, and carbido ligands; crystal structures of the compounds [Ru2Pt(Î¼-CH2)(Î¼-CO)(CO)2{P(cyclo-C6H11)3}(Î·-C5H5)2], [Ru2Pt2(Î¼-H)(Î¼4-CH)(Î¼-CO)(CO)2(PPr3i)2(Î·-C5H5)2], and [Ru2Pt2(Î¼-H)2(Î¼4-C)(Î¼-CO)2(PPr3i)2(Î·-C5H5)2]. Journal of Organometallic Chemistry, 1990, 383, 463-480.	2.8	20
56	Chemistry of polynuclear metal complexes with bridging carbene or carbyne ligands. Part 74. Salts of the anions [W(î€‡CR)(CO)2(Î·5-C2B9H9Me2)]â€“(R = C6H4Me-2 or C6H3Me2-2,6) as reagents for the synthesis of compounds with heteronuclear metalâ€“metal bonds: crystal structure of [NEt4][FeW(Âµ-CC6H3Me2-2,6)(CO)5(Î·5-C2B9H9Me2)]. Journal of the Chemical Society Dalton Transactions, 1988, , 1879-1889.	1.1	19
57	Parallelism in computational chemistry. Theoretica Chimica Acta, 1993, 84, 423-441.	0.9	19
58	Comparison of embedded cluster models to study zeolite catalysis: Proton transfer reactions in acidic chabazite. , 1997, 18, 562-568.		19
59	Chemistry of polynuclear metal complexes with bridging carbene or carbyne ligands. Part 75. Reactions of octacarbonyldicobalt with the salts [X][W(î€‡CR)(CO)2(Î·5-C2B9H9Me2)](X = NEt4or PPh4; R =) Tj ETQq1 1 0.784314 rgB [PPh4][Co2W(Âµ3-CPh)(CO)8(Î·5-C2B9H9Me2)]Â·0.5CH2Cl2. Journal of the Chemical Society Dalton Transactions, 1988, , 1891-1897.	1.1	17
60	Germanium-germanium bonding in the high-pressure modification of lithium germanide - a near-Zintl phase. Journal of the American Chemical Society, 1990, 112, 2881-2886.	6.6	16
61	Demonstration of the donor characteristics of Si and O defects in GaN using hybrid QM/MM. Physica Status Solidi (A) Applications and Materials Science, 2017, 214, 1600445.	0.8	16
62	Synthesis and reactions of phosphido-bridged Î¼3-alkylidyne clusters; X-ray crystal structures of the complexes [Co2W(Î¼-PEt2)3(CO)5(Î·-C5H5)], [Co2W{Î¼3-C(R)C(Et)C(Et)C(O)}(Î¼-CO)(CO)4(PPh2{C(Et)î—»CHEt})(Î·-C5H5)], and [CoW{Î¼-C(R)C(Et)C(Et)C(OH)}(CO)4(Î·-C5H5)] (R = C6H4Me-4). Journal of Organometallic Chemistry, 1986, 311, C55-C59.	0.8	14
63	Reactions of ironâ€“molybdenum compounds with alkynes; crystal structures of [MoFe{Âµ-C(C6H4Me-4)C(CHMe)CH2C(Me)C(Me)}(CO)4(Î·-C5H5)], [MoFe{Âµ-C(C6H4Me-4)C(CHMe)CH2}(CO)5(Î·-C5H5)], and [MoFe{Âµ-C(C6H4Me-4)C(CH2PMe3)CHMe}(CO)5(Î·-C5H5)]. Journal of the Chemical Society Dalton Transactions, 1988, , 2431-2442.	1.1	13
64	The Charge Distribution in Amides and Thioamides by Nuclear Quadrupole Coupling, Dipole Moments and Electronic Structure Calculations. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1996, 51, 460-478.	0.7	13
65	Chemistry of polynuclear metal complexes with bridging carbene or carbyne ligands. Part 78. Reactions of [MoFe(Âµ-CC6H4Me-4)(CO)6(Î·-C5H5)] with alkynes; crystal structures of [MoFe{Âµ-C(C6H4Me-4)C(O)C(Et)C(Et)}(Âµ-CO)(CO)4(Î·-C5H5)] and [MoFe{Âµ-C(C6H4Me-4)C(Me)C[C(O)Me]}(CO)5(Î·-C5H5)]. Journal of the Chemical Society Dalton	1.1	12
66	Chemistry of polynuclear metal complexes with bridging carbene or carbyne ligands. Part 69. Reactions of [MoW(î€‡CC6H4Me-4)(CO)7(Î·-C5H5)] with but-2-yne; crystal structures of [MoW{Âµ-C(C6H4Me-4)C(Me)C(Me)}(CO)3(Î·-MeC2Me)2(Î·-C5H5)] and [MoW{Âµ-C(C6H4Me-4)C(î€†CH2)C(H)MeC(O)}(CO)6(Î·-C5H5)]Â·0.5CH2Cl2. Journal of the Chemical Society Dalton Transactions, 1988, , 207-214.	1.1	12
67	Deformations in mixed-valence copper(I)-copper(II) polymers. Inorganic Chemistry, 1989, 28, 509-518.	1.9	12
68	Theoretical study of the metathesis-like reaction between ditungsten hexaalkoxides and alkynesâ€Šâ€. Journal of the Chemical Society Dalton Transactions, 1997, , 3845-3852.	1.1	12
69	Methylene, oxygen, and sulphur addition to a Âµ-alkylidyne ligand in an ironâ€“molybdenum complex: X-ray crystal structures of [FeMo{Âµ-Ïƒ,Î·-C(C6H4Me-4)î€†CH2}(Âµ-CH2)(CO)5(Î·-C5H5)], [FeMo{Âµ-Î·3-C(C6H4Me-4)C(OMe)C(H)}(CO)5(Î·-C5H5)], and [FeMo{Âµ-Î·-SC(C6H4Me-4)}(CO)5(Î·-C5H5)]. Journal of the Chemical Society Chemical Communications, 1986, , 802-804.	2.0	11
70	Chemistry of polynuclear metal complexes with bridging carbene or carbyne ligands. Part 55. Coupling of methylene and alkylidyne groups at a trimetal centre; crystal structures of [Ru2W{Âµ-Ïƒ:Î·-trans-CHî€†C(H)R}(Âµ-CO)(CO)3(Î·-C5H5)2(Î·-C5Me5)]Â·CH2Cl2and [Ru2W(Âµ3-CCH2R)(Âµ-CO)3(CO)(Î·-C5H5)3](R = C6H4Me-4). Journal of the Chemical Society Dalton Transactions, 1987, , 1201-1208.	1.1	11
71	Modelling the chemistry of Mn-doped MgO for bulk and (100) surfaces. Physical Chemistry Chemical Physics, 2016, 18, 28648-28660.	1.3	11
72	Theoretical studies of inorganic and organometallic reaction mechanisms. 8. Hydrogen exchange in the Î²-agostic ethylene complex of cyclopentadienyl rhodium. Journal of Organometallic Chemistry, 1994, 478, 197-203.	0.8	10

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73	Hybrid-DFT Modeling of Lattice and Surface Vacancies in MnO. Journal of Physical Chemistry C, 2019, 123, 8133-8144.	1.5	10
74	Testing Interatomic Potentials for QM/MM Embedded-Cluster Calculations on Ceria Surfaces. E-Journal of Surface Science and Nanotechnology, 2009, 7, 413-420.	0.1	8
75	The carbaborane group Î·5-C2B9H9Me2as a spectator and non-spectator ligand in di- and tri-metal complex chemistry: X-ray crystal structures of [PPh4][Co2W(Âµ3-CPh)(CO)8(Î·5-C2B9H9Me2)].1/2CH2Cl2, [NEt4][FeW(Âµ-CC6H3Me2-2,6)(CO)5-(Î·5-C2B9H9Me2)], and [IrW(Âµ-CC6H4Me-4)(CO)2(PEt3)2(Î·5-C2B9H9Me2)]. Journal of the Chemical Society Chemical Communications, 1987, , 1881-1884.	2.0	7
76	Chemistry of polynuclear metal complexes with bridging carbene or carbyne ligands. Part 50. Synthesis and crystal structures of the complexes [RuW3(Âµ-CO)(Âµ3-Î·-CO)(Âµ-CPh)2(Âµ3-CPh)(CO)2(Î·-C5H5)3] and [RuW3(Âµ-CO)(Âµ3-Î·-CO){Âµ-C(Ph)C(O)}(Âµ-CPh)(Âµ3-CPh)(CO)(PMePh2)(Î·-C5H5)3]. Journal of the Chemical Society Dalton Transactions, 1987, , 51-59.	1.1	7
77	Halogen Nuclear Quadrupole Coupling Constants: Comparison of ab initio Calculations which include Correlation, with Experiment. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1998, 53, 383-395.	0.7	7
78	The electronic structure of the carbonyl dihalides, COF2, COCl2, COBr2, COClF, COBrF and COBrCl: a combined computational and experimental study. Journal of the Chemical Society Dalton Transactions, 1995, , 2359.	1.1	6
79	Reactions between Âµ-alkylidyne ironâ€“molybdenum complexes and but-2-yne: unusually facile Câ€“C bond forming processes accompanied by hydrogen migration between carbon centres. Journal of the Chemical Society Chemical Communications, 1987, , 53-55.	2.0	5
80	Full-potential XANES calculations for HCl using SCF electron densities. Physica B: Condensed Matter, 1995, 208-209, 68-70.	1.3	5
81	Large scale electronic structure calculations in the study of the condensed phase. Computational and Theoretical Chemistry, 2006, 771, 33-41.	1.5	5
82	Ab Initio potential grid based docking: From High Performance Computing to In Silico Screening. AIP Conference Proceedings, 2007, , .	0.3	3
83	From CO2 to Methanol by Hybrid QM/MM Embedding. , 2001, 40, 4437.		1