

Paul Sherwood

List of Publications by Year in descending order

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papers

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citations

94269

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84
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87
all docs

87
docs citations

87
times ranked

10386
citing authors

#	ARTICLE	IF	CITATIONS
1	Band alignment of rutile and anatase TiO ₂ . <i>Nature Materials</i> , 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. <i>Computational and Theoretical Chemistry</i> , 2003, 632, 1-28.	1.5	887
3	Understanding the Behavior of Halogens as Hydrogen Bond Acceptors. <i>Crystal Growth and Design</i> , 2001, 1, 277-290.	1.4	631
4	The GAMESS-UK electronic structure package: algorithms, developments and applications. <i>Molecular Physics</i> , 2005, 103, 719-747.	0.8	484
5	DL-FIND: An Open-Source Geometry Optimizer for Atomistic Simulations. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11856-11865.	1.1	466
6	Supramolecular Chemistry of Halogens: Complementary Features of Inorganic (M ⁿ⁺ X) and Organic (C ⁿ⁺ X ^{m-}) Halogens Applied to M ⁿ⁺ X ^{m-} Halogen Bond Formation. <i>Journal of the American Chemical Society</i> , 2005, 127, 5979-5989.	6.6	365
7	<sc>C</sc>hem<sc>S</sc>hellâ€”a modular software package for <sc>QM</sc>/<sc>MM</sc> simulations. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2014, 4, 101-110.	6.2	351
8	Zeolite Structure and Reactivity by Combined Quantum-Chemical/Classical Calculations. <i>Journal of Physical Chemistry B</i> , 1999, 103, 6133-6141.	1.2	343
9	Superlinearly converging dimer method for transition state search. <i>Journal of Chemical Physics</i> , 2008, 128, 014106.	1.2	282
10	Computer simulation of zeolite structure and reactivity using embedded cluster methods. <i>Faraday Discussions</i> , 1997, 106, 79-92.	1.6	190
11	Multiscale methods for macromolecular simulations. <i>Current Opinion in Structural Biology</i> , 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. <i>Journal of Chemical Physics</i> , 2002, 117, 10534-10547.	1.2	173
13	Designing Intermolecular Interactions between Halogenated Peripheries of Inorganic and Organic Molecules: Electrostatically Directed M ⁿ⁺ X ^{m-} Halogen Bonds. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 435-440.	1.2	152
14	Point defects in ZnO. <i>Faraday Discussions</i> , 2007, 134, 267-282.	1.6	151
15	Hydrogen bonding and perhalometallate ions: A supramolecular synthetic strategy for new inorganic materials. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002, 99, 4956-4961.	3.3	126
16	Quantum-chemical studies of alkene chemisorption in chabazite: A comparison of cluster and embedded-cluster models. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1998, 94, 3401-3408.	1.7	121
17	From CO ₂ 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 Syntex for funding. K. Waugh, L. Whitmore, S. Cristol, and P. Sushko are thanked for their helpful insights. QM/MM=quantum mechanics/molecular mechanics.. <i>Angewandte Chemie - International Edition</i> , 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. <i>Theoretical Chemistry Accounts</i> , 2003, 109, 140-148.	0.5	100

#	ARTICLE	IF	CITATIONS
19	Hybrid QM/MM embedding approach for the treatment of localized surface states in ionic materials. <i>International Journal of Quantum Chemistry</i> , 2004, 99, 695-712.	1.0	97
20	Identification and Characterization of Active Sites and Their Catalytic Processes of the Cu/ZnO Methanol Catalyst. <i>Topics in Catalysis</i> , 2003, 24, 161-172.	1.3	87
21	Fluoride ligands exhibit marked departures from the hydrogen bond acceptor behavior of their heavier halogen congeners. <i>New Journal of Chemistry</i> , 1999, 23, 965-968.	1.4	85
22	Et ₃ NH ⁺ Co(CO) ₄ ⁻ : hydrogen-bonded adduct or simple ion pair? Single-crystal neutron diffraction study at 15 K. <i>Organometallics</i> , 1992, 11, 2339-2341.	1.1	81
23	A parallel second-order Møller-Plesset gradient. <i>Molecular Physics</i> , 1997, 91, 431-438.	0.8	78
24	An embedded cluster study of the formation of water on interstellar dust grains. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 5431.	1.3	78
25	Adsorption of water and methanol on zeolite Brønsted acid sites: An ab initio, embedded cluster study including electron correlation. <i>Journal of Chemical Physics</i> , 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(η ⁵ -C ₅ H ₅)(CO) ₂ (η ¹ -C ₅ H ₅)] (R = C ₆ H ₃ Me _{2-2,6} , M = Cr, Ti, Zr, Hf, Nb, Ta, Mo, W, Re, Os, Ir, Pt, Au, Hg, Tl, Pb, Bi, Po, At, Rn, Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144, 145, 146, 147, 148, 149, 150, 151, 152, 153, 154, 155, 156, 157, 158, 159, 160, 161, 162, 163, 164, 165, 166, 167, 168, 169, 170, 171, 172, 173, 174, 175, 176, 177, 178, 179, 180, 181, 182, 183, 184, 185, 186, 187, 188, 189, 190, 191, 192, 193, 194, 195, 196, 197, 198, 199, 200, 201, 202, 203, 204, 205, 206, 207, 208, 209, 210, 211, 212, 213, 214, 215, 216, 217, 218, 219, 220, 221, 222, 223, 224, 225, 226, 227, 228, 229, 230, 231, 232, 233, 234, 235, 236, 237, 238, 239, 240, 241, 242, 243, 244, 245, 246, 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37	Chemistry of polynuclear metal complexes with bridging carbene or carbyne ligands. Part 56. Synthesis of iron-molybdenum compounds; crystal structures of $[\text{FeMo}(\mu\text{-CR})(\text{CO})_6(\text{i-C}_5\text{H}_5)]$ and $[\text{FeMo}_2(\mu_3\text{-RC}_2\text{R})(\text{CO})_6(\text{i-C}_5\text{H}_5)_2]$ ($\text{R} = \text{C}_6\text{H}_4\text{Me-4}$). 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 NH_3 and NH_4^+ 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 μ -methylene-diruthenium complexes into tetranuclear metal clusters with μ_4 -methylidyne and μ_4 -carbido groups: X-ray crystal structures of $[\text{Ru}_2\text{Pt}_2(\mu\text{-H})(\mu_4\text{-CH})(\mu\text{-CO})(\text{CO})_2(\text{PPri}_3)_2(\text{i-C}_5\text{H}_5)_2]$ and $[\text{Ru}_2\text{Pt}_2(\mu\text{-H})_2(\mu_4\text{-C})(\mu\text{-CO})_2(\text{PPri}_3)_2(\text{i-C}_5\text{H}_5)_2]$. Journal of the Chemical Society Chemical Communications, 1987, , 454-456.	2.0	27
43	Strengthening of $\text{Na}^+\text{H}^+\text{Co}$ 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 $[\text{WIr}(\mu\text{-CC}_6\text{H}_4\text{Me-4})(\text{CO})_2(\text{PEt}_3)_2(\text{i-C}_2\text{B}_9\text{H}_9\text{Me}_2)]$. Journal of the Chemical Society Dalton Transactions, 1989, , 1845-1854.	1.1	24
47	The Growth of Copper Clusters over ZnO: the Competition between Planar and Polyhedral Clusters. Journal of Physical Chemistry C, 2008, 112, 7420-7430.	1.5	24
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