

Thomas W Keal

List of Publications by Year in descending order

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29
papers

4,747
citations

331259

21
h-index

476904

29
g-index

30
all docs

30
docs citations

30
times ranked

7297
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	DL-FIND: An Open-Source Geometry Optimizer for Atomistic Simulations. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11856-11865.	1.1	466
3	Assessment of a Coulomb-attenuated exchange–correlation energy functional. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 558-562.	1.3	437
4	ChemSHELL—a modular software package for QM/MM simulations. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2014, 4, 101-110.	6.2	351
5	The exchange-correlation potential in Kohn–Sham nuclear magnetic resonance shielding calculations. <i>Journal of Chemical Physics</i> , 2003, 119, 3015-3024.	1.2	254
6	Implementation of surface hopping molecular dynamics using semiempirical methods. <i>Chemical Physics</i> , 2008, 349, 334-347.	0.9	219
7	A semiempirical generalized gradient approximation exchange-correlation functional. <i>Journal of Chemical Physics</i> , 2004, 121, 5654-5660.	1.2	211
8	Semiempirical hybrid functional with improved performance in an extensive chemical assessment. <i>Journal of Chemical Physics</i> , 2005, 123, 121103.	1.2	131
9	Comparison of algorithms for conical intersection optimisation using semiempirical methods. <i>Theoretical Chemistry Accounts</i> , 2007, 118, 837-844.	0.5	126
10	GIAO shielding constants and indirect spin–spin coupling constants: performance of density functional methods. <i>Chemical Physics Letters</i> , 2004, 391, 374-379.	1.2	87
11	Limits to Doping of Wide Band Gap Semiconductors. <i>Chemistry of Materials</i> , 2013, 25, 2924-2926.	3.2	57
12	Choice of exchange-correlation functional for computing NMR indirect spin–spin coupling constants. <i>Chemical Physics Letters</i> , 2006, 425, 163-166.	1.2	54
13	Improved NMR chemical shifts in density functional theory. <i>Chemical Physics Letters</i> , 2003, 380, 70-77.	1.2	53
14	Assessment of semiempirical methods for the photoisomerisation of a protonated Schiff base. <i>Theoretical Chemistry Accounts</i> , 2009, 123, 145-156.	0.5	49
15	Donor and acceptor characteristics of native point defects in GaN. <i>Journal Physics D: Applied Physics</i> , 2019, 52, 335104.	1.3	49
16	Open-Source, Python-Based Redevelopment of the ChemShell Multiscale QM/MM Environment. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1317-1328.	2.3	46
17	Combining insights from solid-state NMR and first principles calculation: applications to the ¹⁹ F NMR of octafluoronaphthalene. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 2389.	1.3	39
18	Activation of Carbon Dioxide over Zinc Oxide by Localised Electrons. <i>ChemPhysChem</i> , 2012, 13, 3453-3456.	1.0	34

#	ARTICLE	IF	CITATIONS
19	Enzyme catalysis captured using multiple structures from one crystal at varying temperatures. IUCrj, 2018, 5, 283-292.	1.0	26
20	Selenium chemistry with DFT: molecular structures and ^{77}Se NMR shielding constants. Molecular Physics, 2005, 103, 1007-1011.	0.8	25
21	Prediction of multiband luminescence due to the gallium vacancy-oxygen defect complex in GaN. Applied Physics Letters, 2018, 112, .	1.5	25
22	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
23	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
24	Modelling the chemistry of Mn-doped MgO for bulk and (100) surfaces. Physical Chemistry Chemical Physics, 2016, 18, 28648-28660.	1.3	11
25	Active-site protein dynamics and solvent accessibility in native <i>Achromobacter cycloclastes</i> copper nitrite reductase. IUCrj, 2017, 4, 495-505.	1.0	11
26	Hybrid-DFT Modeling of Lattice and Surface Vacancies in MnO. Journal of Physical Chemistry C, 2019, 123, 8133-8144.	1.5	10
27	Materials and Molecular Modeling at the Exascale. Computing in Science and Engineering, 2022, 24, 36-45.	1.2	7
28	A QM/MM Study of Nitrite Binding Modes in a Three-Domain Heme-Cu Nitrite Reductase. Molecules, 2018, 23, 2997.	1.7	5
29	QM/MM Simulations of Protein Crystal Reactivity Guided by MSOX Crystallography: A Copper Nitrite Reductase Case Study. Journal of Physical Chemistry B, 2021, 125, 9102-9114.	1.2	3