Thomas W Keal

List of Publications by Year
in descending order

29 papers	4,747 citations	331670 21 h-index	477307 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 TiO2. Nature Materials, 2013, 12, 798-801.	27.5	1,924
2	DL-FIND: An Open-Source Geometry Optimizer for Atomistic Simulations. Journal of Physical Chemistry A, 2009, 113, 11856-11865.	2.5	466
3	Assessment of a Coulomb-attenuated exchangeâ€“correlation energy functional. Physical Chemistry Chemical Physics, 2006, 8, 558-562.	2.8	437
4	<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.	14.6	351
5	The exchange-correlation potential in Kohnâ€“Sham nuclear magnetic resonance shielding calculations. Journal of Chemical Physics, 2003, 119, 3015-3024.	3.0	254
6	Implementation of surface hopping molecular dynamics using semiempirical methods. Chemical Physics, 2008, 349, 334-347.	1.9	219
7	A semiempirical generalized gradient approximation exchange-correlation functional. Journal of Chemical Physics, 2004, 121, 5654-5660.	3.0	211
8	Semiempirical hybrid functional with improved performance in an extensive chemical assessment. Journal of Chemical Physics, 2005, 123, 121103.	3.0	131
9	Comparison of algorithms for conical intersection optimisation using semiempirical methods. Theoretical Chemistry Accounts, 2007, 118, 837-844.	1.4	126
10	GIAO shielding constants and indirect spinâ€“spin coupling constants: performance of density functional methods. Chemical Physics Letters, 2004, 391, 374-379.	2.6	87
11	Limits to Doping of Wide Band Gap Semiconductors. Chemistry of Materials, 2013, 25, 2924-2926.	6.7	57
12	Choice of exchange-correlation functional for computing NMR indirect spinâ€“spin coupling constants. Chemical Physics Letters, 2006, 425, 163-166.	2.6	54
13	Improved NMR chemical shifts in density functional theory. Chemical Physics Letters, 2003, 380, 70-77.	2.6	53
14	Assessment of semiempirical methods for the photoisomerisation of a protonated Schiff base. Theoretical Chemistry Accounts, 2009, 123, 145-156.	1.4	49
15	Donor and acceptor characteristics of native point defects in GaN. Journal Physics D: Applied Physics, 2019, 52, 335104.	2.8	49
16	Open-Source, Python-Based Redevelopment of the ChemShell Multiscale QM/MM Environment. Journal of Chemical Theory and Computation, 2019, 15, 1317-1328.	5.3	46
17	Combining insights from solid-state NMR and first principles calculation: applications to the 19F NMR of octafluoronaphthalene. Physical Chemistry Chemical Physics, 2007, 9, 2389.	2.8	39
18	Activation of Carbon Dioxide over Zinc Oxide by Localised Electrons. ChemPhysChem, 2012, 13, 3453-3456.	2.1	34

#	Article	IF	Citations
19	Enzyme catalysis captured using multiple structures from one crystal at varying temperatures. IUCrJ, 2018, 5, 283-292.	2.2	26
20	Selenium chemistry with DFT: molecular structures and⁷⁷Se NMR shielding constants. Molecular Physics, 2005, 103, 1007-1011.	1.7	25
21	Prediction of multiband luminescence due to the gallium vacancyâ€“oxygen defect complex in GaN. Applied Physics Letters, 2018, 112, .	3.3	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.	2.1	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.	1.8	16
24	Modelling the chemistry of Mn-doped MgO for bulk and (100) surfaces. Physical Chemistry Chemical Physics, 2016, 18, 28648-28660.	2.8	11
25	Active-site protein dynamics and solvent accessibility in nativeAchromobacter cycloclastescopper nitrite reductase. IUCrJ, 2017, 4, 495-505.	2.2	11
26	Hybrid-DFT Modeling of Lattice and Surface Vacancies in MnO. Journal of Physical Chemistry C, 2019, 123, 8133-8144.	3.1	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.	3.8	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.	2.6	3