Michael Walter

List of Publications by Year
in descending order

93	8,723	136950	42399
papers	citations	32	92
		h-index	g-index

95	95	95	9085
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The atomic simulation environmentâ€”a Python library for working with atoms. Journal of Physics Condensed Matter, 2017, 29, 273002.	1.8	1,933
2	A unified view of ligand-protected gold clusters as superatom complexes. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 9157-9162.	7.1	1,472
3	Electronic structure calculations with GPAW: a real-space implementation of the projector augmented-wave method. Journal of Physics Condensed Matter, 2010, 22, 253202.	1.8	1,451
4	On the Structure of Thiolate-Protected Au₂₅. Journal of the American Chemical Society, 2008, 130, 3756-3757.	13.7	682
5	Divide and Protect:Â Capping Gold Nanoclusters with Molecular Goldâ^'Thiolate Rings. Journal of Physical Chemistry B, 2006, 110, 9927-9931.	2.6	405
6	Time-dependent density-functional theory in the projector augmented-wave method. Journal of Chemical Physics, 2008, 128, 244101.	3.0	187
7	Photo-double ionization of molecular hydrogen. Journal of Physics B: Atomic, Molecular and Optical Physics, 1999, 32, 2487-2501.	1.5	134
8	Quantum Well States in Two-Dimensional Gold Clusters on MgO Thin Films. Physical Review Letters, 2009, 102, 206801.	7.8	128
9	Theoretical Characterization of Cyclic Thiolated Gold Clusters. Journal of the American Chemical Society, 2006, 128, 10268-10275.	13.7	118
10	Hydrogen treated anatase TiO₂: a new experimental approach and further insights from theory. Journal of Materials Chemistry A, 2016, 4, 2670-2681.	10.3	117
11	Thiolate-Protected Au₂₅ Superatoms as Building Blocks: Dimers and Crystals. Journal of Physical Chemistry C, 2010, 114, 15986-15994.	3.1	109
12	A hollow tetrahedral cage of hexadecagold dianion provides a robust backbone for a tuneable sub-nanometer oxidation and reduction agent via endohedral doping. Physical Chemistry Chemical Physics, 2006, 8, 5407-5411.	2.8	98
13	Ligand-Protected Gold Alloy Clusters: Doping the Superatom. Journal of Physical Chemistry C, 2009, 113, 15834-15837.	3.1	97
14	Synthesis, Stabilization, Functionalization and, DFT Calculations of Gold Nanoparticles in Fluorous Phases (PTFE and Ionic Liquids). Chemistry - A European Journal, 2009, 15, 10047-10059.	3.3	84
15	Stop-and-go, stepwise and â€œligand-freeâ€•nucleation, nanocrystal growth and formation of Au-NPs in ionic liquids (ILs). Chemical Communications, 2010, 46, 1159.	4.1	77
16	Electrospun Black Titania Nanofibers: Influence of Hydrogen Plasma-Induced Disorder on the Electronic Structure and Photoelectrochemical Performance. Journal of Physical Chemistry C, 2015, 119, 18835-18842.	3.1	68
17	Activation and mechanochemical breaking of Câ€“C bonds initiate wear of diamond (110) surfaces in contact with silica. Carbon, 2016, 98, 474-483.	10.3	61
18	Simplified continuum solvent model with a smooth cavity based on volumetric data. Journal of Chemical Physics, 2014, 141, 174108.	3.0	58

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19	Ab initio study of CO2 hydrogenation mechanisms on inverse ZnO/Cu catalysts. Journal of Catalysis, 2018, 360, 168-174.	6.2	58
20	Au<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>40</mml:mn></mml:msub></mml:math>: A large tetrahedral magic cluster. Physical Review B, 2011, 84, .	3.2	57
21	On the Structure of a Thiolated Gold Cluster: Au₄₄(SR)₂₈^{2â^'}. Journal of Physical Chemistry C, 2010, 114, 15883-15889.	3.1	54
22	Electronic Structure of MgO-Supported Au Clusters: Quantum Dots Probed by Scanning Tunneling Microscopy. Physical Review Letters, 2007, 99, 096102.	7.8	49
23	A mechanochromic donor-acceptor torsional spring. Nature Communications, 2021, 12, 4243.	12.8	47
24	Bit Threads and Holographic Monogamy. Communications in Mathematical Physics, 2020, 376, 609-648.	2.2	45
25	A 58-electron superatom-complex model for the magic phosphine-protected gold clusters (Schmid-gold, NanogoldÂ®) of 1.4-nm dimension. Chemical Science, 2011, 2, 1583.	7.4	44
26	Oxidation State and Symmetry of Magnesia-Supported Pd₁₃O_x Nanocatalysts Influence Activation Barriers of CO Oxidation. Journal of the American Chemical Society, 2012, 134, 7690-7699.	13.7	43
27	Interactions of polymers with reduced graphene oxide: van der Waals binding energies of benzene on graphene with defects. Physical Chemistry Chemical Physics, 2014, 16, 33-37.	2.8	43
28	Oxidation of Magnesia-Supported Pd₃₀ Nanoclusters and Catalyzed CO Combustion: Size-Selected Experiments and First-Principles Theory. Journal of Physical Chemistry C, 2012, 116, 9594-9607.	3.1	40
29	Progressive Shortening of sp-Hybridized Carbon Chains through Oxygen-Induced Cleavage. Journal of Physical Chemistry C, 2011, 115, 24653-24661.	3.1	38
30	Squeezing, Then Stacking: From Breathing Pores to Threeâ€Dimensional Ionic Selfâ€Assembly under Electrochemical Control. Angewandte Chemie - International Edition, 2014, 53, 12951-12954.	13.8	36
31	Ultralow Friction of Steel Surfaces Using a 1,3-Diketone Lubricant in the Thin Film Lubrication Regime. Langmuir, 2015, 31, 11033-11039.	3.5	35
32	Gold Sulfide Nanoclusters: A Unique Coreâ€Inâ€Cage Structure. Chemistry - A European Journal, 2010, 16, 4999-5003.	3.3	34
33	Effective Polarizability Models. Journal of Physical Chemistry A, 2017, 121, 9742-9751.	2.5	33
34	The halogen analogs of thiolated gold nanoclusters. Nanoscale, 2012, 4, 4234.	5.6	31
35	Energy sharing and asymmetry parameters for photo double ionization of helium 100 eV above threshold in single-particle and Jacobi coordinates. Journal of Physics B: Atomic, Molecular and Optical Physics, 2002, 35, L521-L526.	1.5	30
36	â€œLigandâ€Freeâ€•Cluster Quantized Charging in an Ionic Liquid. Angewandte Chemie - International Edition, 2011, 50, 9735-9738.	13.8	30

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37	Ultralow Friction Induced by Tribochemical Reactions: A Novel Mechanism of Lubrication on Steel Surfaces. Langmuir, 2013, 29, 5207-5213.	3.5	30
38	A Simply Synthesized, Tough Polyarylene with Transient Mechanochromic Response. Angewandte Chemie - International Edition, 2018, 57, 997-1000.	13.8	30
39	Photoelectron spectra from first principles: from the many-body to the single-particle picture. New Journal of Physics, 2008, 10, 043018.	2.9	29
40	Optical absorption of magnesia-supported gold clusters and nanoscale catalysts: Effects due to the support, clusters, and adsorbants. Physical Review B, 2005, 72, .	3.2	28
41	High molecular weight mechanochromic spiropyran main chain copolymers via reproducible microwave-assisted Suzuki polycondensation. Polymer Chemistry, 2015, 6, 3694-3707.	3.9	27
42	pH Tuning of Waterâ€Soluble Arylazopyrazole Photoswitches. Chemistry - A European Journal, 2020, 26, 13203-13212.	3.3	27
43	Soluble and stable alternating main-chain merocyanine copolymers through quantitative spiropyranâ€“merocyanine conversion. Polymer Chemistry, 2014, 5, 443-453.	3.9	26
44	Substituent Correlations Characterized by Hammett Constants in the Spiropyranâ€“Merocyanine Transition. Journal of Physical Chemistry A, 2017, 121, 2683-2687.	2.5	26
45	Selection Rules and Isotope Effects in the Full Fragmentation of the Hydrogen Molecule. Physical Review Letters, 2000, 85, 1630-1633.	7.8	24
46	Appearance of non-first-Born effects in (e, 3e) on helium. Journal of Physics B: Atomic, Molecular and Optical Physics, 2003, 36, L77-L83.	1.5	23
47	Chemical Substitution - Alignment of the Surface Potentials for Efficient Charge Transport in Nanocrystalline TiO₂ Photocatalysts. Chemistry of Materials, 2016, 28, 4223-4230.	6.7	22
48	The effect of dynamical screening on helium (e, 3e) differential cross-sections. Journal of Physics B: Atomic, Molecular and Optical Physics, 2005, 38, 1569-1579.	1.5	20
49	An old workhorse for new applications: Fe(dpm)₃ as a precursor for low-temperature PECVD of iron(<scp>iii</scp>) oxide. Physical Chemistry Chemical Physics, 2015, 17, 11174-11181.	2.8	20
50	Cross-sections for (e, 3e) collisions on helium: the DS6C wavefunction. Journal of Physics B: Atomic, Molecular and Optical Physics, 2006, 39, 4365-4377.	1.5	19
51	Density functional theory and chromium: Insights from the dimers. Journal of Chemical Physics, 2015, 142, 124316.	3.0	18
52	Alkyl-substituted spiropyrans: electronic effects, model compounds and synthesis of aliphatic main-chain copolymers. Polymer Chemistry, 2017, 8, 5407-5414.	3.9	18
53	1,3-Diketone Fluids and Their Complexes with Iron. Journal of Physical Chemistry A, 2013, 117, 3369-3376.	2.5	17
54	Macroscopic Superlow Friction of Steel and Diamond-Like Carbon Lubricated with a Formanisotropic 1,3-Diketone. ACS Omega, 2017, 2, 8330-8342.	3.5	17

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55	Effects of Gas-Phase Conditions and Particle Size on the Properties of Cu(111)-Supported Zn_yO_x Particles Revealed by Global Optimization and Ab Initio Thermodynamics. Journal of Physical Chemistry C, 2019, 123, 30903-30916.	3.1	17
56	Ab Initio Wavelength-Dependent Raman Spectra: Placzek Approximation and Beyond. Journal of Chemical Theory and Computation, 2020, 16, 576-586.	5.3	17
57	Stabilization of Liâ€“S batteries with a lean electrolyte via ion-exchange trapping of lithium polysulfides using a cationic, polybenzimidazolium binder. Sustainable Energy and Fuels, 2020, 4, 1180-1190.	4.9	15
58	Offset-corrected<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="normal">Î”</mml:mi></mml:math>-Kohn-Sham scheme for semiempirical prediction of absolute x-ray photoelectron energies in molecules and solids. Physical Review B, 2016, 94, .	3.2	14
59	Molecular symmetry in two-electron excited and ionized states. Journal of Physics B: Atomic, Molecular and Optical Physics, 2000, 33, 2907-2927.	1.5	13
60	Reversible Anionâ€Driven Switching of an Organic 2D Crystal at a Solidâ€“Liquid Interface. Small, 2017, 13, 1702379.	10.0	12
61	Experimental and theoretical 2p core-level spectra of size-selected gas-phase aluminum and silicon cluster cations: chemical shifts, geometric structure, and coordination-dependent screening. Physical Chemistry Chemical Physics, 2019, 21, 6651-6661.	2.8	12
62	Temperature and loading rate dependent rupture forces from universal paths in mechanochemistry. Physical Review Materials, 2018, 2, .	2.4	12
63	Multi-particle photoionization by a single photon. Journal of Physics B: Atomic, Molecular and Optical Physics, 2003, 36, 4561-4579.	1.5	11
64	Stability and IR Spectroscopy of Zwitterionic Form of Î²-Alanine in Water Clusters. Journal of Physical Chemistry B, 2019, 123, 4392-4399.	2.6	10
65	Symmetry-induced long-lived excited state in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msubsup><mml:mi mathvariant="normal">Au</mml:mi><mml:mn>6</mml:mn><mml:mo>â^’</mml:mo></mml:msubsup></mml:math>. Physical Review B, 2007, 76, .	3.2	9
66	Macroscopic quantum electrodynamics and density functional theory approaches to dispersion interactions between fullerenes. Physical Chemistry Chemical Physics, 2020, 22, 23295-23306.	2.8	9
67	Dispersion forces in inhomogeneous planarly layered media: A one-dimensional model for effective polarizabilities. Physical Review A, 2019, 99, .	2.5	8
68	Ambient Bistable Single Dipole Switching in a Molecular Monolayer. Angewandte Chemie - International Edition, 2020, 59, 14049-14053.	13.8	8
69	Shape-Amplitude Representation ofN-Particle Photofragmentation Processes. Physical Review Letters, 2003, 90, 233001.	7.8	7
70	Charging properties of gold clusters in different environments. Physical Review B, 2013, 87, .	3.2	7
71	Optical signatures of pentacene in soft rare-gas environments. Journal of Chemical Physics, 2019, 150, 244703.	3.0	7
72	Impact of effective polarisability models on the near-field interaction of dissolved greenhouse gases at ice and air interfaces. Physical Chemistry Chemical Physics, 2019, 21, 21296-21304.	2.8	7

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73	Ab Initio Modeling of the ZnO-Cu(111) Interface. Journal of Physical Chemistry C, 2022, 126, 764-771.	3.1	7
74	Photoionisation using Kohn-Sham wave functions. European Physical Journal D, 2005, 33, 393-398.	1.3	5
75	ZusammenrÃ¼cken und Stapeln: von atmenden Poren zu dreidimensionaler ionischer Selbstorganisation unter elektrochemischer Kontrolle. Angewandte Chemie, 2014, 126, 13165-13168.	2.0	5
76	Semifluorinated, kinked polyarylenesviadirect arylation polycondensation. Polymer Chemistry, 2020, 11, 6928-6934.	3.9	5
77	Reliable Computational Prediction of the Supramolecular Ordering of Complex Molecules under Electrochemical Conditions. Journal of Chemical Theory and Computation, 2020, 16, 5227-5243.	5.3	5
78	Fragmentation of s Rydberg states in H3molecules. Journal of Physics B: Atomic, Molecular and Optical Physics, 2005, 38, 1845-1855.	1.5	4
79	How to observe the oxidation of magnesiaâ€supported Pd clusters by scanning tunnelling microscopy. Physica Status Solidi (B): Basic Research, 2010, 247, 1016-1022.	1.5	4
80	Spectroscopic signatures of triplet states in acenes. Journal of Physics B: Atomic, Molecular and Optical Physics, 2017, 50, 154007.	1.5	4
81	Understanding Superatomic Ag Nanohydrides. Small, 2021, 17, e2004808.	10.0	4
82	Effective screening of medium-assisted van der Waals interactions between embedded particles. Journal of Chemical Physics, 2021, 154, 104102.	3.0	4
83	Computational study on noncovalent interactions between (n, n) singleâ€walled <scp>carbon nanotubes</scp> and simple lignin modelâ€compounds. Journal of Computational Chemistry, 2022, 43, 340-348.	3.3	4
84	Nodes of entangledN-particle wave functions. Physical Review A, 2006, 74, .	2.5	3
85	Tuning Intermolecular Interaction Between Lignin and Carbon Nanotubes in Fiber Composites â€“ A Combined Experimental and Ab-Initio Modeling Study. Journal of Renewable Materials, 2018, , .	2.2	3
86	Charge Transfer Excitations with Range Separated Functionals Using Improved Virtual Orbitals. Journal of Chemical Theory and Computation, 2018, 14, 3667-3676.	5.3	3
87	Ambient Bistable Single Dipole Switching in a Molecular Monolayer. Angewandte Chemie, 2020, 132, 14153-14157.	2.0	3
88	Ligand Protected Gold Alloy Clusters asÂSuperatoms. , 2011, , 29-41.		3
89	Oscillatory Structure of Molecular Photoionization Cross Sections. Physics Essays, 2000, 13, 297-302.	0.4	3
90	Excitation dynamics in polyacene molecules on rare-gas clusters. Journal of Chemical Physics, 2022, 156, 034305.	3.0	3

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91	Organogels from Diketopyrrolopyrrole Copolymer Ionene/Polythiophene Blends Exhibit Ground-State Single Electron Transfer in the Solid State. Macromolecules, 2022, 55, 4979-4994.	4.8	2
92	Substituent effects on the Su-Schrieffer-Heeger electron-phonon coupling in conjugated polyenes. Physical Review B, 2019, 100, .	3.2	1
93	A Simply Synthesized, Tough Polyarylene with Transient Mechanochromic Response. Angewandte Chemie, 2018, 130, 1009-1012.	2.0	0