Michael Walter

List of Publications by Year
in descending order

93	8,723	136940 32	42393 92
papers	citations	h-index	g-index

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

#	Article	IF	Citations
1	Excitation dynamics in polyacene molecules on rare-gas clusters. Journal of Chemical Physics, 2022, 156, 034305.	3.0	3
2	Ab Initio Modeling of the ZnO-Cu(111) Interface. Journal of Physical Chemistry C, 2022, 126, 764-771.	3.1	7
3	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
4	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
5	Understanding Superatomic Ag Nanohydrides. Small, 2021, 17, e2004808.	10.0	4
6	Effective screening of medium-assisted van der Waals interactions between embedded particles. Journal of Chemical Physics, 2021, 154, 104102.	3.0	4
7	A mechanochromic donor-acceptor torsional spring. Nature Communications, 2021, 12, 4243.	12.8	47
8	Bit Threads and Holographic Monogamy. Communications in Mathematical Physics, 2020, 376, 609-648.	2.2	45
9	Ab Initio Wavelength-Dependent Raman Spectra: Placzek Approximation and Beyond. Journal of Chemical Theory and Computation, 2020, 16, 576-586.	5.3	17
10	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
11	Semifluorinated, kinked polyarylenesviadirect arylation polycondensation. Polymer Chemistry, 2020, 11, 6928-6934.	3.9	5
12	Macroscopic quantum electrodynamics and density functional theory approaches to dispersion interactions between fullerenes. Physical Chemistry Chemical Physics, 2020, 22, 23295-23306.	2.8	9
13	pH Tuning of Waterâ€Soluble Arylazopyrazole Photoswitches. Chemistry - A European Journal, 2020, 26, 13203-13212.	3.3	27
14	Ambient Bistable Single Dipole Switching in a Molecular Monolayer. Angewandte Chemie - International Edition, 2020, 59, 14049-14053.	13.8	8
15	Ambient Bistable Single Dipole Switching in a Molecular Monolayer. Angewandte Chemie, 2020, 132, 14153-14157.	2.0	3
16	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
17	Optical signatures of pentacene in soft rare-gas environments. Journal of Chemical Physics, 2019, 150, 244703.	3.0	7
18	Dispersion forces in inhomogeneous planarly layered media: A one-dimensional model for effective polarizabilities. Physical Review A, 2019, 99, .	2.5	8

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19	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
20	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
21	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
22	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
23	Substituent effects on the Su-Schrieffer-Heeger electron-phonon coupling in conjugated polyenes. Physical Review B, 2019, 100, .	3.2	1
24	Ab initio study of CO2 hydrogenation mechanisms on inverse ZnO/Cu catalysts. Journal of Catalysis, 2018, 360, 168-174.	6.2	58
25	A Simply Synthesized, Tough Polyarylene with Transient Mechanochromic Response. Angewandte Chemie, 2018, 130, 1009-1012.	2.0	0
26	A Simply Synthesized, Tough Polyarylene with Transient Mechanochromic Response. Angewandte Chemie - International Edition, 2018, 57, 997-1000.	13.8	30
27	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
28	Charge Transfer Excitations with Range Separated Functionals Using Improved Virtual Orbitals. Journal of Chemical Theory and Computation, 2018, 14, 3667-3676.	5.3	3
29	Temperature and loading rate dependent rupture forces from universal paths in mechanochemistry. Physical Review Materials, 2018, 2, .	2.4	12
30	The atomic simulation environmentâ€”a Python library for working with atoms. Journal of Physics Condensed Matter, 2017, 29, 273002.	1.8	1,933
31	Substituent Correlations Characterized by Hammett Constants in the Spiropyranâ€“Merocyanine Transition. Journal of Physical Chemistry A, 2017, 121, 2683-2687.	2.5	26
32	Reversible Anionâ€Đriven Switching of an Organic 2D Crystal at a Solidâ€“Liquid Interface. Small, 2017, 13, 1702379.	10.0	12
33	Spectroscopic signatures of triplet states in acenes. Journal of Physics B: Atomic, Molecular and Optical Physics, 2017, 50, 154007.	1.5	4
34	Alkyl-substituted spiropyrans: electronic effects, model compounds and synthesis of aliphatic main-chain copolymers. Polymer Chemistry, 2017, 8, 5407-5414.	3.9	18
35	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
36	Effective Polarizability Models. Journal of Physical Chemistry A, 2017, 121, 9742-9751.	2.5	33

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37	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
38	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
39	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
40	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
41	Density functional theory and chromium: Insights from the dimers. Journal of Chemical Physics, 2015, 142, 124316.	3.0	18
42	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
43	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
44	High molecular weight mechanochromic spiropyran main chain copolymers via reproducible microwave-assisted Suzuki polycondensation. Polymer Chemistry, 2015, 6, 3694-3707.	3.9	27
45	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
46	Simplified continuum solvent model with a smooth cavity based on volumetric data. Journal of Chemical Physics, 2014, 141, 174108.	3.0	58
47	Soluble and stable alternating main-chain merocyanine copolymers through quantitative spiropyranâ€“merocyanine conversion. Polymer Chemistry, 2014, 5, 443-453.	3.9	26
48	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
49	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
50	ZusammenrÃ¼cken und Stapeln: von atmenden Poren zu dreidimensionaler ionischer Selbstorganisation unter elektrochemischer Kontrolle. Angewandte Chemie, 2014, 126, 13165-13168.	2.0	5
51	Charging properties of gold clusters in different environments. Physical Review B, 2013, 87, .	3.2	7
52	1,3-Diketone Fluids and Their Complexes with Iron. Journal of Physical Chemistry A, 2013, 117, 3369-3376.	2.5	17
53	Ultralow Friction Induced by Tribochemical Reactions: A Novel Mechanism of Lubrication on Steel Surfaces. Langmuir, 2013, 29, 5207-5213.	3.5	30
54	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

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55	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
56	The halogen analogs of thiolated gold nanoclusters. Nanoscale, 2012, 4, 4234.	5.6	31
57	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
58	Progressive Shortening of sp-Hybridized Carbon Chains through Oxygen-Induced Cleavage. Journal of Physical Chemistry C, 2011, 115, 24653-24661.	3.1	38
59	â€œLigandâ€Freeâ€•Cluster Quantized Charging in an Ionic Liquid. Angewandte Chemie - International Edition, 2011, 50, 9735-9738.	13.8	30
60	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
61	Ligand Protected Gold Alloy Clusters asÂSuperatoms. , 2011, , 29-41.		3
62	On the Structure of a Thiolated Gold Cluster: Au₄₄(SR)₂₈^{2â^'}. Journal of Physical Chemistry C, 2010, 114, 15883-15889.	3.1	54
63	Gold Sulfide Nanoclusters: A Unique Coreâ€Inâ€Cage Structure. Chemistry - A European Journal, 2010, 16, 4999-5003.	3.3	34
64	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
65	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
66	Thiolate-Protected Au₂₅ Superatoms as Building Blocks: Dimers and Crystals. Journal of Physical Chemistry C, 2010, 114, 15986-15994.	3.1	109
67	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
68	Quantum Well States in Two-Dimensional Gold Clusters on MgO Thin Films. Physical Review Letters, 2009, 102, 206801.	7.8	128
69	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
70	Ligand-Protected Gold Alloy Clusters: Doping the Superatom. Journal of Physical Chemistry C, 2009, 113, 15834-15837.	3.1	97
71	On the Structure of Thiolate-Protected Au₂₅. Journal of the American Chemical Society, 2008, 130, 3756-3757.	13.7	682
72	Time-dependent density-functional theory in the projector augmented-wave method. Journal of Chemical Physics, 2008, 128, 244101.	3.0	187

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73	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
74	Photoelectron spectra from first principles: from the many-body to the single-particle picture. New Journal of Physics, 2008, 10, 043018.	2.9	29
75	Electronic Structure of MgO-Supported Au Clusters: Quantum Dots Probed by Scanning Tunneling Microscopy. Physical Review Letters, 2007, 99, 096102.	7.8	49
76	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
77	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
78	Divide and Protect:Â Capping Gold Nanoclusters with Molecular Goldâ^'Thiolate Rings. Journal of Physical Chemistry B, 2006, 110, 9927-9931.	2.6	405
79	Theoretical Characterization of Cyclic Thiolated Gold Clusters. Journal of the American Chemical Society, 2006, 128, 10268-10275.	13.7	118
80	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
81	Nodes of entangledN-particle wave functions. Physical Review A, 2006, 74, .	2.5	3
82	Photoionisation using Kohn-Sham wave functions. European Physical Journal D, 2005, 33, 393-398.	1.3	5
83	Fragmentation of s Rydberg states in H3molecules. Journal of Physics B: Atomic, Molecular and Optical Physics, 2005, 38, 1845-1855.	1.5	4
84	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
85	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
86	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
87	Shape-Amplitude Representation ofN-Particle Photofragmentation Processes. Physical Review Letters, 2003, 90, 233001.	7.8	7
88	Multi-particle photoionization by a single photon. Journal of Physics B: Atomic, Molecular and Optical Physics, 2003, 36, 4561-4579.	1.5	11
89	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
90	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

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91	Selection Rules and Isotope Effects in the Full Fragmentation of the Hydrogen Molecule. Physical Review Letters, 2000, 85, 1630-1633.	7.8	24
92	Oscillatory Structure of Molecular Photoionization Cross Sections. Physics Essays, 2000, 13, 297-302.	0.4	3
93	Photo-double ionization of molecular hydrogen. Journal of Physics B: Atomic, Molecular and Optical Physics, 1999, 32, 2487-2501.	1.5	134