Bryan M Wong

List of Publications by Year
in descending order

185 papers	8,015 citations	38742 50 h-index	64796 79 g-index
242 all docs	242 docs citations	242 times ranked	10058 citing authors

#	Article	IF	Citations
1	A Transparent, Selfâ€Healing, Highly Stretchable Ionic Conductor. Advanced Materials, 2017, 29, 1605099.	21.0	447
2	Defluorination of Per- and Polyfluoroalkyl Substances (PFASs) with Hydrated Electrons: Structural Dependence and Implications to PFAS Remediation and Management. Environmental Science & Technology, 2019, 53, 3718-3728.	10.0	297
3	Optoelectronic and Excitonic Properties of Oligoacenes: Substantial Improvements from Range-Separated Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2010, 6, 3704-3712.	5.3	248
4	Nonempirically Tuned Range-Separated DFT Accurately Predicts Both Fundamental and Excitation Gaps in DNA and RNA Nucleobases. Journal of Chemical Theory and Computation, 2012, 8, 2682-2687.	5.3	203
5	Stress Sensing in Polycaprolactone Films via an Embedded Photochromic Compound. ACS Applied Materials & Interfaces, 2010, 2, 1594-1600.	8.0	177
6	A Highly Stretchy, Transparent Elastomer with the Capability to Automatically Selfâ€Heal Underwater. Advanced Materials, 2018, 30, e1804602.	21.0	167
7	Coumarin dyes for dye-sensitized solar cells: A long-range-corrected density functional study. Journal of Chemical Physics, 2008, 129, 214703.	3.0	166
8	Novel metalâ€“organic framework linkers for light harvesting applications. Chemical Science, 2014, 5, 2081-2090.	7.4	152
9	Absorption and fluorescence properties of oligothiophene biomarkers from long-range-corrected time-dependent density functional theory. Physical Chemistry Chemical Physics, 2009, 11, 4498.	2.8	145
10	Non-proteinaceous hydrolase comprised of a phenylalanine metallo-supramolecular amyloid-like structure. Nature Catalysis, 2019, 2, 977-985.	34.4	142
11	Machine Learning: New Ideas and Tools in Environmental Science and Engineering. Environmental Science & Technology, 2021, 55, 12741-12754.	10.0	140
12	Optoelectronic Properties of Carbon Nanorings: Excitonic Effects from Time-Dependent Density Functional Theory. Journal of Physical Chemistry C, 2009, 113, 21921-21927.	3.1	132
13	Color Detection Using Chromophore-Nanotube Hybrid Devices. Nano Letters, 2009, 9, 1028-1033.	9.1	115
14	Synthesis, Characterization, and Computational Studies of Cycloparaphenylene Dimers. Journal of the American Chemical Society, 2012, 134, 19709-19715.	13.7	115
15	Optical, Structural, and Numerical Investigations of GaAs/AlGaAs Coreâ€“Multishell Nanowire Quantum Well Tubes. Nano Letters, 2013, 13, 1016-1022.	9.1	106
16	Energy and charge transfer by donorâ€“acceptor pairs confined in a metalâ€“organic framework: a spectroscopic and computational investigation. Journal of Materials Chemistry A, 2014, 2, 3389-3398.	10.3	100
17	Nanoscale Effects on Heterojunction Electron Gases in GaN/AlGaN Core/Shell Nanowires. Nano Letters, 2011, 11, 3074-3079.	9.1	97
18	Electronically Excited States of Vitamin B₁₂: Benchmark Calculations Including Time-Dependent Density Functional Theory and Correlated ab Initio Methods. Journal of Physical Chemistry A, 2011, 115, 1280-1292.	2.5	94

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19	Results for aliovalent doping of CeBr3 with Ca2+. Journal of Applied Physics, 2014, 115, .	2.5	91
20	A Machine Learning Approach for Predicting Defluorination of Per- and Polyfluoroalkyl Substances (PFAS) for Their Efficient Treatment and Removal. Environmental Science and Technology Letters, 2019, 6, 624-629.	8.7	90
21	An embedded-atom method interatomic potential for Pdâ€“H alloys. Journal of Materials Research, 2008, 23, 704-718.	2.6	86
22	Degradation of Perfluoroalkyl Ether Carboxylic Acids with Hydrated Electrons: Structureâ€“Reactivity Relationships and Environmental Implications. Environmental Science & Technology, 2020, 54, 2489-2499.	10.0	86
23	A Non-Thermal Plasma Route to Plasmonic TiN Nanoparticles. Journal of Physical Chemistry C, 2017, 121, 2316-2322.	3.1	82
24	Isolation of Pristine Electronics Grade Semiconducting Carbon Nanotubes by Switching the Rigidity of the Wrapping Polymer Backbone on Demand. ACS Nano, 2015, 9, 10203-10213.	14.6	78
25	Polarizabilities of Ï€-Conjugated Chains Revisited: Improved Results from Broken-Symmetry Range-Separated DFT and New CCSD(T) Benchmarks. Journal of Chemical Theory and Computation, 2016, 12, 3593-3602.	5.3	75
26	Breaking Badly: DFT-D2 Gives Sizeable Errors for Tensile Strengths in Palladium-Hydride Solids. Journal of Chemical Theory and Computation, 2015, 11, 5426-5435.	5.3	74
27	A high-spin ground-state donor-acceptor conjugated polymer. Science Advances, 2019, 5, eaav2336.	10.3	72
28	Noncovalent interactions in supramolecular complexes: A study on corannulene and the double concave buckycatcher. Journal of Computational Chemistry, 2009, 30, 51-56.	3.3	71
29	Structural and Electronic Properties of Graphdiyne Carbon Nanotubes from Large-Scale DFT Calculations. Journal of Physical Chemistry C, 2016, 120, 18871-18877.	3.1	70
30	Donorâ€“acceptor polymers with tunable infrared photoresponse. Polymer Chemistry, 2017, 8, 2922-2930.	3.9	70
31	Comparison of Molecular Dynamics with Classical Density Functional and Poissonâ€“Boltzmann Theories of the Electric Double Layer in Nanochannels. Journal of Chemical Theory and Computation, 2012, 8, 2012-2022.	5.3	69
32	Solid state lithiationâ€“delithiation of sulphur in sub-nano confinement: a new concept for designing lithiumâ€“sulphur batteries. Chemical Science, 2016, 7, 1224-1232.	7.4	69
33	The Importance of Short- and Long-Range Exchange on Various Excited State Properties of DNA Monomers, Stacked Complexes, and Watsonâ€“Crick Pairs. Journal of Chemical Theory and Computation, 2015, 11, 2199-2209.	5.3	68
34	Potential-Driven Electron Transfer Lowers the Dissociation Energy of the Câ€“F Bond and Facilitates Reductive Defluorination of Perfluorooctane Sulfonate (PFOS). ACS Applied Materials & Interfaces, 2019, 11, 33913-33922.	8.0	67
35	Halogen Bonding Interactions: Revised Benchmarks and a New Assessment of Exchange vs Dispersion. Journal of Chemical Theory and Computation, 2018, 14, 180-190.	5.3	66
36	Single amino acid bionanozyme for environmental remediation. Nature Communications, 2022, 13, 1505.	12.8	66

#	Article	IF	Citations
37	Heterogeneous CPU+GPU-Enabled Simulations for DFTB Molecular Dynamics of Large Chemical and Biological Systems. Journal of Chemical Theory and Computation, 2019, 15, 2807-2815.	5.3	65
38	Analytical bond-order potential for the cadmium telluride binary system. Physical Review B, 2012, 85, .	3.2	64
39	Structural Dependence of Reductive Defluorination of Linear PFAS Compounds in a UV/Electrochemical System. Environmental Science & Technology, 2020, 54, 10668-10677.	10.0	62
40	Electronic Properties of Vinylene-Linked Heterocyclic Conducting Polymers: Predictive Design and Rational Guidance from DFT Calculations. Journal of Physical Chemistry C, 2011, 115, 18333-18341.	3.1	61
41	Confined Lithiumâ€“Sulfur Reactions in Narrow-Diameter Carbon Nanotubes Reveal Enhanced Electrochemical Reactivity. ACS Nano, 2018, 12, 9775-9784.	14.6	61
42	Photophysical and theoretical investigations of the [8]cycloparaphenylene radical cation and its charge-resonance dimer. Chemical Science, 2013, 4, 4285.	7.4	59
43	Accurate Electron Affinities and Orbital Energies of Anions from a Nonempirically Tuned Range-Separated Density Functional Theory Approach. Journal of Chemical Theory and Computation, 2017, 13, 1656-1666.	5.3	56
44	Effect of quantum tunneling on the efficiency of excitation energy transfer in plasmonic nanoparticle chain waveguides. Journal of Materials Chemistry C, 2018, 6, 5857-5864.	5.5	56
45	Iterative Reductive Aromatization/Ring-Closing Metathesis Strategy toward the Synthesis of Strained Aromatic Belts. Journal of the American Chemical Society, 2016, 138, 6577-6582.	13.7	55
46	Inconsistencies in the Electronic Properties of Phosphorene Nanotubes: New Insights from Large-Scale DFT Calculations. Journal of Physical Chemistry Letters, 2016, 7, 4340-4345.	4.6	54
47	Electronic structure of the S₁ state in methylcobalamin: Insight from CASSCF/MCâ€XQDPT2, EOMâ€CCSD, and TDâ€DFT calculations. Journal of Computational Chemistry, 2013, 34, 987-1004.	3.3	53
48	Bridgehead Imine Substituted Cyclopentadithiophene Derivatives: An Effective Strategy for Band Gap Control in Donorâ€“Acceptor Polymers. Macromolecules, 2013, 46, 1337-1342.	4.8	51
49	Polycation Binders: An Effective Approach toward Lithium Polysulfide Sequestration in Liâ€“S Batteries. ACS Energy Letters, 2017, 2, 2591-2597.	17.4	51
50	Thermoelectric Performance of an Open-Shell Donorâ€“Acceptor Conjugated Polymer Doped with a Radical-Containing Small Molecule. Macromolecules, 2018, 51, 3886-3894.	4.8	51
51	Spectroscopic, Structural, and Theoretical Studies of Halide Complexes with a Urea-Based Tripodal Receptor. Inorganic Chemistry, 2012, 51, 4274-4284.	4.0	50
52	Investigating the Reactivity of 1,4-Anthracene-Incorporated Cycloparaphenylene. Organic Letters, 2016, 18, 1574-1577.	4.6	49
53	Real-Time Quantum Dynamics of Long-Range Electronic Excitation Transfer in Plasmonic Nanoantennas. Journal of Chemical Theory and Computation, 2017, 13, 3442-3454.	5.3	49
54	Spectroscopic Properties of Nanotubeâ€“Chromophore Hybrids. ACS Nano, 2011, 5, 7767-7774.	14.6	48

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55	Sulfate radical oxidation of aromatic contaminants: a detailed assessment of density functional theory and high-level quantum chemical methods. Environmental Sciences: Processes and Impacts, 2017, 19, 395-404.	3.5	48
56	Chemical and Radiation Stability of Ionic Liquids: A Computational Screening Study. Journal of Physical Chemistry C, 2016, 120, 27757-27767.	3.1	45
57	Degradation of Per- and Polyfluoroalkyl Substances with Hydrated Electrons: A New Mechanism from First-Principles Calculations. Environmental Science & Technology, 2022, 56, 8167-8175.	10.0	44
58	A Self-Assembled Fluorideâ€“Water Cyclic Cluster of [F(H₂O)]₄^{4â€“} in a Molecular Box. Journal of the American Chemical Society, 2012, 134, 11892-11895.	13.7	43
59	Giant Raman Response to the Encapsulation of Sulfur in Narrow Diameter Single-Walled Carbon Nanotubes. Journal of the American Chemical Society, 2016, 138, 40-43.	13.7	43
60	Rational design of a macrocycle-based chemosensor for anions. Tetrahedron Letters, 2010, 51, 1329-1332.	1.4	42
61	Reversible, opto-mechanically induced spin-switching in a nanoribbon-spiropyran hybrid material. Nanoscale, 2012, 4, 1321.	5.6	42
62	Thermochemistry of Alane Complexes for Hydrogen Storage: A Theoretical and Experimental Investigation. Journal of Physical Chemistry C, 2011, 115, 7778-7786.	3.1	41
63	Spectral- and Pulse-Shape Discrimination in Triplet-Harvesting Plastic Scintillators. IEEE Transactions on Nuclear Science, 2012, 59, 3312-3319.	2.0	41
64	Assessing backbone solvation effects in the conformational propensities of amino acid residues in unfolded peptides. Physical Chemistry Chemical Physics, 2015, 17, 24917-24924.	2.8	41
65	A new approach toward transition state spectroscopy. Faraday Discussions, 2013, 163, 33.	3.2	39
66	Real-Time Quantum Dynamics Reveals Complex, Many-Body Interactions in Solvated Nanodroplets. Journal of Chemical Theory and Computation, 2016, 12, 1862-1871.	5.3	39
67	Indirect but Efficient: Laser-Excited Electrons Can Drive Ultrafast Polarization Switching in Ferroelectric Materials. Journal of Physical Chemistry Letters, 2019, 10, 3402-3407.	4.6	39
68	Ultrafast photoinduced band splitting and carrier dynamics in chiral tellurium nanosheets. Nature Communications, 2020, 11, 3991.	12.8	39
69	Formation of an Amine-Water Cyclic Pentamer: A New Type of Water Cluster in a Polyazacryptand. Crystal Growth and Design, 2010, 10, 1486-1488.	3.0	37
70	Accuracy of existing atomic potentials for the CdTe semiconductor compound. Journal of Chemical Physics, 2011, 134, 244703.	3.0	37
71	Temperature and Molecular Size Dependence of the High-Pressure Limit. Journal of Physical Chemistry A, 2003, 107, 6206-6211.	2.5	36
72	Real-time degradation dynamics of hydrated per- and polyfluoroalkyl substances (PFASs) in the presence of excess electrons. Physical Chemistry Chemical Physics, 2020, 22, 6804-6808.	2.8	36

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73	Understanding Gas Phase Modifier Interactions in Rapid Analysis by Differential Mobility-Tandem Mass Spectrometry. Journal of the American Society for Mass Spectrometry, 2014, 25, 1098-1113.	2.8	35
74	Materials Compatibility in Rechargeable Aluminum Batteries: Chemical and Electrochemical Properties between Vanadium Pentoxide and Chloroaluminate Ionic Liquids. Chemistry of Materials, 2019, 31, 7238-7247.	6.7	35
75	Functionalization of Single-Wall Carbon Nanotubes with Chromophores of Opposite Internal Dipole Orientation. ACS Applied Materials & Interfaces, 2013, 5, 9355-9361.	8.0	34
76	Is a cross-Î²-sheet structure of low molecular weight peptides necessary for the formation of fibrils and peptide hydrogels?. Physical Chemistry Chemical Physics, 2018, 20, 18158-18168.	2.8	33
77	Photochemistry of Plasmonic Titanium Nitride Nanocrystals. Journal of Physical Chemistry C, 2019, 123, 21796-21804.	3.1	33
78	Orientation of a Monolayer of Dipolar Molecules on Graphene from X-ray Absorption Spectroscopy. Langmuir, 2014, 30, 2559-2565.	3.5	32
79	Effect of Dipolar Molecule Structure on the Mechanism of Graphene-Enhanced Raman Scattering. Journal of Physical Chemistry C, 2016, 120, 13815-13824.	3.1	32
80	Highly selective and sensitive macrocycle-based dinuclear foldamer for fluorometric and colorimetric sensing of citrate in water. Scientific Reports, 2018, 8, 286.	3.3	31
81	Self-assembled cyclic oligothiophene nanotubes: Electronic properties from a dispersion-corrected hybrid functional. Physical Review B, 2011, 84, .	3.2	30
82	Analytical bond-order potential for the Cd-Zn-Te ternary system. Physical Review B, 2012, 86, .	3.2	30
83	Molecular Dynamics Studies of Dislocations in CdTe Crystals from a New Bond Order Potential. Journal of Physical Chemistry C, 2012, 116, 17563-17571.	3.1	30
84	Raman Enhancement of a Dipolar Molecule on Graphene. Journal of Physical Chemistry C, 2014, 118, 2077-2084.	3.1	30
85	Absorption and fluorescence signatures of 1,2,3-triazole based regioisomers: challenging compounds for TD-DFT. Physical Chemistry Chemical Physics, 2014, 16, 9064-9073.	2.8	29
86	Preferential Charge Generation at Aggregate Sites in Narrow Band Gap Infrared Photoresponsive Polymer Semiconductors. Advanced Optical Materials, 2018, 6, 1701138.	7.3	29
87	An Experimental and Modeling Study of Nanoparticle Formation and Growth from Dimethylamine and Nitric Acid. Journal of Physical Chemistry A, 2019, 123, 5640-5648.	2.5	29
88	Stability of Calcium Ion Battery Electrolytes: Predictions from Ab Initio Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2021, 13, 13114-13122.	8.0	29
89	Improved band gaps and structural properties from Wannierâ€“Fermiâ€“LÃ¶wdin self-interaction corrections for periodic systems. Journal of Physics Condensed Matter, 2021, 33, 115501.	1.8	29
90	Accurate Inertias for Large-Amplitude Motions:Â Improvements on Prevailing Approximations. Journal of Physical Chemistry A, 2006, 110, 7406-7413.	2.5	28

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91	A C₃ Symmetric Nitrate Complex with a Thiophene-Based Tripodal Receptor. Crystal Growth and Design, 2011, 11, 959-963.	3.0	28
92	Atomistic potentials for palladiumâ€“silver hydrides. Modelling and Simulation in Materials Science and Engineering, 2013, 21, 045005.	2.0	28
93	A quantum defect model for the s, p, d, and f Rydberg series of CaF. Journal of Chemical Physics, 2011, 134, 114313.	3.0	27
94	On the nonâ€thermal plasma synthesis of nickel nanoparticles. Plasma Processes and Polymers, 2018, 15, 1700104.	3.0	27
95	Covalent Atomic Bridges Enable Unidirectional Enhancement of Electronic Transport in Aligned Carbon Nanotubes. ACS Applied Materials & Interfaces, 2019, 11, 19315-19323.	8.0	27
96	Anomalous Optoelectronic Properties of Chiral Carbon Nanoringsâ€¦ and One Ring to Rule Them All. Journal of Physical Chemistry Letters, 2011, 2, 2702-2706.	4.6	26
97	Correlating Li⁺-Solvation Structure and its Electrochemical Reaction Kinetics with Sulfur in Subnano Confinement. Journal of Physical Chemistry Letters, 2018, 9, 1739-1745.	4.6	26
98	Size resolved chemical composition of nanoparticles from reactions of sulfuric acid with ammonia and dimethylamine. Aerosol Science and Technology, 2018, 52, 1120-1133.	3.1	26
99	Self-assembly of ordered water tetramers in an encapsulated [Br(H2O)12]âˆ’ complex. Chemical Communications, 2012, 48, 8631.	4.1	25
100	An exclusive fluoride receptor: fluoride-induced proton transfer to a quinoline-based thiourea. Tetrahedron Letters, 2014, 55, 1467-1470.	1.4	25
101	A highly efficient dinuclear Cu(<scp>ii</scp>) chemosensor for colorimetric and fluorescent detection of cyanide in water. RSC Advances, 2014, 4, 54263-54267.	3.6	24
102	Linear polarizabilities and second hyperpolarizabilities of streptocyanines: Results from brokenâ€Symmetry DFT and new CCSD(T) benchmarks. Journal of Computational Chemistry, 2018, 39, 2350-2359.	3.3	24
103	Charge-Assisted Encapsulation of Two Chlorides by a Hexaprotonated Azamacrocycle. Crystal Growth and Design, 2010, 10, 1478-1481.	3.0	23
104	Solutionâ€Processable Donorâ€“Acceptor Polymers with Modular Electronic Properties and Very Narrow Bandgaps. Macromolecular Rapid Communications, 2014, 35, 1516-1521.	3.9	23
105	Binding and selectivity of dihydrogen phosphate by H-bond donors and acceptors in a tripodal-based thiourea receptor. Tetrahedron Letters, 2015, 56, 115-118.	1.4	23
106	The diamine cation is not a chemical example where density functional theory fails. Nature Communications, 2018, 9, 4733.	12.8	23
107	Anion directed conformational diversities of an arene based hexa-amide receptor and recognition of the [F₄(H₂O)₆]^{4âˆ’}cluster. RSC Advances, 2014, 4, 62689-62693.	3.6	22
108	Harnessing Plasma Environments for Ammonia Catalysis: Mechanistic Insights from Experiments and Large-Scale Ab Initio Molecular Dynamics. Journal of Physical Chemistry Letters, 2020, 11, 10469-10475.	4.6	22

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109	Effects of magnetic, electric, and intense laser fields on the optical properties of AlGaAs/GaAs quantum wells for terahertz photodetectors. Physica B: Condensed Matter, 2022, 635, 413838.	2.7	22
110	A theoretical and experimental kinetic study of phenyl radical addition to butadiene. Proceedings of the Combustion Institute, 2005, 30, 1049-1056.	3.9	21
111	Sultam-Based Hetero[5]helicene: Synthesis, Structure, and Crystallization-Induced Emission Enhancement. ACS Omega, 2016, 1, 1336-1342.	3.5	21
112	Electronic Signatures of Large Amplitude Motions:Â Dipole Moments of Vibrationally Excited Local-Bend and Local-Stretch States of S0Acetyleneâ€. Journal of Physical Chemistry B, 2006, 110, 18912-18920.	2.6	20
113	Evolution of Chemical Bonding during HCNâ‡„HNC Isomerization as Revealed through Nuclear Quadrupole Hyperfine Structure. Angewandte Chemie - International Edition, 2008, 47, 2969-2972.	13.8	20
114	A Long-Range Electric Field Solver for Molecular Dynamics Based on Atomistic-to-Continuum Modeling. Journal of Chemical Theory and Computation, 2011, 7, 1736-1749.	5.3	20
115	Electron beam synthesis of metal and semiconductor nanoparticles using metalâ€“organic frameworks as ordered precursors. Nanotechnology, 2011, 22, 375601.	2.6	20
116	Melt-Growth Dynamics in CdTe Crystals. Physical Review Letters, 2012, 108, 245503.	7.8	20
117	Ab initio metadynamics calculations reveal complex interfacial effects in acetic acid deprotonation dynamics. Journal of Molecular Liquids, 2021, 330, 115624.	4.9	20
118	High-fidelity simulations of CdTe vapor deposition from a bond-order potential-based molecular dynamics method. Physical Review B, 2012, 85, .	3.2	19
119	Quantum confinement of excitons in wurtzite InP nanowires. Journal of Applied Physics, 2015, 117, .	2.5	19
120	Nanoarchitectonics of Metal-Free Porous Polyketone as Photocatalytic Assemblies for Artificial Photosynthesis. ACS Applied Materials & Interfaces, 2022, 14, 771-783.	8.0	19
121	Anion Complexation Studies of 3-Nitrophenyl-Substituted Tripodal Thiourea Receptor: A Naked-Eye Detection of Sulfate via Fluoride Displacement Assay. ACS Omega, 2017, 2, 9057-9066.	3.5	18
122	Determination of the level of hexavalent, trivalent, and total chromium in the discharged effluent of Bahir Dar tannery using ICP-OES and UVâ€“Visible spectrometry. Cogent Chemistry, 2018, 4, 1534566.	2.5	18
123	High Magnetic Field Detunes Vibronic Resonances in Photosynthetic Light Harvesting. Journal of Physical Chemistry Letters, 2018, 9, 5548-5554.	4.6	18
124	A new interpretation of the structure and solvent dependence of the far UV circular dichroism spectrum of short oligopeptides. Chemical Communications, 2019, 55, 5701-5704.	4.1	18
125	Charge density wave hampers exciton condensation in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:mi>T</mml:mi><mml:mtext>-</mml:mtext>â^’</mml:m Physical Review B, 2019, 100, .	3.2	18
126	Ring currents modulate optoelectronic properties of aromatic chromophores at 25 T. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 11289-11298.	7.1	18

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127	Photo-induced degradation of PFASs: Excited-state mechanisms from real-time time-dependent density functional theory. Journal of Hazardous Materials, 2022, 423, 127026.	12.4	18
128	PAMELA: An open-source software package for calculating nonlocal exact exchange effects on electron gases in core-shell nanowires. AIP Advances, 2012, 2, 032173.	1.3	17
129	Water-Mediated Electronic Structure of Oligopeptides Probed by Their UV Circular Dichroism, Absorption Spectra, and Time-Dependent DFT Calculations. Journal of Physical Chemistry B, 2020, 124, 2579-2590.	2.6	17
130	Field Programmable Gate Arrays for Enhancing the Speed and Energy Efficiency of Quantum Dynamics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 2085-2098.	5.3	17
131	Ab initio metadynamics calculations of dimethylamine for probing pK_b variations in bulk vs. surface environments. Physical Chemistry Chemical Physics, 2020, 22, 26265-26277.	2.8	17
132	Separation of long-range and short-range interactions in Rydberg states of diatomic molecules. Journal of Chemical Physics, 2008, 128, 194301.	3.0	16
133	Defect formation dynamics during CdTe overlayer growth. Physical Review B, 2012, 85, .	3.2	16
134	Colorimetric and optical discrimination of halides by a simple chemosensor. RSC Advances, 2015, 5, 38733-38741.	3.6	16
135	Harnessing deep neural networks to solve inverse problems in quantum dynamics: machine-learned predictions of time-dependent optimal control fields. Physical Chemistry Chemical Physics, 2020, 22, 22889-22899.	2.8	16
136	High-Temperature Decomposition of Diisopropyl Methylphosphonate on Alumina: Mechanistic Predictions from Ab Initio Molecular Dynamics. Journal of Physical Chemistry C, 2021, 125, 21922-21932.	3.1	16
137	Electrocatalytic water oxidation performance in an extended porous organic framework with a covalent alliance of distinct Ru sites. Nanoscale, 2022, 14, 7621-7633.	5.6	16
138	Effects of large-amplitude torsions on partition functions: beyond the conventional separability assumption. Molecular Physics, 2005, 103, 1027-1034.	1.7	15
139	Enhanced photocurrent efficiency of a carbon nanotube pâ€“n junction electromagnetically coupled to a photonic structure. Journal Physics D: Applied Physics, 2009, 42, 055111.	2.8	15
140	A refined parameterization of the analytical Cdâ€“Znâ€“Te bond-order potential. Journal of Molecular Modeling, 2013, 19, 5469-5477.	1.8	14
141	Chirality Induced Spin Selectivity of Photoexcited Electrons in Carbonâ€Sulfur [n]Helicenes. ChemPhotoChem, 2019, 3, 770-777.	3.0	14
142	Modulating the conductance in graphene nanoribbons with multi-barriers under an applied voltage. Results in Physics, 2021, 27, 104505.	4.1	14
143	Predicting Complex Erosion Profiles in Steam Distribution Headers with Convolutional and Recurrent Neural Networks. Industrial & Engineering Chemistry Research, 2022, 61, 8520-8529.	3.7	14
144	Physical removal of metallic carbon nanotubes from nanotube network devices using a thermal and fluidic process. Nanotechnology, 2013, 24, 105202.	2.6	13

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145	Analytical Bond-Order Potential for the Cdâ€“Teâ€“Se Ternary System. Journal of Physical Chemistry C, 2014, 118, 20661-20679.	3.1	13
146	A prediction of dislocationâ€free CdTe/CdS photovoltaic multilayers via nanoâ€patterning and composition grading. Progress in Photovoltaics: Research and Applications, 2015, 23, 1837-1846.	8.1	13
147	Additional Insights between Fermiâ€“LÃ¶wdin Orbital SIC and the Localization Equation Constraints in SIC-DFT. Journal of Physical Chemistry Letters, 2018, 9, 6456-6462.	4.6	13
148	Fractional occupation numbers and selfâ€interaction correctionâ€scaling methods with the Fermiâ€LÃ¶wdin orbital selfâ€interaction correction approach. Journal of Computational Chemistry, 2020, 41, 1200-1208.	3.3	13
149	Thermodynamic calculations for molecules with asymmetric internal rotorsâ€”application to 1,3-butadiene. Journal of Computational Chemistry, 2007, 28, 759-766.	3.3	12
150	An Efficient and Accurate Formalism for the Treatment of Large Amplitude Intramolecular Motion. Journal of Chemical Theory and Computation, 2012, 8, 2713-2724.	5.3	12
151	Acceleration vs Accuracy: Influence of Basis Set Quality on the Mechanism and Dynamics Predicted by Ab Initio Molecular Dynamics. Journal of Physical Chemistry C, 2019, 123, 25113-25120.	3.1	12
152	NIC-CAGE: An open-source software package for predicting optimal control fields in photo-excited chemical systems. Computer Physics Communications, 2021, 258, 107541.	7.5	12
153	A quinoline based bis-urea receptor for anions: a selective receptor for hydrogen sulfate. Natural Product Communications, 2012, 7, 301-4.	0.5	12
154	6â€‰nm super-resolution optical transmission and scattering spectroscopic imaging of carbon nanotubes using a nanometer-scale white light source. Nature Communications, 2021, 12, 6868.	12.8	12
155	Thermodynamic calculations for molecules with asymmetric internal rotors. II. Application to the 1,2â€dihaloethanes. Journal of Computational Chemistry, 2008, 29, 481-487.	3.3	11
156	Nuclear quadrupole hyperfine structure in HC14N/H14NC and DC15N/D15NC isomerization: a diagnostic tool for characterizing vibrational localization. Physical Chemistry Chemical Physics, 2008, 10, 5599.	2.8	11
157	Unusual Bandgap Oscillations in Template-Directed Ï€-Conjugated Porphyrin Nanotubes. Journal of Physical Chemistry Letters, 2016, 7, 2362-2367.	4.6	10
158	Quantum tunneling mechanisms in monolayer graphene modulated by multiple electrostatic barriers. Results in Physics, 2021, 26, 104403.	4.1	10
159	Large-scale atomistic simulations of helium-3 bubble growth in complex palladium alloys. Journal of Chemical Physics, 2016, 144, 194705.	3.0	9
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