Bryan M Wong

List of Publications by Citations

179 papers	5,728 citations	42 h-index	66 g-index
242 ext. papers	6,876 ext. citations	6.2 avg, IF	6.28 L-index

#	Paper	IF	Citations
179	A Transparent, Self-Healing, Highly Stretchable Ionic Conductor. *Advanced Materials*, **2017**, 29, 1605099	24	321
178	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	6.4	213
177	Coumarin dyes for dye-sensitized solar cells: A long-range-corrected density functional study. *Journal of Chemical Physics*, **2008**, 129, 214703	3.9	152
176	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	6.4	150
175	Stress sensing in polycaprolactone films via an embedded photochromic compound. *ACS Applied Materials & Interfaces*, **2010**, 2, 1594-600	9.5	149
174	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	10.3	137
173	Novel metal□organic framework linkers for light harvesting applications. *Chemical Science*, **2014**, 5, 2081-2090	9.1	136
172	Absorption and fluorescence properties of oligothiophene biomarkers from long-range-corrected time-dependent density functional theory. *Physical Chemistry Chemical Physics*, **2009**, 11, 4498-508	3.6	131
171	Optoelectronic Properties of Carbon Nanorings: Excitonic Effects from Time-Dependent Density Functional Theory. *Journal of Physical Chemistry C*, **2009**, 113, 21921-21927	3.8	122
170	A Highly Stretchy, Transparent Elastomer with the Capability to Automatically Self-Heal Underwater. *Advanced Materials*, **2018**, 30, e1804602	24	109
169	Color detection using chromophore-nanotube hybrid devices. *Nano Letters*, **2009**, 9, 1028-33	11.5	104
168	Synthesis, characterization, and computational studies of cycloparaphenylene dimers. *Journal of the American Chemical Society*, **2012**, 134, 19709-15	16.4	97
167	Optical, structural, and numerical investigations of GaAs/AlGaAs core-multishell nanowire quantum well tubes. *Nano Letters*, **2013**, 13, 1016-22	11.5	94
166	Nanoscale effects on heterojunction electron gases in GaN/AlGaN core/shell nanowires. *Nano Letters*, **2011**, 11, 3074-9	11.5	92
165	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, 1280-92	2.8	86
164	Results for aliovalent doping of CeBr3 with Ca2+. *Journal of Applied Physics*, **2014**, 115, 034908	2.5	81
163	Energy and charge transfer by donor□cceptor pairs confined in a metal□rganic framework: a spectroscopic and computational investigation. *Journal of Materials Chemistry A*, **2014**, 2, 3389-3398	13	79

162	Noncovalent interactions in supramolecular complexes: a study on corannulene and the double concave buckycatcher. *Journal of Computational Chemistry*, **2009**, 30, 51-6	3.5	69
161	An embedded-atom method interatomic potential for Pd alloys. *Journal of Materials Research*, **2008**, 23, 704-718	2.5	69
160	Isolation of Pristine Electronics Grade Semiconducting Carbon Nanotubes by Switching the Rigidity of the Wrapping Polymer Backbone on Demand. *ACS Nano*, **2015**, 9, 10203-13	16.7	67
159	Non-proteinaceous hydrolase comprised of a phenylalanine metallo-supramolecular amyloid-like structure. *Nature Catalysis*, **2019**, 2, 977-985	36.5	65
158	Comparison of Molecular Dynamics with Classical Density Functional and Poisson-Boltzmann Theories of the Electric Double Layer in Nanochannels. *Journal of Chemical Theory and Computation* , **2012**, 8, 2012-2022	6.4	60
157	A Non-Thermal Plasma Route to Plasmonic TiN Nanoparticles. *Journal of Physical Chemistry C*, **2017**, 121, 2316-2322	3.8	59
156	Structural and Electronic Properties of Graphdiyne Carbon Nanotubes from Large-Scale DFT Calculations. *Journal of Physical Chemistry C*, **2016**, 120, 18871-18877	3.8	57
155	Solid state lithiation-delithiation of sulphur in sub-nano confinement: a new concept for designing lithium-sulphur batteries. *Chemical Science*, **2016**, 7, 1224-1232	9.4	56
154	Photophysical and theoretical investigations of the [8]cycloparaphenylene radical cation and its charge-resonance dimer. *Chemical Science*, **2013**, 4, 4285	9.4	55
153	Analytical bond-order potential for the cadmium telluride binary system. *Physical Review B*, **2012**, 85,	3.3	54
152	Polarizabilities of Conjugated Chains Revisited: Improved Results from Broken-Symmetry Range-Separated DFT and New CCSD(T) Benchmarks. *Journal of Chemical Theory and Computation*, **2016**, 12, 3593-602	6.4	53
151	The Importance of Short- and Long-Range Exchange on Various Excited State Properties of DNA Monomers, Stacked Complexes, and Watson-Crick Pairs. *Journal of Chemical Theory and Computation*, **2015**, 11, 2199-209	6.4	52
150	Breaking Badly: DFT-D2 Gives Sizeable Errors for Tensile Strengths in Palladium-Hydride Solids. *Journal of Chemical Theory and Computation*, **2015**, 11, 5426-35	6.4	50
149	Electronic structure of the S1 state in methylcobalamin: insight from CASSCF/MC-XQDPT2, EOM-CCSD, and TD-DFT calculations. *Journal of Computational Chemistry*, **2013**, 34, 987-1004	3.5	49
148	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	3.8	49
147	Donor cceptor polymers with tunable infrared photoresponse. *Polymer Chemistry*, **2017**, 8, 2922-2930	4.9	48
146	Spectroscopic, structural, and theoretical studies of halide complexes with a urea-based tripodal receptor. *Inorganic Chemistry*, **2012**, 51, 4274-84	5.1	47
145	Bridgehead Imine Substituted Cyclopentadithiophene Derivatives: An Effective Strategy for Band Gap Control in Donor cceptor Polymers. *Macromolecules*, **2013**, 46, 1337-1342	5.5	46

144	Spectroscopic properties of nanotube-chromophore hybrids. *ACS Nano*, **2011**, 5, 7767-74	16.7	46
143	A high-spin ground-state donor-acceptor conjugated polymer. *Science Advances*, **2019**, 5, eaav2336	14.3	44
142	Iterative Reductive Aromatization/Ring-Closing Metathesis Strategy toward the Synthesis of Strained Aromatic Belts. *Journal of the American Chemical Society*, **2016**, 138, 6577-82	16.4	44
141	Halogen Bonding Interactions: Revised Benchmarks and a New Assessment of Exchange vs Dispersion. *Journal of Chemical Theory and Computation*, **2018**, 14, 180-190	6.4	44
140	Confined Lithium-Sulfur Reactions in Narrow-Diameter Carbon Nanotubes Reveal Enhanced Electrochemical Reactivity. *ACS Nano*, **2018**, 12, 9775-9784	16.7	44
139	Degradation of Perfluoroalkyl Ether Carboxylic Acids with Hydrated Electrons: Structure-Reactivity Relationships and Environmental Implications. *Environmental Science & Technology*, **2020**, 54, 2489-2499	10.3	42
138	Inconsistencies in the Electronic Properties of Phosphorene Nanotubes: New Insights from Large-Scale DFT Calculations. *Journal of Physical Chemistry Letters*, **2016**, 7, 4340-4345	6.4	42
137	A self-assembled fluoride-water cyclic cluster of [F(H2O)]4(4-) in a molecular box. *Journal of the American Chemical Society*, **2012**, 134, 11892-5	16.4	42
136	Polycation Binders: An Effective Approach toward Lithium Polysulfide Sequestration in Li–S Batteries. *ACS Energy Letters*, **2017**, 2, 2591-2597	20.1	39
135	Rational design of a macrocyclic-based chemosensor for anions. *Tetrahedron Letters*, **2010**, 51, 1329-1332	2	39
134	Investigating the Reactivity of 1,4-Anthracene-Incorporated Cycloparaphenylene. *Organic Letters*, **2016**, 18, 1574-7	6.2	38
133	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	11	36
132	Reversible, opto-mechanically induced spin-switching in a nanoribbon-spiropyran hybrid material. *Nanoscale*, **2012**, 4, 1321-7	7.7	36
131	Formation of an Amine-Water Cyclic Pentamer: A New Type of Water Cluster in a Polyazacryptand. *Crystal Growth and Design*, **2010**, 10, 1486-1488	3.5	36
130	Thermochemistry of Alane Complexes for Hydrogen Storage: A Theoretical and Experimental Investigation. *Journal of Physical Chemistry C*, **2011**, 115, 7778-7786	3.8	36
129	Chemical and Radiation Stability of Ionic Liquids: A Computational Screening Study. *Journal of Physical Chemistry C*, **2016**, 120, 27757-27767	3.8	35
128	Accuracy of existing atomic potentials for the CdTe semiconductor compound. *Journal of Chemical Physics*, **2011**, 134, 244703	3.9	35
127	A new approach toward transition state spectroscopy. *Faraday Discussions*, **2013**, 163, 33-57; discussion 117-38	3.6	34

126	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	7.1	34
125	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	6.4	33
124	Assessing backbone solvation effects in the conformational propensities of amino acid residues in unfolded peptides. *Physical Chemistry Chemical Physics*, **2015**, 17, 24917-24	3.6	33
123	Spectral- and Pulse-Shape Discrimination in Triplet-Harvesting Plastic Scintillators. *IEEE Transactions on Nuclear Science*, **2012**, 59, 3312-3319	1.7	33
122	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	4.3	32
121	Thermoelectric Performance of an Open-Shell Donor–Acceptor Conjugated Polymer Doped with a Radical-Containing Small Molecule. *Macromolecules*, **2018**, 51, 3886-3894	5.5	32
120	Giant Raman Response to the Encapsulation of Sulfur in Narrow Diameter Single-Walled Carbon Nanotubes. *Journal of the American Chemical Society*, **2016**, 138, 40-3	16.4	31
119	Potential-Driven Electron Transfer Lowers the Dissociation Energy of the C-F Bond and Facilitates Reductive Defluorination of Perfluorooctane Sulfonate (PFOS). *ACS Applied Materials & Interfaces*, **2019**, 11, 33913-33922	9.5	30
118	Effect of Dipolar Molecule Structure on the Mechanism of Graphene-Enhanced Raman Scattering. *Journal of Physical Chemistry C*, **2016**, 120, 13815-13824	3.8	30
117	Functionalization of single-wall carbon nanotubes with chromophores of opposite internal dipole orientation. *ACS Applied Materials & Interfaces*, **2013**, 5, 9355-61	9.5	30
116	Real-Time Quantum Dynamics of Long-Range Electronic Excitation Transfer in Plasmonic Nanoantennas. *Journal of Chemical Theory and Computation*, **2017**, 13, 3442-3454	6.4	29
115	Temperature and Molecular Size Dependence of the High-Pressure Limit. *Journal of Physical Chemistry A*, **2003**, 107, 6206-6211	2.8	29
114	Understanding gas phase modifier interactions in rapid analysis by differential mobility-tandem mass spectrometry. *Journal of the American Society for Mass Spectrometry*, **2014**, 25, 1098-113	3.5	28
113	Self-assembled cyclic oligothiophene nanotubes: Electronic properties from a dispersion-corrected hybrid functional. *Physical Review B*, **2011**, 84,	3.3	28
112	A C Symmetric Nitrate Complex with a Thiophene-Based Tripodal Receptor. *Crystal Growth and Design*, **2011**, 11, 959-963	3.5	27
111	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	6.4	26
110	Orientation of a monolayer of dipolar molecules on graphene from X-ray absorption spectroscopy. *Langmuir*, **2014**, 30, 2559-65	4	26
109	Molecular Dynamics Studies of Dislocations in CdTe Crystals from a New Bond Order Potential. *Journal of Physical Chemistry C*, **2012**, 116, 17563-17571	3.8	26

108	Accurate inertias for large-amplitude motions: improvements on prevailing approximations. *Journal of Physical Chemistry A*, **2006**, 110, 7406-13	2.8	26
107	Machine Learning: New Ideas and Tools in Environmental Science and Engineering. *Environmental Science & Technology*, **2021**, 55, 12741-12754	10.3	26
106	Highly selective and sensitive macrocycle-based dinuclear foldamer for fluorometric and colorimetric sensing of citrate in water. *Scientific Reports*, **2018**, 8, 286	4.9	25
105	Raman Enhancement of a Dipolar Molecule on Graphene. *Journal of Physical Chemistry C*, **2014**, 118, 2077-2084	3.8	25
104	Covalent Atomic Bridges Enable Unidirectional Enhancement of Electronic Transport in Aligned Carbon Nanotubes. *ACS Applied Materials & Interfaces*, **2019**, 11, 19315-19323	9.5	24
103	Photochemistry of Plasmonic Titanium Nitride Nanocrystals. *Journal of Physical Chemistry C*, **2019**, 123, 21796-21804	3.8	24
102	Self-assembly of ordered water tetramers in an encapsulated [Br(H2O)12]- complex. *Chemical Communications*, **2012**, 48, 8631-3	5.8	24
101	Charge-assisted encapsulation of two chlorides by a hexaprotonated azamacrocycle. *Crystal Growth and Design*, **2010**, 10, 1478-1781	3.5	23
100	A quantum defect model for the s, p, d, and f Rydberg series of CaF. *Journal of Chemical Physics*, **2011**, 134, 114313	3.9	23
99	Analytical bond-order potential for the Cd-Zn-Te ternary system. *Physical Review B*, **2012**, 86,	3.3	23
98	Materials Compatibility in Rechargeable Aluminum Batteries: Chemical and Electrochemical Properties between Vanadium Pentoxide and Chloroaluminate Ionic Liquids. *Chemistry of Materials*, **2019**, 31, 7238-7247	9.6	22
97	A highly efficient dinuclear Cu(II) chemosensor for colorimetric and fluorescent detection of cyanide in water. *RSC Advances*, **2014**, 4, 54263-54267	3.7	22
96	An exclusive fluoride receptor: Fluoride-induced proton transfer to a quinoline-based thiourea. *Tetrahedron Letters*, **2014**, 55, 1467-1470	2	22
95	Absorption and fluorescence signatures of 1,2,3-triazole based regioisomers: challenging compounds for TD-DFT. *Physical Chemistry Chemical Physics*, **2014**, 16, 9064-73	3.6	22
94	Structural Dependence of Reductive Defluorination of Linear PFAS Compounds in a UV/Electrochemical System. *Environmental Science & Technology*, **2020**, 54, 10668-10677	10.3	22
93	Is a cross-β sheet structure of low molecular weight peptides necessary for the formation of fibrils and peptide hydrogels?. *Physical Chemistry Chemical Physics*, **2018**, 20, 18158-18168	3.6	21
92	Preferential Charge Generation at Aggregate Sites in Narrow Band Gap Infrared Photoresponsive Polymer Semiconductors. *Advanced Optical Materials*, **2018**, 6, 1701138	8.1	21
91	Real-Time Quantum Dynamics Reveals Complex, Many-Body Interactions in Solvated Nanodroplets. *Journal of Chemical Theory and Computation*, **2016**, 12, 1862-71	6.4	21

90	Solution-processable donor-acceptor polymers with modular electronic properties and very narrow bandgaps. *Macromolecular Rapid Communications*, **2014**, 35, 1516-21	4.8	21
89	Anomalous Optoelectronic Properties of Chiral Carbon Nanorings: One Ring to Rule Them All. *Journal of Physical Chemistry Letters*, **2011**, 2, 2702-2706	6.4	21
88	Anion directed conformational diversities of an arene based hexa-amide receptor and recognition of the [F4(H2O)6]4− cluster. *RSC Advances*, **2014**, 4, 62689-62693	3.7	20
87	Melt-growth dynamics in CdTe crystals. *Physical Review Letters*, **2012**, 108, 245503	7.4	19
86	Evolution of chemical bonding during HCN HNC isomerization as revealed through nuclear quadrupole hyperfine structure. *Angewandte Chemie - International Edition*, **2008**, 47, 2969-72	16.4	18
85	Quantum confinement of excitons in wurtzite InP nanowires. *Journal of Applied Physics*, **2015**, 117, 194306	2.5	17
84	Binding and selectivity of dihydrogen phosphate by H-bond donors and acceptors in a tripodal-based thiourea receptor. *Tetrahedron Letters*, **2015**, 56, 115-118	2	17
83	On the non-thermal plasma synthesis of nickel nanoparticles. *Plasma Processes and Polymers*, **2018**, 15, 1700104	3.4	17
82	High-fidelity simulations of CdTe vapor deposition from a bond-order potential-based molecular dynamics method. *Physical Review B*, **2012**, 85,	3.3	17
81	Electronic signatures of large amplitude motions: dipole moments of vibrationally excited local-bend and local-stretch states of S0 acetylene. *Journal of Physical Chemistry B*, **2006**, 110, 18912-20	3.4	17
80	A theoretical and experimental kinetic study of phenyl radical addition to butadiene. *Proceedings of the Combustion Institute*, **2005**, 30, 1049-1056	5.9	17
79	Colorimetric and Optical Discrimination of Halides by a Simple Chemosensor. *RSC Advances*, **2015**, 5, 38733-38741	3.7	16
78	Correlating Li-Solvation Structure and its Electrochemical Reaction Kinetics with Sulfur in Subnano Confinement. *Journal of Physical Chemistry Letters*, **2018**, 9, 1739-1745	6.4	16
77	Atomistic potentials for palladium–silver hydrides. *Modelling and Simulation in Materials Science and Engineering*, **2013**, 21, 045005	2	16
76	Sultam-Based Hetero[5]helicene: Synthesis, Structure, and Crystallization-Induced Emission Enhancement. *ACS Omega*, **2016**, 1, 1336-1342	3.9	16
75	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	3.9	15
74	Defect formation dynamics during CdTe overlayer growth. *Physical Review B*, **2012**, 85,	3.3	15
73	Electron beam synthesis of metal and semiconductor nanoparticles using metal-organic frameworks as ordered precursors. *Nanotechnology*, **2011**, 22, 375601	3.4	15

72	PAMELA: An open-source software package for calculating nonlocal exact exchange effects on electron gases in core-shell nanowires. *AIP Advances*, **2012**, 2, 032173	1.5	15
71	Separation of long-range and short-range interactions in Rydberg states of diatomic molecules. *Journal of Chemical Physics*, **2008**, 128, 194301	3.9	15
70	Indirect but Efficient: Laser-Excited Electrons Can Drive Ultrafast Polarization Switching in Ferroelectric Materials. *Journal of Physical Chemistry Letters*, **2019**, 10, 3402-3407	6.4	14
69	Effects of large-amplitude torsions on partition functions: beyond the conventional separability assumption. *Molecular Physics*, **2005**, 103, 1027-1034	1.7	14
68	Size resolved chemical composition of nanoparticles from reactions of sulfuric acid with ammonia and dimethylamine. *Aerosol Science and Technology*, **2018**, 52, 1120-1133	3.4	14
67	A Long-Range Electric Field Solver for Molecular Dynamics Based on Atomistic-to-Continuum Modeling. *Journal of Chemical Theory and Computation*, **2011**, 7, 1736-49	6.4	13
66	Enhanced photocurrent efficiency of a carbon nanotube p□ junction electromagnetically coupled to a photonic structure. *Journal Physics D: Applied Physics*, **2009**, 42, 055111	3	13
65	Determination of the level of hexavalent, trivalent, and total chromium in the discharged effluent of Bahir Dar tannery using ICP-OES and UV□Visible spectrometry. *Cogent Chemistry*, **2018**, 4, 1534566	2.5	13
64	An Experimental and Modeling Study of Nanoparticle Formation and Growth from Dimethylamine and Nitric Acid. *Journal of Physical Chemistry A*, **2019**, 123, 5640-5648	2.8	12
63	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	5.8	12
62	A quinoline based bis-urea receptor for anions: a selective receptor for hydrogen sulfate. *Natural Product Communications*, **2012**, 7, 301-4	0.9	12
61	The diamine cation is not a chemical example where density functional theory fails. *Nature Communications*, **2018**, 9, 4733	17.4	12
60	Linear polarizabilities and second hyperpolarizabilities of streptocyanines: Results from broken-Symmetry DFT and new CCSD(T) benchmarks. *Journal of Computational Chemistry*, **2018**, 39, 2350-2359	3.5	12
59	High Magnetic Field Detunes Vibronic Resonances in Photosynthetic Light Harvesting. *Journal of Physical Chemistry Letters*, **2018**, 9, 5548-5554	6.4	12
58	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	3.6	11
57	A refined parameterization of the analytical Cd-Zn-Te bond-order potential. *Journal of Molecular Modeling*, **2013**, 19, 5469-77	2	11
56	A prediction of dislocation-free CdTe/CdS photovoltaic multilayers via nano-patterning and composition grading. *Progress in Photovoltaics: Research and Applications*, **2015**, 23, 1837-1846	6.8	11
55	An Efficient and Accurate Formalism for the Treatment of Large Amplitude Intramolecular Motion. *Journal of Chemical Theory and Computation*, **2012**, 8, 2713-2724	6.4	11

54	Thermodynamic calculations for molecules with asymmetric internal rotors--application to 1,3-butadiene. *Journal of Computational Chemistry*, **2007**, 28, 759-66	3.5	11
53	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	11.5	10
52	Analytical Bond-Order Potential for the Cd□Te□Se Ternary System. *Journal of Physical Chemistry C*, **2014**, 118, 20661-20679	3.8	10
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50	Nuclear quadrupole hyperfine structure in HC14N/H14NC and DC15N/D15NC isomerization: a diagnostic tool for characterizing vibrational localization. *Physical Chemistry Chemical Physics*, **2008**, 10, 5599-606	3.6	10
49	Thermodynamic calculations for molecules with asymmetric internal rotors. II. Application to the 1,2-dihaloethanes. *Journal of Computational Chemistry*, **2008**, 29, 481-7	3.5	10
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47	Additional Insights between Fermi-L□wdin Orbital SIC and the Localization Equation Constraints in SIC-DFT. *Journal of Physical Chemistry Letters*, **2018**, 9, 6456-6462	6.4	10
46	Charge density wave hampers exciton condensation in 1T□TiSe2. *Physical Review B*, **2019**, 100,	3.3	9
45	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	2.8	9
44	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	3.4	8
43	Unusual Bandgap Oscillations in Template-Directed □Conjugated Porphyrin Nanotubes. *Journal of Physical Chemistry Letters*, **2016**, 7, 2362-7	6.4	8
42	Ultrafast photoinduced band splitting and carrier dynamics in chiral tellurium nanosheets. *Nature Communications*, **2020**, 11, 3991	17.4	8
41	Ab initio metadynamics calculations reveal complex interfacial effects in acetic acid deprotonation dynamics. *Journal of Molecular Liquids*, **2021**, 330, 115624	6	8
40	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	3.8	7
39	metadynamics calculations of dimethylamine for probing p variations in bulk surface environments. *Physical Chemistry Chemical Physics*, **2020**, 22, 26265-26277	3.6	7
38	Stability of Calcium Ion Battery Electrolytes: Predictions from Ab Initio Molecular Dynamics Simulations. *ACS Applied Materials & Interfaces*, **2021**, 13, 13114-13122	9.5	7
37	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	6.4	6

36	Fractional occupation numbers and self-interaction correction-scaling methods with the Fermi-Löwdin orbital self-interaction correction approach. *Journal of Computational Chemistry*, **2020**, 41, 1200-1208	3.5	6
35	Studies of intersystem crossing dynamics in acetylene. *Journal of Chemical Physics*, **2007**, 126, 184307	3.9	6
34	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	3.6	6
33	Large-scale atomistic simulations of helium-3 bubble growth in complex palladium alloys. *Journal of Chemical Physics*, **2016**, 144, 194705	3.9	6
32	Single amino acid bionanozyme for environmental remediation.. *Nature Communications*, **2022**, 13, 1505	17.4	6
31	Chirality Induced Spin Selectivity of Photoexcited Electrons in Carbon-Sulfur [n]Helicenes. *ChemPhotoChem*, **2019**, 3, 770-777	3.3	5
30	(E)-2-{Eth-yl[4-(4-nitro-phenyl-diazen-yl)phen-yl]amino}ethyl anthracene-9-carboxyl-ate. *Acta Crystallographica Section E: Structure Reports Online*, **2008**, 64, o595		5
29	6 nm super-resolution optical transmission and scattering spectroscopic imaging of carbon nanotubes using a nanometer-scale white light source. *Nature Communications*, **2021**, 12, 6868	17.4	5
28	Improved band gaps and structural properties from Wannier-Fermi-Löwdin self-interaction corrections for periodic systems. *Journal of Physics Condensed Matter*, **2021**, 33, 115501	1.8	5
27	Modulating the conductance in graphene nanoribbons with multi-barriers under an applied voltage. *Results in Physics*, **2021**, 27, 104505	3.7	5
26	Persistent radical anion polymers based on naphthalenediimide and a vinylene spacer.. *RSC Advances*, **2018**, 8, 14760-14764	3.7	4
25	An MM and QM Study of Biomimetic Catalysis of Diels-Alder Reactions Using Cyclodextrins. *Catalysts*, **2018**, 8,	4	4
24	Poly((2-alkylbenzo[1,2,3]triazole-4,7-diyl)vinylene)s for organic solar cells. *Journal of Polymer Science, Part B: Polymer Physics*, **2015**, 53, 1539-1545	2.6	4
23	Charge-density induced discrimination of halides with a rigid dinuclear copper(II) complex. *Molecular Systems Design and Engineering*, **2020**, 5, 996-1002	4.6	4
22	Nanoarchitectonics of Metal-Free Porous Polyketone as Photocatalytic Assemblies for Artificial Photosynthesis.. *ACS Applied Materials & Interfaces*, **2021**,	9.5	4
21	Solvation Structure of Surface-Supported Amine Fragments: A Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2017**, 121, 22156-22163	3.8	3
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19	Electric potential invariants and ions-in-molecules effective potentials for molecular Rydberg states. *Journal of Chemical Physics*, **2016**, 145, 234301	3.9	3

18	NIC-CAGE: An open-source software package for predicting optimal control fields in photo-excited chemical systems. *Computer Physics Communications*, **2021**, 258, 107541	4.2	3
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16	Analytical calculations of molecular integrals for multielectron R-matrix methods. *Journal of Chemical Physics*, **2006**, 124, 14106	3.9	2
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