Jeffrey R Reimers

List of Publications by Year
in descending order

202 papers	8,764 citations	34016 52 h-index	54797 84 g-index
217 all docs	217 docs citations	217 times ranked	8268 citing authors

#	Article	IF	Citations
1	A practical method for the use of curvilinear coordinates in calculations of normal-mode-projected displacements and Duschinsky rotation matrices for large molecules. Journal of Chemical Physics, 2001, 115, 9103-9109.	1.2	546
2	Failure of density-functional theory and time-dependent density-functional theory for large extended Ï€ systems. Journal of Chemical Physics, 2002, 117, 5543-5549.	1.2	317
3	Density Functional Theory for Charge Transfer:Â The Nature of the N-Bands of Porphyrins and Chlorophylls Revealed through CAM-B3LYP, CASPT2, and SAC-CI Calculations. Journal of Physical Chemistry B, 2006, 110, 15624-15632.	1.2	315
4	Formalism, analytical model, and a priori Greenâ€™s-function-based calculations of the currentâ€“voltage characteristics of molecular wires. Journal of Chemical Physics, 2000, 112, 1510-1521.	1.2	274
5	The Solvation of Acetonitrile. Journal of the American Chemical Society, 1999, 121, 3730-3744.	6.6	235
6	Identifying carbon as the source of visible single-photon emission from hexagonal boron nitride. Nature Materials, 2021, 20, 321-328.	13.3	210
7	The structure, energetics, and nature of the chemical bonding of phenylthiol adsorbed on the Au(111) surface: Implications for density-functional calculations of molecular-electronic conduction. Journal of Chemical Physics, 2005, 122, 094708.	1.2	150
8	Adsorption of Benzene on Copper, Silver, and Gold Surfaces. Journal of Chemical Theory and Computation, 2006, 2, 1093-1105.	2.3	141
9	Molecular dynamics of the A+BC reaction in rare gas solution. Journal of Chemical Physics, 1986, 85, 5625-5643.	1.2	134
10	The Low-Lying Excited States of Pyridine. Journal of Physical Chemistry A, 2000, 104, 8389-8408.	1.1	125
11	Defect states in hexagonal boron nitride: Assignments of observed properties and prediction of properties relevant to quantum computation. Physical Review B, 2018, 97, .	1.1	125
12	Gold surfaces and nanoparticles are protected by Au(0)â€“thiyl species and are destroyed when Au(I)â€“thiolates form. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E1424-33.	3.3	116
13	Adsorption of Pyridine on the Gold(111) Surface:â€‰ Implications for â€œAlligator Clipsâ€•for Molecular Wires. Journal of Physical Chemistry B, 2002, 106, 6740-6747.	1.2	113
14	Adsorption of ammonia on the gold (111) surface. Journal of Chemical Physics, 2002, 116, 8981-8987.	1.2	112
15	Demonstration and interpretation of significant asymmetry in the low-resolution and high-resolution Q y fluorescence and absorption spectra of bacteriochlorophyll a. Journal of Chemical Physics, 2011, 134, 024506.	1.2	112
16	Assignment of the Q-Bands of the Chlorophylls: Coherence Loss via Qx â^’ Qy Mixing. Scientific Reports, 2013, 3, 2761.	1.6	110
17	The Appropriateness of Density-Functional Theory for the Calculation of Molecular Electronics Properties. Annals of the New York Academy of Sciences, 2003, 1006, 235-251.	1.8	107
18	Switchable Electronic Coupling in Model Oligoporphyrin Molecular Wires Examined through the Measurement and Assignment of Electronic Absorption Spectra. Journal of the American Chemical Society, 2002, 124, 9299-9309.	6.6	106

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19	Single-photon emitters in hexagonal boron nitride: a review of progress. Reports on Progress in Physics, 2020, 83, 044501.	8.1	104
20	Understanding the inelastic electron-tunneling spectra of alkanedithiols on gold. Journal of Chemical Physics, 2006, 124, 094704.	1.2	103
21	Solvent Effects on the Electronic Spectra of Transition Metal Complexes. Chemical Reviews, 2000, 100, 775-786.	23.0	96
22	Competition of van der Waals and chemical forces on goldâ€“sulfur surfaces and nanoparticles. Nature Reviews Chemistry, 2017, 1, .	13.8	95
23	Weak, strong, and coherent regimes of FrÃ¶hlich condensation and their applications to terahertz medicine and quantum consciousness. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 4219-4224.	3.3	94
24	Electron and energy transfer through bridged systems. 6. Molecular switches: the critical field in electric field activated bistable molecules. Journal of the American Chemical Society, 1990, 112, 4192-4197.	6.6	89
25	Long-lived long-distance photochemically induced spin-polarized charge separation in Î²,Î²â€²-pyrrolic fused ferrocene-porphyrin-fullerene systems. Chemical Science, 2012, 3, 257-269.	3.7	88
26	Chemical Analysis of the Superatom Model for Sulfur-Stabilized Gold Nanoparticles. Journal of the American Chemical Society, 2010, 132, 8378-8384.	6.6	87
27	Rigid Fused Oligoporphyrins as Potential Versatile Molecular Wires. 2. B3LYP and SCF Calculated Geometric and Electronic Properties of 98 Oligoporphyrin and Related Molecules. Journal of Physical Chemistry A, 1999, 103, 4385-4397.	1.1	83
28	Simulation of theAu(111)â^š(22Ã—3)surface reconstruction. Physical Review B, 2007, 75, .	1.1	80
29	A priorimethod for propensity rules for inelastic electron tunneling spectroscopy of single-molecule conduction. Physical Review B, 2007, 75, .	1.1	80
30	Coexistence of Multiple Conformations in Cysteamine Monolayers on Au(111). Journal of Physical Chemistry B, 2005, 109, 15355-15367.	1.2	79
31	Photoinduced electron transfer in a Î²,Î²â€²-pyrrolic fused ferroceneâ€“(zinc porphyrin)â€“fullerene. Physical Chemistry Chemical Physics, 2007, 9, 5260.	1.3	78
32	Efficient Methods for the Quantum Chemical Treatment of Protein Structures: The Effects of London-Dispersion and Basis-Set Incompleteness on Peptide and Water-Cluster Geometries. Journal of Chemical Theory and Computation, 2013, 9, 3240-3251.	2.3	75
33	Challenges facing an understanding of the nature of low-energy excited states in photosynthesis. Biochimica Et Biophysica Acta - Bioenergetics, 2016, 1857, 1627-1640.	0.5	74
34	Successful a Priori Modeling of CO Adsorption on Pt(111) Using Periodic Hybrid Density Functional Theory. Journal of the American Chemical Society, 2007, 129, 10402-10407.	6.6	73
35	A Unified Description of the Electrochemical, Charge Distribution, and Spectroscopic Properties of the Special-Pair Radical Cation in Bacterial Photosynthesis. Journal of the American Chemical Society, 2004, 126, 4132-4144.	6.6	72
36	Understanding and Improving Solid-State Polymer/C60-Fullerene Bulk-Heterojunction Solar Cells Using Ternary Porphyrin Blends. Journal of Physical Chemistry C, 2007, 111, 15415-15426.	1.5	72

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37	Understanding and Calibrating Density-Functional-Theory Calculations Describing the Energy and Spectroscopy of Defect Sites in Hexagonal Boron Nitride. Journal of Chemical Theory and Computation, 2018, 14, 1602-1613.	2.3	69
38	Complex time dependent wave packet technique for thermal equilibrium systems: Electronic spectra. Journal of Chemical Physics, 1983, 79, 4749-4757.	1.2	67
39	Challenges for the Accurate Simulation of Anisotropic Charge Mobilities through Organic Molecular Crystals: The Î² Phase of mer-Tris(8-hydroxyquinolinato)aluminum(III) (Alq3) Crystal. Journal of Physical Chemistry C, 2012, 116, 14826-14836.	1.5	66
40	Ab Initio and Density-Functional Calculations of the Vibrational Structure of the Singlet and Triplet Excited States of Pyrazine. Journal of Physical Chemistry A, 1999, 103, 9830-9841.	1.1	65
41	The First Singlet (n,Ï€*) and (Ï€,Ï€*) Excited States of the Hydrogen-Bonded Complex between Water and Pyridine. Journal of Physical Chemistry A, 2002, 106, 8769-8778.	1.1	63
42	Density-functional geometry optimization of the 150â€‰000-atom photosystem-I trimer. Journal of Chemical Physics, 2006, 124, 024301.	1.2	62
43	Photoluminescence, photophysics, and photochemistry of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:msub><mml:mi mathvariant="normal">V</mml:mi><mml:mi mathvariant="normal">B</mml:mi></mml:msub></mml:mrow><mml:mo>â^’</mml:mo></mml:msup></mml:math> defect in hexagonal boron nitride. Physical Review B, 2020, 102, .	1.1	60
44	Time-dependent density-functional determination of arbitrary singlet and triplet excited-state potential energy surfaces: Application to the water molecule. Journal of Chemical Physics, 2000, 113, 7084-7096.	1.2	58
45	Macrocyclic ligand design. X-Ray, DFT and solution studies of the effect of N-methylation and N-benzylation of 1,4,10,13-tetraoxa-7,16-diazacyclooctadecane on its affinity for selected transition and post-transition metal ions. Dalton Transactions RSC, 2001, , 614-620.	2.3	58
46	Assignment of the Q_y Absorption Spectrum of Photosystem-I from Thermosynechococcus elongatus Based on CAM-B3LYP Calculations at the PW91-Optimized Protein Structure. Journal of Physical Chemistry B, 2007, 111, 9923-9930.	1.2	58
47	Penrose-Hameroff orchestrated objective-reduction proposal for human consciousness is not biologically feasible. Physical Review E, 2009, 80, 021912.	0.8	57
48	Quantum entanglement between electronic and vibrational degrees of freedom in molecules. Journal of Chemical Physics, 2011, 135, 244110.	1.2	56
49	Dipole Order in Halide Perovskites: Polarization and Rashba Band Splittings. Journal of Physical Chemistry C, 2017, 121, 23045-23054.	1.5	56
50	Binding to gold(0): Accurate computational methods with application to AuNH3. Journal of Chemical Physics, 2002, 116, 10277-10286.	1.2	54
51	Quinoxalino[2,3-bâ€˜]porphyrins Behave as Ï€-Expanded Porphyrins upon One-Electron Reduction:â€‰ Broad Control of the Degree of Delocalization through Substitution at the Macrocycle Periphery. Journal of Physical Chemistry B, 2007, 111, 8762-8774.	1.2	54
52	Modeling the Bacterial Photosynthetic Reaction Center. 4. The Structural, Electrochemical, and Hydrogen-Bonding Properties of 22 Mutants ofRhodobacter sphaeroides. Journal of the American Chemical Society, 2001, 123, 8550-8563.	6.6	53
53	Recommending Hartreeâ€“Fock Theory with London-Dispersion and Basis-Set-Superposition Corrections for the Optimization or Quantum Refinement of Protein Structures. Journal of Physical Chemistry B, 2014, 118, 14612-14626.	1.2	53
54	Modeling the Bacterial Photosynthetic Reaction Center. 1. Magnesium Parameters for the Semiempirical AM1 Method Developed Using a Genetic Algorithm. Journal of Physical Chemistry B, 1998, 102, 8080-8090.	1.2	52

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55	Modeling the Bacterial Photosynthetic Reaction Center. 2. A Combined Quantum Mechanical/Molecular Mechanical Study of the Structure of the Cofactors in the Reaction Centers of Purple Bacteria. Journal of Physical Chemistry B, 1999, 103, 4906-4915.	1.2	52
56	Ab Initio and Density Functional Calculations of the Energies of the Singlet and Triplet Valence Excited States of Pyrazine. Journal of Physical Chemistry A, 1999, 103, 9821-9829.	1.1	52
57	Application of time-dependent density-functional theory to the 3Î£uâ^' first excited state of H2. Journal of Chemical Physics, 2000, 112, 527-530.	1.2	52
58	Inter-porphyrin coupling: how strong should it be for molecular electronics applications?. Journal of Porphyrins and Phthalocyanines, 2002, 06, 795-805.	0.4	52
59	Optimization and Chemical Control of Porphyrin-Based Molecular Wires and Switches. Annals of the New York Academy of Sciences, 1998, 852, 1-21.	1.8	49
60	Reaction Force and Its Link to Diabatic Analysis: A Unifying Approach to Analyzing Chemical Reactions. Journal of Physical Chemistry Letters, 2010, 1, 2858-2862.	2.1	46
61	Singlet and Triplet Valence Excited States of Pyrimidine. Journal of Physical Chemistry A, 2003, 107, 3093-3106.	1.1	45
62	The Mechanism of Covalent Bonding. Journal of Chemical Education, 1997, 74, 1494.	1.1	44
63	Non-adiabatic effects in thermochemistry, spectroscopy and kinetics: the general importance of all three Bornâ€“Oppenheimer breakdown corrections. Physical Chemistry Chemical Physics, 2015, 17, 24641-24665.	1.3	43
64	Electronic Couplings and Energy Transfer Dynamics in the Oxidized Primary Electron Donor of the Bacterial Reaction Center. Journal of Physical Chemistry B, 2004, 108, 1753-1765.	1.2	42
65	Molecular Origins of Conduction Channels Observed in Shot-Noise Measurements. Nano Letters, 2006, 6, 2431-2437.	4.5	42
66	A priori calculations of the free energy of formation from solution of polymorphic self-assembled monolayers. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E6101-10.	3.3	42
67	Synthesis and physical properties of biquinoxalinyl bridged bis-porphyrins: models for aspects of Photosynthetic Reaction Centres. Organic and Biomolecular Chemistry, 2003, 1, 2777.	1.5	41
68	Charge Delocalization in the Special-Pair Radical Cation of Mutant Reaction Centers ofRhodobactersphaeroidesfrom Stark Spectra and Nonadiabatic Spectral Simulations. Journal of Physical Chemistry B, 2006, 110, 18688-18702.	1.2	40
69	Modeling the bacterial photosynthetic reaction center. VII. Full simulation of the intervalence holeâ€“transfer absorption spectrum of the special-pair radical cation. Journal of Chemical Physics, 2003, 119, 3262-3277.	1.2	39
70	Formation of Goldâ^'Methanethiyl Self-Assembled Monolayers. Journal of the American Chemical Society, 2007, 129, 14532-14533.	6.6	39
71	Vibrational Stark Spectroscopy 3. Accurate Benchmark ab Initio and Density Functional Calculations for CO and CN-. Journal of Physical Chemistry A, 1999, 103, 10580-10587.	1.1	37
72	Successes and failures of time-dependent density functional theory for the low-lying excited states of chlorophylls. Molecular Physics, 2005, 103, 1057-1065.	0.8	37

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73	Gold Mining by Alkanethiol Radicals: Vacancies and Pits in the Self-Assembled Monolayers of 1-Propanethiol and 1-Butanethiol on Au(111). Journal of Physical Chemistry C, 2011, 115, 10630-10639.	1.5	36
74	Accurate prediction of the properties of materials using the <scp>CAMâ€B3LYP</scp> density functional. Journal of Computational Chemistry, 2021, 42, 1486-1497.	1.5	35
75	Hydrogen bonding and reactivity of water to azines in their S1 (n,Ï€*) electronic excited states in the gas phase and in solution. Physical Chemistry Chemical Physics, 2012, 14, 8791.	1.3	34
76	The symmetry of single-molecule conduction. Journal of Chemical Physics, 2006, 125, 184702.	1.2	33
77	van der Waals forces control ferroelectricâ€“antiferroelectric ordering in CuInP₂S₆ and CuBiP₂Se₆ laminar materials. Chemical Science, 2018, 9, 7620-7627.	3.7	33
78	A new fundamental type of conformational isomerism. Nature Chemistry, 2018, 10, 615-624.	6.6	33
79	The Green's Function Density Functional Tight-Binding (gDFTB) Method for Molecular Electronic Conductionâ€. Journal of Physical Chemistry A, 2007, 111, 5692-5702.	1.1	32
80	Bioferroelectric Properties of Glycine Crystals. Journal of Physical Chemistry Letters, 2019, 10, 1319-1324.	2.1	32
81	Hamiltonian operators including both symmetric and antisymmetric vibrational modes for vibronic coupling and intervalence charge-transfer applications. Chemical Physics, 2004, 299, 79-82.	0.9	31
82	Control of the Orbital Delocalization and Implications for Molecular Rectification in the Radical Anions of Porphyrins with Coplanar 90Â° and 180Â° Î²,Î²â€˜-Fused Extensions. Journal of Physical Chemistry A, 2008, 112, 556-570.	1.1	31
83	Evanescent-Field Spectroscopy using Structured Optical Fibers: Detection of Charge-Transfer at the Porphyrin-Silica Interface. Journal of the American Chemical Society, 2009, 131, 2925-2933.	6.6	31
84	Controlling the Stereochemistry and Regularity of Butanethiol Self-Assembled Monolayers on Au(111). Journal of the American Chemical Society, 2014, 136, 17087-17094.	6.6	31
85	Sulfur ligand mediated electrochemistry of gold surfaces and nanoparticles: What, how, and why. Current Opinion in Electrochemistry, 2017, 1, 7-15.	2.5	31
86	Classical and semiclassical approximations for incoherent neutron scattering. Physical Review A, 1987, 36, 2613-2627.	1.0	30
87	The Effect of Alkylation of N- and O-Donor Atoms on Their Strength of Coordination to Silver(I). Journal of Physical Chemistry A, 2001, 105, 6567-6574.	1.1	30
88	Towards a comprehensive model for the electronic and vibrational structure of the Creutzâ€“Taube ion. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2008, 366, 15-31.	1.6	30
89	Chain-Branching Control of the Atomic Structure of Alkanethiol-Based Goldâ€“Sulfur Interfaces. Journal of the American Chemical Society, 2011, 133, 14856-14859.	6.6	30
90	Spontaneous Sâ€“Si bonding of alkanethiols to Si(111)â€“H: towards Siâ€“moleculeâ€“Si circuits. Chemical Science, 2020, 11, 5246-5256.	3.7	30

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91	Dynamics of the A + BC reaction in solution. Chemical Physics Letters, 1986, 123, 394-398.	1.2	29
92	Modeling the Bacterial Photosynthetic Reaction Center 3:Â Interpretation of Effects of Site-Directed Mutagenesis on the Special-Pair Midpoint Potentialâ€. Biochemistry, 2000, 39, 16185-16189.	1.2	29
93	Electronâ€“vibration entanglement in the Bornâ€“Oppenheimer description of chemical reactions and spectroscopy. Physical Chemistry Chemical Physics, 2015, 17, 24666-24682.	1.3	29
94	CASSCFâ€wave packet ab initio prediction of electronic and vibrational spectra: Application to the A(2Î)â€‰â†â€‰X(2Î£+) absorption of C2H at 3000 K. Journal of Chemical Physics, 1985, 82, 5064-5077.	1.2	28
95	Single molecule conductivity: The role of junction-orbital degeneracy in the artificially high currents predicted by ab initio approaches. Journal of Chemical Physics, 2004, 121, 6615-6627.	1.2	28
96	Edge effects on optically detected magnetic resonance of vacancy defects in hexagonal boron nitride. Communications Physics, 2020, 3, .	2.0	28
97	Examination of the Photophysical Processes of Chlorophyll d Leading to a Clarification of Proposed Uphill Energy Transfer Processes in Cells of Acaryochloris marinaÂ¶. Photochemistry and Photobiology, 2003, 77, 628.	1.3	26
98	Overcoming computational uncertainties to reveal chemical sensitivity in single molecule conduction calculations. Journal of Chemical Physics, 2005, 122, 224502.	1.2	26
99	Control of the site and potential of reduction and oxidation processes in Ï€-expanded quinoxalinoporphyrins. Physical Chemistry Chemical Physics, 2008, 10, 268-280.	1.3	26
100	Scanning Tunneling Microscopic Observation of Adatom-Mediated Motifs on Goldâ^'Thiol Self-Assembled Monolayers at High Coverage. Journal of Physical Chemistry C, 2009, 113, 19601-19608.	1.5	26
101	Models for the Structure and Electronic Transmission of Carbon Nanotubes Covalently Linked by a Molecular Bridge via Amide Couplings. Journal of Physical Chemistry C, 2007, 111, 3700-3704.	1.5	25
102	Chemisorbed and Physisorbed Structures for 1,10-Phenanthroline and Dipyrido[3,2-a:2â€˜,3â€˜-c]phenazine on Au(111). Journal of Physical Chemistry C, 2007, 111, 17285-17296.	1.5	25
103	The Lowest Singlet (n,Ï€*) and (Ï€,Ï€*) Excited States of the Hydrogen-Bonded Complex between Water and Pyrazine. Journal of Physical Chemistry A, 2007, 111, 954-962.	1.1	25
104	The Need for Quantum-Mechanical Treatment of Capacitance and Related Properties of Nanoelectrodes. Journal of Physical Chemistry B, 2001, 105, 8979-8988.	1.2	24
105	A priori evaluation of the solvent contribution to the reorganization energy accompanying intramolecular electron transfer: Predicting the nature of the Creutzâ€“Taube ion. Chemical Physics, 2005, 319, 39-51.	0.9	24
106	Ultraviolet photodissociation action spectroscopy of the N-pyridinium cation. Journal of Chemical Physics, 2015, 142, 014301.	1.2	24
107	Q | R: quantum-based refinement. Acta Crystallographica Section D: Structural Biology, 2017, 73, 45-52.	1.1	24
108	Electron and Energy Transfer through Bridged Systems. 9. Toward a Priori Evaluation of the Intermetallic Coupling in Bis-metal Complexes. Journal of Physical Chemistry A, 1999, 103, 3066-3072.	1.1	23

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109	Modelling the bacterial photosynthetic reaction center. V. Assignment of the electronic transition observed at 2200 cmâ¯1 in the special-pair radical-cation as a second-highest occupied molecular orbital to highest occupied molecular orbital transition. Journal of Chemical Physics, 2003, 119, 3240-3248.	1.2	23
110	Modelling the bacterial photosynthetic reaction center. VI. Use of density-functional theory to determine the nature of the vibronic coupling between the four lowest-energy electronic states of the special-pair radical cation. Journal of Chemical Physics, 2003, 119, 3249-3261.	1.2	23
111	Explanation of the Anomalous Complexation of Silver(I) with Ammonia in Terms of the Poor Affinity of the Ion for Water. Journal of Physical Chemistry A, 2004, 108, 8434-8438.	1.1	23
112	Bond angle variations in XH₃ [X = N, P, As, Sb, Bi]: the critical role of Rydberg orbitals exposed using a diabatic state model. Physical Chemistry Chemical Physics, 2015, 17, 24618-24640.	1.3	23
113	Nature of the special-pair radical cation in bacterial photosynthesis. International Journal of Quantum Chemistry, 2000, 80, 1224-1243.	1.0	22
114	An azanorbornadiene anchor for molecular-level construction on silicon(100). Nanotechnology, 2004, 15, 324-332.	1.3	22
115	Synthetically tuneable biomimetic artificial photosynthetic reaction centres that closely resemble the natural system in purple bacteria. Chemical Science, 2016, 7, 6534-6550.	3.7	22
116	Covalent Linkages of Molecules and Proteins to Siâ€“H Surfaces Formed by Disulfide Reduction. Langmuir, 2020, 36, 14999-15009.	1.6	22
117	Atomic-Resolution Kinked Structure of an Alkylporphyrin on Highly Ordered Pyrolytic Graphite. Journal of Physical Chemistry Letters, 2011, 2, 62-66.	2.1	21
118	Polymorphism in porphyrin monolayers: the relation between adsorption configuration and molecular conformation. Physical Chemistry Chemical Physics, 2013, 15, 12451.	1.3	21
119	van der Waals Forces Control the Internal Chemical Structure of Monolayers within the Lamellar Materials CuInP₂S₆ and CuBiP₂Se₆. Journal of Physical Chemistry C, 2018, 122, 22675-22687.	1.5	21
120	Energy flow in the Photosystem I supercomplex: Comparison of approximative theories with DM-HEOM. Chemical Physics, 2018, 515, 262-271.	0.9	21
121	INDO/S parameters for gold. International Journal of Quantum Chemistry, 2002, 90, 424-438.	1.0	20
122	Peptide Ligations Accelerated byN-Terminal Aspartate and Glutamate Residues. Organic Letters, 2011, 13, 4770-4773.	2.4	20
123	A unified diabatic description for electron transfer reactions, isomerization reactions, proton transfer reactions, and aromaticity. Physical Chemistry Chemical Physics, 2015, 17, 24598-24617.	1.3	20
124	Solving the scalability issue in quantum-based refinement: Q|R#1. Acta Crystallographica Section D: Structural Biology, 2017, 73, 1020-1028.	1.1	20
125	Multistate density functional theory applied with 3 unpaired electrons in 3 orbitals: The singdoublet and tripdoublet states of the ethylene cation. Chemical Physics Letters, 2019, 736, 136803.	1.2	19
126	Complexation, Computational, Magnetic, and Structural Studies of the Maillard Reaction Product Isomaltol Including Investigation of an Uncommon Ï€ Interaction with Copper(II). Inorganic Chemistry, 2011, 50, 1498-1505.	1.9	18

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127	Intermixed Adatom and Surfaceâ€Bound Adsorbates in Regular Selfâ€Assembled Monolayers of Racemic 2â€Butanethiol on Au(111). ChemPhysChem, 2015, 16, 928-932.	1.0	18
128	Molecular quantum cellular automata cell design trade-offs: latching vs. power dissipation. Physical Chemistry Chemical Physics, 2018, 20, 17881-17888.	1.3	18
129	The exact eigenfunctions and eigenvalues of a twoâ€dimensional rigid rotor obtained using Gaussian wave packet dynamics. Journal of Chemical Physics, 1985, 83, 511-515.	1.2	17
130	Absorption-emission symmetry breaking and the different origins of vibrational structures of the 1Qy and 1Qx electronic transitions of pheophytin a. Journal of Chemical Physics, 2019, 151, 165102.	1.2	17
131	Theoretical spectroscopy of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">V</mml:mi><mml:mi mathvariant="normal">N</mml:mi></mml:msub><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mi mathvariant="normal">B</mml:mi></mml:msub></mml:mrow></mml:math> defect in hexagonal boron	1.1	17
132	Understanding the Chemisorption of 2-Methyl-2-propanethiol on Au(111). Journal of Physical Chemistry C, 2007, 111, 10878-10885.	1.5	16
133	The conduction properties of Î±,Ï‰-diaminoalkanes and hydrazine bridging gold electrodes. Chemical Physics Letters, 2008, 454, 284-288.	1.2	16
134	From Chaos to Order: Chain-Length Dependence of the Free Energy of Formation of Meso-tetraalkylporphyrin Self-Assembled Monolayer Polymorphs. Journal of Physical Chemistry C, 2016, 120, 1739-1748.	1.5	16
135	Application of the Computationally Efficient Self-Consistent-Charge Density-Functional Tight-Binding Method to Magnesium-Containing Moleculesâ€. Journal of Physical Chemistry A, 2007, 111, 5743-5750.	1.1	15
136	Title is missing!. Photosynthesis Research, 1998, 55, 163-171.	1.6	14
137	Inter-porphyrin coupling: rotation-modulation of inter-ring coupling in a Î¼-oxo-silicon phthalocyanine dimer. Chemical Physics Letters, 2003, 378, 654-659.	1.2	14
138	Molecular Electronics: From Basic Chemical Principles to Photosynthesis to Steady-State Through-Molecule Conductivity to Computer Architectures. Australian Journal of Chemistry, 2004, 57, 1133.	0.5	14
139	First Singlet (n,Ï€*) Excited State of Hydrogen-Bonded Complexes between Water and Pyrimidine. Journal of Physical Chemistry A, 2005, 109, 1576-1586.	1.1	13
140	The Manganiteâ^'Water Interface. Journal of Physical Chemistry C, 2007, 111, 10427-10437.	1.5	13
141	Problems, successes and challenges for the application of dispersion-corrected density-functional theory combined with dispersion-based implicit solvent models to large-scale hydrophobic self-assembly and polymorphism. Molecular Simulation, 2016, 42, 494-510.	0.9	13
142	On the relationship between the classical, semiclassical, and quantum dynamics of a Morse oscillator. The Journal of Physical Chemistry, 1988, 92, 3225-3235.	2.9	12
143	Modeling the adsorption of norbornadiene on the Si(001) surface: The predominance of non-[2+2]-cycloaddition products. Journal of Chemical Physics, 2003, 119, 1115-1126.	1.2	12
144	An Atomistic Approach to Conduction Between Nanoelectrodes Through a Single Molecule. Annals of the New York Academy of Sciences, 2002, 960, 100-130.	1.8	12

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145	Formation of waterâ€“chlorophyll clusters in dilute samples of chlorophyll-a in ether at low temperature. Physical Chemistry Chemical Physics, 2014, 16, 2323-2330.	1.3	12
146	An analytical data inversion method for magnetic circular dichroism spectra dominated by the â€œB-termâ€. Physical Chemistry Chemical Physics, 2014, 16, 2315-2322.	1.3	12
147	The revised Penroseâ€“Hameroff orchestrated objective-reduction proposal for human consciousness is not scientifically justified. Physics of Life Reviews, 2014, 11, 101-103.	1.5	12
148	Faraday cage screening reveals intrinsic aspects of the van der Waals attraction. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E10295-E10302.	3.3	12
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