Jeffrey R Reimers

List of Publications by Year in Descending Order

207 papers	7,364 citations	49 h-index	76 g-index
217 ext. papers	8,075 ext. citations	5.3 avg, IF	6.12 L-index

#	Paper	IF	Citations
207	Density functionals with asymptotic-potential corrections are required for the simulation of spectroscopic properties of materials.. *Chemical Science*, **2022**, 13, 1492-1503	9.4	0
206	Silicon - single molecule - silicon circuits.. *Chemical Science*, **2021**, 12, 15870-15881	9.4	1
205	Accurate prediction of the properties of materials using the CAM-B3LYP density functional. *Journal of Computational Chemistry*, **2021**, 42, 1486-1497	3.5	11
204	Identifying carbon as the source of visible single-photon emission from hexagonal boron nitride. *Nature Materials*, **2021**, 20, 321-328	27	78
203	Spontaneous S-Si bonding of alkanethiols to Si(111)-H: towards Si-molecule-Si circuits. *Chemical Science*, **2020**, 11, 5246-5256	9.4	15
202	Single-photon emitters in hexagonal boron nitride: a review of progress. *Reports on Progress in Physics*, **2020**, 83, 044501	14.4	52
201	Source code, input data, and sample output concerning the application of multistate density functional theory to the singdoublet and tripdoublet states of the ethylene cation. *Data in Brief*, **2020**, 28, 104984	1.2	1
200	Photoluminescence, photophysics, and photochemistry of the VB□ defect in hexagonal boron nitride. *Physical Review B*, **2020**, 102,	3.3	21
199	Theoretical spectroscopy of the VNNB defect in hexagonal boron nitride. *Physical Review B*, **2020**, 102,	3.3	8
198	Asymmetry in the Fluorescence and Absorption Spectra of Chlorophyll Pertaining to Exciton Dynamics. *Frontiers in Chemistry*, **2020**, 8, 588289	5	3
197	Covalent Linkages of Molecules and Proteins to Si-H Surfaces Formed by Disulfide Reduction. *Langmuir*, **2020**, 36, 14999-15009	4	12
196	Convergence of Defect Energetics Calculations. *Journal of Physical Chemistry C*, **2020**, 124, 21178-21183	3.8	9
195	Edge effects on optically detected magnetic resonance of vacancy defects in hexagonal boron nitride. *Communications Physics*, **2020**, 3,	5.4	13
194	Competition between charge migration and charge transfer induced by nuclear motion following core ionization: Model systems and application to Li. *Journal of Chemical Physics*, **2019**, 151, 124108	3.9	1
193	Decomposition of Ferrocene on Pt(111) and Its Effect on Molecular Electronic Junctions. *Journal of Physical Chemistry C*, **2019**, 123, 15569-15574	3.8	3
192	Noel S. Hush. *Journal of Physical Chemistry A*, **2019**, 123, 3935-3936	2.8	
191	Noel S. Hush. *Journal of Physical Chemistry B*, **2019**, 123, 3885-3886	3.4	

190	Bioferroelectric Properties of Glycine Crystals. *Journal of Physical Chemistry Letters*, **2019**, 10, 1319-1324	6.4	17
189	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	2.5	14
188	Absorption-emission symmetry breaking and the different origins of vibrational structures of the Q and Q electronic transitions of pheophytin a. *Journal of Chemical Physics*, **2019**, 151, 165102	3.9	8
187	Defect states in hexagonal boron nitride: Assignments of observed properties and prediction of properties relevant to quantum computation. *Physical Review B*, **2018**, 97,	3.3	81
186	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	6.4	42
185	Understanding non-linear effects from Hill-type dynamics with application to decoding of p53 signaling. *Scientific Reports*, **2018**, 8, 2147	4.9	1
184	Polarization effect within a protein crystal: A molecular dynamics simulation study. *Chemical Physics Letters*, **2018**, 706, 303-307	2.5	4
183	Molecular quantum cellular automata cell design trade-offs: latching vs. power dissipation. *Physical Chemistry Chemical Physics*, **2018**, 20, 17881-17888	3.6	12
182	How Equilibrium Gets Mimicked During Kinetic and Thermodynamic Control in Porphyrin and Phthalocyanine Self-Assembled Monolayers. *Langmuir*, **2018**, 34, 18-22	4	2
181	Cyanine platelet single crystals: growth, crystal structure and optical spectra. *Physical Chemistry Chemical Physics*, **2018**, 20, 29166-29173	3.6	3
180	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	11.5	9
179	van der Waals forces control ferroelectric-antiferroelectric ordering in CuInPS and CuBiPSe laminar materials. *Chemical Science*, **2018**, 9, 7620-7627	9.4	21
178	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	3.8	11
177	A new fundamental type of conformational isomerism. *Nature Chemistry*, **2018**, 10, 615-624	17.6	22
176	Energy flow in the Photosystem I supercomplex: Comparison of approximative theories with DM-HEOM. *Chemical Physics*, **2018**, 515, 262-271	2.3	13
175	Competition of van der Waals and chemical forces on gold–sulfur surfaces and nanoparticles. *Nature Reviews Chemistry*, **2017**, 1,	34.6	72
174	Relating transition-state spectroscopy to standard chemical spectroscopic processes. *Chemical Physics Letters*, **2017**, 683, 467-477	2.5	1
173	Diabatic models with transferrable parameters for generalized chemical reactions. *Journal of Physics: Conference Series*, **2017**, 833, 012014	0.3	0

172	Sulfur ligand mediated electrochemistry of gold surfaces and nanoparticles: What, how, and why. *Current Opinion in Electrochemistry*, **2017**, 1, 7-15	7.2	26
171	The critical role of the transition-state cusp diameter in understanding adiabatic and non-adiabatic electron transfer. *Russian Journal of Electrochemistry*, **2017**, 53, 1042-1053	1.2	2
170	Solving the scalability issue in quantum-based refinement: Q|R#1. *Acta Crystallographica Section D: Structural Biology*, **2017**, 73, 1020-1028	5.5	14
169	Q|R: quantum-based refinement. *Acta Crystallographica Section D: Structural Biology*, **2017**, 73, 45-52	5.5	21
168	Dipole Order in Halide Perovskites: Polarization and Rashba Band Splittings. *Journal of Physical Chemistry C*, **2017**, 121, 23045-23054	3.8	39
167	Surface Adsorption **2017**, 387-416		3
166	Synthetically tuneable biomimetic artificial photosynthetic reaction centres that closely resemble the natural system in purple bacteria. *Chemical Science*, **2016**, 7, 6534-6550	9.4	16
165	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	2	13
164	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	3.8	13
163	Challenges facing an understanding of the nature of low-energy excited states in photosynthesis. *Biochimica Et Biophysica Acta - Bioenergetics*, **2016**, 1857, 1627-1640	4.6	59
162	Putting David Craig's Legacy to Work in Nanotechnology and Biotechnology. *Australian Journal of Chemistry*, **2016**, 69, 1331	1.2	2
161	Gold surfaces and nanoparticles are protected by Au(0)-thiyl species and are destroyed when Au(I)-thiolates form. *Proceedings of the National Academy of Sciences of the United States of America* , **2016**, 113, E1424-33	11.5	83
160	Ultraviolet photodissociation action spectroscopy of the N-pyridinium cation. *Journal of Chemical Physics*, **2015**, 142, 014301	3.9	21
159	A unified diabatic description for electron transfer reactions, isomerization reactions, proton transfer reactions, and aromaticity. *Physical Chemistry Chemical Physics*, **2015**, 17, 24598-617	3.6	13
158	Non-adiabatic effects in thermochemistry, spectroscopy and kinetics: the general importance of all three Born-Oppenheimer breakdown corrections. *Physical Chemistry Chemical Physics*, **2015**, 17, 24641-65	3.6	32
157	Electron-vibration entanglement in the Born-Oppenheimer description of chemical reactions and spectroscopy. *Physical Chemistry Chemical Physics*, **2015**, 17, 24666-82	3.6	22
156	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	11.5	32
155	Free energies for the coordination of ligands to the magnesium of chlorophyll-a in solvents. *Molecular Physics*, **2015**, 113, 1648-1654	1.7	1

154	The Importance of Motions that Accompany Those Occurring Along the Reaction Coordinate. *Australian Journal of Chemistry*, **2015**, 68, 1202	1.2	4
153	Intermixed adatom and surface-bound adsorbates in regular self-assembled monolayers of racemic 2-butanethiol on Au(111). *ChemPhysChem*, **2015**, 16, 928-32	3.2	18
152	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, 24618-40	3.6	18
151	Formation of water-chlorophyll clusters in dilute samples of chlorophyll-a in ether at low temperature. *Physical Chemistry Chemical Physics*, **2014**, 16, 2323-30	3.6	7
150	An analytical data inversion method for Magnetic Circular Dichroism spectra dominated by the "B-term". *Physical Chemistry Chemical Physics*, **2014**, 16, 2315-22	3.6	7
149	The revised Penrose-Hameroff orchestrated objective-reduction proposal for human consciousness is not scientifically justified: comment on "Consciousness in the universe: a review of the 'Orch OR' theory" by Hameroff and Penrose. *Physics of Life Reviews*, **2014**, 11, 101-3; discussion 104-12	2.1	8
148	Recommending Hartree-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, 14612-26	3.4	46
147	Controlling the stereochemistry and regularity of butanethiol self-assembled monolayers on au(111). *Journal of the American Chemical Society*, **2014**, 136, 17087-94	16.4	28
146	A multiscale simulation technique for molecular electronics: design of a directed self-assembled molecular n-bit shift register memory device. *Nanotechnology*, **2013**, 24, 505202	3.4	1
145	Polymorphism in porphyrin monolayers: the relation between adsorption configuration and molecular conformation. *Physical Chemistry Chemical Physics*, **2013**, 15, 12451-8	3.6	17
144	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, 3240-51	6.4	61
143	Assignment of the Q-bands of the chlorophylls: coherence loss via Qx - Qy mixing. *Scientific Reports*, **2013**, 3, 2761	4.9	86
142	Toward ab initio refinement of protein X-ray crystal structures: interpreting and correlating structural fluctuations. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	7
141	Long-lived long-distance photochemically induced spin-polarized charge separation in β-pyrrolic fused ferrocene-porphyrin-fullerene systems. *Chemical Science*, **2012**, 3, 257-269	9.4	80
140	Hydrogen bonding and reactivity of water to azines in their S1 (n,π) electronic excited states in the gas phase and in solution. *Physical Chemistry Chemical Physics*, **2012**, 14, 8791-802	3.6	31
139	Challenges for the Accurate Simulation of Anisotropic Charge Mobilities through Organic Molecular Crystals: The β Phase of mer-Tris(8-hydroxyquinolinato)aluminum(III) (Alq3) Crystal. *Journal of Physical Chemistry C*, **2012**, 116, 14826-14836	3.8	61
138	BIOPHYSCHEM2011: A Joint Meeting of the Australian Society for Biophysics and the RACI Physical Chemistry Division. *Australian Journal of Chemistry*, **2012**, 65, 439	1.2	
137	Frequency-based Quantum Computers from a Chemist's Perspective. *Australian Journal of Chemistry*, **2012**, 65, 512	1.2	3

136	First Steps Towards Quantum Refinement of Protein X-Ray Structures **2012**, 87-120		6
135	Toward ab initio refinement of protein X-ray crystal structures: interpreting and correlating structural fluctuations **2012**, 21-36		
134	SIESTA: A Linear-Scaling Method for Density Functional Calculations **2011**, 45-75		4
133	Chain-branching control of the atomic structure of alkanethiol-based gold-sulfur interfaces. *Journal of the American Chemical Society*, **2011**, 133, 14856-9	16.4	27
132	Self-Consistent-Charge Density Functional Tight-Binding Method: An Efficient Approximation of Density Functional Theory **2011**, 287-307		5
131	Introduction to Effective Low-Energy Hamiltonians in Condensed Matter Physics and Chemistry **2011**, 309-366		5
130	Coupled-Cluster Calculations for Large Molecular and Extended Systems **2011**, 167-200		9
129	Evaluation of Nonlinear Optical Properties of Large Conjugated Molecular Systems by Long-Range-Corrected Density Functional Theory **2011**, 475-491		
128	MNDO-Like Semiempirical Molecular Orbital Theory and Its Application to Large Systems **2011**, 259-286		18
127	Calculating Molecular Conductance **2011**, 615-648		0
126	Large-Scale Plane-Wave-Based Density Functional Theory: Formalism, Parallelization, and Applications **2011**, 77-116		25
125	Principles of Density Functional Theory: Equilibrium and Nonequilibrium Applications **2011**, 1-44		
124	Interference-induced electron- and hole-conduction asymmetry. *Theoretical Chemistry Accounts*, **2011**, 130, 815-828	1.9	4
123	Atomic-Resolution Kinked Structure of an Alkylporphyrin on Highly Ordered Pyrolytic Graphite. *Journal of Physical Chemistry Letters*, **2011**, 2, 62-6	6.4	21
122	Peptide ligations accelerated by N-terminal aspartate and glutamate residues. *Organic Letters*, **2011**, 13, 4770-3	6.2	19
121	Complexation, computational, magnetic, and structural studies of the Maillard reaction product isomaltol including investigation of an uncommon interaction with copper(II). *Inorganic Chemistry*, **2011**, 50, 1498-505	5.1	16
120	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	3.8	32
119	Quantum entanglement between electronic and vibrational degrees of freedom in molecules. *Journal of Chemical Physics*, **2011**, 135, 244110	3.9	47

118	SIESTA: Properties and Applications **2011**, 367-395		1
117	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	3.9	98
116	Reaction Force and Its Link to Diabatic Analysis: A Unifying Approach to Analyzing Chemical Reactions. *Journal of Physical Chemistry Letters*, **2010**, 1, 2858-2862	6.4	42
115	Accurate and computationally efficient third-nearest-neighbor tight-binding model for large graphene fragments. *Physical Review B*, **2010**, 81,	3.3	6
114	Chemical analysis of the superatom model for sulfur-stabilized gold nanoparticles. *Journal of the American Chemical Society*, **2010**, 132, 8378-84	16.4	80
113	Weak, strong, and coherent regimes of Fröhlich 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, 4219-24	11.5	74
112	Scanning Tunneling Microscopic Observation of Adatom-Mediated Motifs on Gold□thiol Self-Assembled Monolayers at High Coverage. *Journal of Physical Chemistry C*, **2009**, 113, 19601-19608	3.8	26
111	Evanescent-field spectroscopy using structured optical fibers: detection of charge-transfer at the porphyrin-silica interface. *Journal of the American Chemical Society*, **2009**, 131, 2925-33	16.4	24
110	Norbornadiene-Based Molecules for Functionalizing The Si(001) Surface. *Journal of Physical Chemistry C*, **2009**, 113, 16094-16103	3.8	4
109	N-Silylamine Junctions for Molecular Wires to Gold: The Effect of Binding Atom Hybridization on the Electronic Transmission. *Journal of Physical Chemistry C*, **2009**, 113, 20458-20462	3.8	1
108	Penrose-Hameroff orchestrated objective-reduction proposal for human consciousness is not biologically feasible. *Physical Review E*, **2009**, 80, 021912	2.4	48
107	Polymeric di- and discrete trinuclear silver(I) assemblies incorporating gamma-carbon bonded, neutral acetylacetone-imine motifs assembled from racemic and diastereopure N,N'-bis(acetylacetone)cyclohexanediimine units. *Dalton Transactions*, **2009**, 4896-900	4.3	10
106	Control of the site and potential of reduction and oxidation processes in pi-expanded quinoxalinoporphyrins. *Physical Chemistry Chemical Physics*, **2008**, 10, 515-27	3.6	23
105	Control of the orbital delocalization and implications for molecular rectification in the radical anions of porphyrins with coplanar 90 degrees and 180 degrees beta,beta'-fused extensions. *Journal of Physical Chemistry A*, **2008**, 112, 556-70	2.8	27
104	Two-dimensional, phenanthroline-based, extended □conjugated molecules for single-molecule conduction. *Journal of Physics Condensed Matter*, **2008**, 20, 295208	1.8	4
103	Towards a comprehensive model for the electronic and vibrational structure of the Creutz-Taube ion. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2008**, 366, 15-31	3	27
102	The conduction properties of □diaminoalkanes and hydrazine bridging gold electrodes. *Chemical Physics Letters*, **2008**, 454, 284-288	2.5	16
101	Control of the site and potential of reduction and oxidation processes in pi-expanded quinoxalinoporphyrins. *Physical Chemistry Chemical Physics*, **2008**, 10, 268-80	3.6	1

100	Understanding the Chemisorption of 2-Methyl-2-propanethiol on Au(111). *Journal of Physical Chemistry C*, **2007**, 111, 10878-10885	3.8	16
99	Photoinduced electron transfer in a beta,beta'-pyrrolic fused ferrocene-(zinc porphyrin)-fullerene. *Physical Chemistry Chemical Physics*, **2007**, 9, 5260-6	3.6	71
98	Assignment of the Qy 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, 9923-30	3.4	50
97	Formation of gold-methanethiyl self-assembled monolayers. *Journal of the American Chemical Society*, **2007**, 129, 14532-3	16.4	39
96	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	3.8	23
95	Quinoxalino[2,3-b']porphyrins behave as pi-expanded porphyrins upon one-electron reduction: broad control of the degree of delocalization through substitution at the macrocycle periphery. *Journal of Physical Chemistry B*, **2007**, 111, 8762-74	3.4	49
94	Application of the computationally efficient self-consistent-charge density-functional tight-binding method to magnesium-containing molecules. *Journal of Physical Chemistry A*, **2007**, 111, 5743-50	2.8	14
93	Successful a priori modeling of CO adsorption on Pt(111) using periodic hybrid density functional theory. *Journal of the American Chemical Society*, **2007**, 129, 10402-7	16.4	67
92	Chemisorbed and Physisorbed Structures for 1,10-Phenanthroline and Dipyrido[3,2-a:2□3□-c]phenazine on Au(111). *Journal of Physical Chemistry C*, **2007**, 111, 17285-17296	3.8	25
91	The lowest singlet (n,pi*) and (pi,pi*) excited states of the hydrogen-bonded complex between water and pyrazine. *Journal of Physical Chemistry A*, **2007**, 111, 954-62	2.8	22
90	The Manganite□Water Interface. *Journal of Physical Chemistry C*, **2007**, 111, 10427-10437	3.8	12
89	The Green's function density functional tight-binding (gDFTB) method for molecular electronic conduction. *Journal of Physical Chemistry A*, **2007**, 111, 5692-702	2.8	28
88	Examination of the Photophysical Processes of Chlorophyll d Leading to a Clarification of Proposed Uphill Energy Transfer Processes in Cells of Acaryochloris marina□. *Photochemistry and Photobiology*, **2007**, 77, 628-637	3.6	0
87	Simulation of the Au(111)□(22□3) surface reconstruction. *Physical Review B*, **2007**, 75,	3.3	71
86	A priori method for propensity rules for inelastic electron tunneling spectroscopy of single-molecule conduction. *Physical Review B*, **2007**, 75,	3.3	77
85	Pressure-induced spectral changes for the special-pair radical cation of the bacterial photosynthetic reaction center. *Journal of Chemical Physics*, **2007**, 126, 215102	3.9	10
84	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	3.8	68
83	□he molecules and methods of chemical, biochemical, and nanoscale electron transfer□*Chemical Physics*, **2006**, 324, 1-2	2.3	1

82	Physically based molecular device model in a transient circuit simulator. *Chemical Physics*, **2006**, 326, 188-196	2.3	5
81	The symmetry of single-molecule conduction. *Journal of Chemical Physics*, **2006**, 125, 184702	3.9	33
80	Understanding the inelastic electron-tunneling spectra of alkanedithiols on gold. *Journal of Chemical Physics*, **2006**, 124, 94704	3.9	96
79	Density-functional geometry optimization of the 150,000-atom photosystem-I trimer. *Journal of Chemical Physics*, **2006**, 124, 024301	3.9	57
78	FUNCTIONALIZATION OF SEMICONDUCTOR SURFACES BY ORGANIC LAYERS: CONCERTED CYCLOADDITION VERSUS STEPWISE FREE-RADICAL REACTION MECHANISMS **2006**, 333-360		6
77	Adsorption of Benzene on Copper, Silver, and Gold Surfaces. *Journal of Chemical Theory and Computation*, **2006**, 2, 1093-105	6.4	130
76	Molecular origins of conduction channels observed in shot-noise measurements. *Nano Letters*, **2006** , 6, 2431-7	11.5	38
75	Charge delocalization in the special-pair radical cation of mutant reaction centers of Rhodobacter sphaeroides from Stark spectra and nonadiabatic spectral simulations. *Journal of Physical Chemistry B*, **2006**, 110, 18688-702	3.4	35
74	Density functional theory for charge transfer: 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, 15624-32	3.4	260
73	The Nature of the Special-pair Radical Cation Produced by Primary Charge Separation During Photosynthesis **2006**, 109-126		
72	The molecules and methods of chemical, biochemical, and nanoscale electron transfer *Chemical Physics*, **2006**, 326, 1-2	2.3	4
71	Successes and failures of time-dependent density functional theory for the low-lying excited states of chlorophylls. *Molecular Physics*, **2005**, 103, 1057-1065	1.7	32
70	First singlet (n,pi*) excited state of hydrogen-bonded complexes between water and pyrimidine. *Journal of Physical Chemistry A*, **2005**, 109, 1576-86	2.8	13
69	Coexistence of multiple conformations in cysteamine monolayers on Au(111). *Journal of Physical Chemistry B*, **2005**, 109, 15355-67	3.4	75
68	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	3.9	141
67	A priori evaluation of the solvent contribution to the reorganization energy accompanying intramolecular electron transfer: Predicting the nature of the Creutz Taube ion. *Chemical Physics*, **2005**, 319, 39-51	2.3	21
66	Overcoming computational uncertainties to reveal chemical sensitivity in single molecule conduction calculations. *Journal of Chemical Physics*, **2005**, 122, 224502	3.9	25
65	An azanorbornadiene anchor for molecular-level construction on silicon(100). *Nanotechnology*, **2004**, 15, 324-332	3.4	22

64	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, 6615-27	3.9	26
63	Molecular Electronics: From Basic Chemical Principles to Photosynthesis to Steady-State Through-Molecule Conductivity to Computer Architectures. *Australian Journal of Chemistry*, **2004**, 57, 1133	1.2	13
62	Hamiltonian operators including both symmetric and antisymmetric vibrational modes for vibronic coupling and intervalence charge-transfer applications. *Chemical Physics*, **2004**, 299, 79-82	2.3	27
61	Flanged nanotube–electrode junctions. *Nanotechnology*, **2004**, 15, 1226-1232	3.4	5
60	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	2.8	17
59	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, 4132-44	16.4	67
58	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	3.4	40
57	Wavepacket propagation using time-sliced semiclassical initial value methods. *Journal of Chemical Physics*, **2004**, 121, 12208-16	3.9	2
56	Examination of the photophysical processes of chlorophyll d leading to a clarification of proposed uphill energy transfer processes in cells of Acaryochloris marinas. *Photochemistry and Photobiology*, **2003**, 77, 628-37	3.6	24
55	The appropriateness of density-functional theory for the calculation of molecular electronics properties. *Annals of the New York Academy of Sciences*, **2003**, 1006, 235-51	6.5	100
54	Inter-porphyrin coupling: rotation-modulation of inter-ring coupling in a bis-oxo-silicon phthalocyanine dimer. *Chemical Physics Letters*, **2003**, 378, 654-659	2.5	12
53	Singlet and Triplet Valence Excited States of Pyrimidine. *Journal of Physical Chemistry A*, **2003**, 107, 3093-3106	2.8	42
52	Synthesis and physical properties of biquinoxalinyl bridged bis-porphyrins: models for aspects of photosynthetic reaction centres. *Organic and Biomolecular Chemistry*, **2003**, 1, 2777-87	3.9	39
51	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	3.9	11
50	Modelling the bacterial photosynthetic reaction center. V. Assignment of the electronic transition observed at 2200 cm^{-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	3.9	21
49	Modeling the bacterial photosynthetic reaction center. VII. Full simulation of the intervalence hole-transfer absorption spectrum of the special-pair radical cation. *Journal of Chemical Physics*, **2003**, 119, 3262-3277	3.9	36
48	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	3.9	20
47	An atomistic approach to conduction between nanoelectrodes through a single molecule. *Annals of the New York Academy of Sciences*, **2002**, 960, 100-30	6.5	11

46	INDO/S parameters for gold. *International Journal of Quantum Chemistry*, **2002**, 90, 424-438	2.1	19
45	Binding to gold(0): Accurate computational methods with application to AuNH3. *Journal of Chemical Physics*, **2002**, 116, 10277-10286	3.9	52
44	Inter-porphyrin coupling: how strong should it be for molecular electronics applications?. *Journal of Porphyrins and Phthalocyanines*, **2002**, 06, 795-805	1.8	49
43	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, 9299-309	16.4	96
42	Adsorption of Pyridine on the Gold(111) Surface: Implications for Alligator Clips for Molecular Wires. *Journal of Physical Chemistry B*, **2002**, 106, 6740-6747	3.4	101
41	Failure of density-functional theory and time-dependent density-functional theory for large extended systems. *Journal of Chemical Physics*, **2002**, 117, 5543-5549	3.9	287
40	The First Singlet (n,) and () Excited States of the Hydrogen-Bonded Complex between Water and Pyridine. *Journal of Physical Chemistry A*, **2002**, 106, 8769-8778	2.8	62
39	Adsorption of ammonia on the gold (111) surface. *Journal of Chemical Physics*, **2002**, 116, 8981-8987	3.9	103
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8	On the relationship between the classical, semiclassical, and quantum dynamics of a Morse oscillator. *The Journal of Physical Chemistry*, **1988**, 92, 3225-3235		12
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