Jeffrey R Reimers

List of Publications by Citations

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	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	3.9	430
206	Failure of density-functional theory and time-dependent density-functional theory for large extended π systems. *Journal of Chemical Physics*, **2002**, 117, 5543-5549	3.9	287
205	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
204	Formalism, analytical model, and a priori Green's-function-based calculations of the current–voltage characteristics of molecular wires. *Journal of Chemical Physics*, **2000**, 112, 1510-1521	3.9	251
203	The Solvation of Acetonitrile. *Journal of the American Chemical Society*, **1999**, 121, 3730-3744	16.4	216
202	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
201	Adsorption of Benzene on Copper, Silver, and Gold Surfaces. *Journal of Chemical Theory and Computation*, **2006**, 2, 1093-105	6.4	130
200	Molecular dynamics of the A+BC reaction in rare gas solution. *Journal of Chemical Physics*, **1986**, 85, 5625-5643	3.9	126
199	The Low-Lying Excited States of Pyridine. *Journal of Physical Chemistry A*, **2000**, 104, 8389-8408	2.8	105
198	Adsorption of ammonia on the gold (111) surface. *Journal of Chemical Physics*, **2002**, 116, 8981-8987	3.9	103
197	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
196	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
195	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
194	Understanding the inelastic electron-tunneling spectra of alkanedithiols on gold. *Journal of Chemical Physics*, **2006**, 124, 94704	3.9	96
193	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
192	Assignment of the Q-bands of the chlorophylls: coherence loss via Qx - Qy mixing. *Scientific Reports*, **2013**, 3, 2761	4.9	86
191	Solvent effects on the electronic spectra of transition metal complexes. *Chemical Reviews*, **2000**, 100, 775-86	68.1	83

190	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
189	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
188	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
187	Chemical analysis of the superatom model for sulfur-stabilized gold nanoparticles. *Journal of the American Chemical Society*, **2010**, 132, 8378-84	16.4	80
186	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	16.4	78
185	Identifying carbon as the source of visible single-photon emission from hexagonal boron nitride. *Nature Materials*, **2021**, 20, 321-328	27	78
184	A priori method for propensity rules for inelastic electron tunneling spectroscopy of single-molecule conduction. *Physical Review B*, **2007**, 75,	3.3	77
183	Coexistence of multiple conformations in cysteamine monolayers on Au(111). *Journal of Physical Chemistry B*, **2005**, 109, 15355-67	3.4	75
182	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
181	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	2.8	74
180	Competition of van der Waals and chemical forces on gold–sulfur surfaces and nanoparticles. *Nature Reviews Chemistry*, **2017**, 1,	34.6	72
179	Photoinduced electron transfer in a beta,beta'-pyrrolic fused ferrocene-(zinc porphyrin)-fullerene. *Physical Chemistry Chemical Physics*, **2007**, 9, 5260-6	3.6	71
178	Simulation of the Au(111)-(22×√3) surface reconstruction. *Physical Review B*, **2007**, 75,	3.3	71
177	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
176	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
175	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
174	Complex time dependent wave packet technique for thermal equilibrium systems: Electronic spectra. *Journal of Chemical Physics*, **1983**, 79, 4749-4757	3.9	64
173	The First Singlet (n,π*) and (π,π*) Excited States of the Hydrogen-Bonded Complex between Water and Pyridine. *Journal of Physical Chemistry A*, **2002**, 106, 8769-8778	2.8	62

172	Challenges for the Accurate Simulation of Anisotropic Charge Mobilities through Organic Molecular Crystals: The Phase of mer-Tris(8-hydroxyquinolinato)aluminum(III) (Alq3) Crystal. *Journal of Physical Chemistry C*, **2012**, 116, 14826-14836	3.8	61
171	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
170	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
169	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	3.9	58
168	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	2.8	58
167	Density-functional geometry optimization of the 150,000-atom photosystem-I trimer. *Journal of Chemical Physics*, **2006**, 124, 024301	3.9	57
166	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		56
165	Binding to gold(0): Accurate computational methods with application to AuNH3. *Journal of Chemical Physics*, **2002**, 116, 10277-10286	3.9	52
164	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	3.4	52
163	Single-photon emitters in hexagonal boron nitride: a review of progress. *Reports on Progress in Physics*, **2020**, 83, 044501	14.4	52
162	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
161	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
160	Inter-porphyrin coupling: how strong should it be for molecular electronics applications?. *Journal of Porphyrins and Phthalocyanines*, **2002**, 06, 795-805	1.8	49
159	Application of time-dependent density-functional theory to the 3 first excited state of H2. *Journal of Chemical Physics*, **2000**, 112, 527-530	3.9	49
158	Penrose-Hameroff orchestrated objective-reduction proposal for human consciousness is not biologically feasible. *Physical Review E*, **2009**, 80, 021912	2.4	48
157	Modeling the bacterial photosynthetic reaction center. 4. The structural, electrochemical, and hydrogen-bonding properties of 22 mutants of Rhodobacter sphaeroides. *Journal of the American Chemical Society*, **2001**, 123, 8550-63	16.4	48
156	Quantum entanglement between electronic and vibrational degrees of freedom in molecules. *Journal of Chemical Physics*, **2011**, 135, 244110	3.9	47
155	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	3.4	47

154	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
153	Optimization and Chemical Control of Porphyrin-Based Molecular Wires and Switches. *Annals of the New York Academy of Sciences*, **1998**, 852, 1-21	6.5	46
152	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	2.8	45
151	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
150	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
149	Singlet and Triplet Valence Excited States of Pyrimidine. *Journal of Physical Chemistry A*, **2003**, 107, 3093-3106	2.8	42
148	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
147	Dipole Order in Halide Perovskites: Polarization and Rashba Band Splittings. *Journal of Physical Chemistry C*, **2017**, 121, 23045-23054	3.8	39
146	Formation of gold-methanethiyl self-assembled monolayers. *Journal of the American Chemical Society*, **2007**, 129, 14532-3	16.4	39
145	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
144	Molecular origins of conduction channels observed in shot-noise measurements. *Nano Letters*, **2006**, 6, 2431-7	11.5	38
143	The Mechanism of Covalent Bonding. *Journal of Chemical Education*, **1997**, 74, 1494	2.4	36
142	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
141	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
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139	The symmetry of single-molecule conduction. *Journal of Chemical Physics*, **2006**, 125, 184702	3.9	33
138	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
137	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

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135	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
134	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
133	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
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128	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
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126	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
125	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
124	Sulfur ligand mediated electrochemistry of gold surfaces and nanoparticles: What, how, and why. *Current Opinion in Electrochemistry*, **2017**, 1, 7-15	7.2	26
123	Scanning Tunneling Microscopic Observation of Adatom-Mediated Motifs on Gold(111) Thiol Self-Assembled Monolayers at High Coverage. *Journal of Physical Chemistry C*, **2009**, 113, 19601-19608	3.8	26
122	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
121	Modeling the bacterial photosynthetic reaction center 3: interpretation of effects of site-directed mutagenesis on the special-pair midpoint potential. *Biochemistry*, **2000**, 39, 16185-9	3.2	26
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119	Large-Scale Plane-Wave-Based Density Functional Theory: Formalism, Parallelization, and Applications **2011**, 77-116		25

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114	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
113	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
112	The Need for Quantum-Mechanical Treatment of Capacitance and Related Properties of Nanoelectrodes. *Journal of Physical Chemistry B*, **2001**, 105, 8979-8988	3.4	23
111	Electron-vibration entanglement in the Born-Oppenheimer description of chemical reactions and spectroscopy. *Physical Chemistry Chemical Physics*, **2015**, 17, 24666-82	3.6	22
110	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
109	An azanorbornadiene anchor for molecular-level construction on silicon(100). *Nanotechnology*, **2004**, 15, 324-332	3.4	22
108	Nature of the special-pair radical cation in bacterial photosynthesis. *International Journal of Quantum Chemistry*, **2000**, 80, 1224-1243	2.1	22
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103	Modelling the bacterial photosynthetic reaction center. V. Assignment of the electronic transition observed at 2200 cm□□ 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
102	A priori evaluation of the solvent contribution to the reorganization energy accompanying intramolecular electron transfer: Predicting the nature of the Creutz□□aube ion. *Chemical Physics*, **2005**, 319, 39-51	2.3	21
101	Photoluminescence, photophysics, and photochemistry of the VB□□defect in hexagonal boron nitride. *Physical Review B*, **2020**, 102,	3.3	21

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98	Peptide ligations accelerated by N-terminal aspartate and glutamate residues. *Organic Letters*, **2011**, 13, 4770-3	6.2	19
97	INDO/S parameters for gold. *International Journal of Quantum Chemistry*, **2002**, 90, 424-438	2.1	19
96	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
95	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
94	MNDO-Like Semiempirical Molecular Orbital Theory and Its Application to Large Systems **2011**, 259-286		18
93	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	2.8	18
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91	Polymorphism in porphyrin monolayers: the relation between adsorption configuration and molecular conformation. *Physical Chemistry Chemical Physics*, **2013**, 15, 12451-8	3.6	17
90	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
89	The exact eigenfunctions and eigenvalues of a two-dimensional rigid rotor obtained using Gaussian wave packet dynamics. *Journal of Chemical Physics*, **1985**, 83, 511-515	3.9	17
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80	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
79	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
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72	Molecular quantum cellular automata cell design trade-offs: latching vs. power dissipation. *Physical Chemistry Chemical Physics*, **2018**, 20, 17881-17888	3.6	12
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65	Accurate prediction of the properties of materials using the CAM-B3LYP density functional. *Journal of Computational Chemistry*, **2021**, 42, 1486-1497	3.5	11

64	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
63	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
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61	Coupled-Cluster Calculations for Large Molecular and Extended Systems **2011**, 167-200		9
60	Comparison of Soliton Geometry and Charge-Density Wave Structure, and Band Gaps, Between Odd Polyene and Symmetrical Polymethine Cyanine (Brooker) Ions and T - Polyacetylene : Scf and Model Hamiltonian Approaches with Implications For Molecular Wires and Switches. *Molecular Crystals and Liquid Crystals*, **1993**, 234, 51-57		9
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