Sharon Hammes-Schiffer

List of Publications by Year in Descending Order

260 papers	14,425 citations	61 h-index	111 g-index
403 ext. papers	16,177 ext. citations	10.2 avg, IF	7.39 L-index

#	Paper	IF	Citations
260	Electrocatalysis in Alkaline Media and Alkaline Membrane-Based Energy Technologies.. *Chemical Reviews*, **2022**,	68.1	25
259	Cavity-Modulated Proton Transfer Reactions.. *Journal of the American Chemical Society*, **2022**,	16.4	5
258	Theoretical Modeling of Electrochemical Proton-Coupled Electron Transfer.. *Chemical Reviews*, **2022**,	68.1	8
257	Analytical gradients for nuclear-electronic orbital multistate density functional theory: Geometry optimizations and reaction paths.. *Journal of Chemical Physics*, **2022**, 156, 114115	3.9	0
256	Theoretical perspectives on non-Born-Oppenheimer effects in chemistry.. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2022**, 380, 20200377	3	3
255	Quantum Simulations of Vibrational Strong Coupling via Path Integrals.. *Journal of Physical Chemistry Letters*, **2022**, 3890-3895	6.4	2
254	Direct Dynamics with Nuclear-Electronic Orbital Density Functional Theory. *Accounts of Chemical Research*, **2021**, 54, 4131-4141	24.3	7
253	Investigation of the p of the Nucleophilic O2′ of the Hairpin Ribozyme. *Journal of Physical Chemistry B*, **2021**, 125, 11869-11883	3.4	1
252	Simulation of the Chiral Sum Frequency Generation Response of Supramolecular Structures Requires Vibrational Couplings. *Journal of Physical Chemistry B*, **2021**, 125, 12072-12081	3.4	4
251	Artificial Neural Networks as Propagators in Quantum Dynamics. *Journal of Physical Chemistry Letters*, **2021**, 12, 10654-10662	6.4	3
250	Computing Proton-Coupled Redox Potentials of Fluorotyrosines in a Protein Environment. *Journal of Physical Chemistry B*, **2021**, 125, 128-136	3.4	4
249	Glutamate Mediates Proton-Coupled Electron Transfer Between Tyrosines 730 and 731 in Ribonucleotide Reductase. *Journal of the American Chemical Society*, **2021**, 143, 6054-6059	16.4	2
248	Excited State Intramolecular Proton Transfer with Nuclear-Electronic Orbital Ehrenfest Dynamics. *Journal of Physical Chemistry Letters*, **2021**, 12, 3497-3502	6.4	13
247	Multicomponent Unitary Coupled Cluster and Equation-of-Motion for Quantum Computation. *Journal of Chemical Theory and Computation*, **2021**, 17, 3252-3258	6.4	6
246	Mechanistic Insights about Electrochemical Proton-Coupled Electron Transfer Derived from a Vibrational Probe. *Journal of the American Chemical Society*, **2021**, 143, 8381-8390	16.4	7
245	Electrocatalytic Oxidation of Alcohol with Cobalt Triphosphine Complexes. *ACS Catalysis*, **2021**, 11, 6384-6389	13.1	3
244	Theoretical Description of the Primary Proton-Coupled Electron Transfer Reaction in the Cytochrome Complex. *Journal of the American Chemical Society*, **2021**, 143, 715-723	16.4	5

243	Multi PCET in symmetrically substituted benzimidazoles. *Chemical Science*, **2021**, 12, 12667-12675	9.4	2
242	Artificial Neural Networks as Mappings between Proton Potentials, Wave Functions, Densities, and Energy Levels. *Journal of Physical Chemistry Letters*, **2021**, 12, 2206-2212	6.4	7
241	Multicomponent Coupled Cluster Singles and Doubles with Density Fitting: Protonated Water Tetramers with Quantized Protons. *Journal of Physical Chemistry Letters*, **2021**, 12, 1631-1637	6.4	7
240	Transition states, reaction paths, and thermochemistry using the nuclear-electronic orbital analytic Hessian. *Journal of Chemical Physics*, **2021**, 154, 054108	3.9	9
239	Nuclear-electronic orbital methods: Foundations and prospects. *Journal of Chemical Physics*, **2021**, 155, 030901	3.9	3
238	Analytical Gradients for Nuclear-Electronic Orbital Time-Dependent Density Functional Theory: Excited-State Geometry Optimizations and Adiabatic Excitation Energies. *Journal of Chemical Theory and Computation*, **2021**, 17, 5110-5122	6.4	2
237	Hydrogen Evolution Mediated by Cobalt Diimine-Dioxime Complexes: Insights into the Role of the Ligand Acid/Base Functionalities.. *ChemElectroChem*, **2021**, 8, 2671-2679	4.3	3
236	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801	3.9	115
235	Proton-Coupled Defects Impact O-H Bond Dissociation Free Energies on Metal Oxide Surfaces. *Journal of Physical Chemistry Letters*, **2021**, 12, 9761-9767	6.4	4
234	Unraveling Two Pathways for Electrochemical Alcohol and Aldehyde Oxidation on NiOOH. *Journal of the American Chemical Society*, **2020**, 142, 21538-21547	16.4	43
233	Proton-Coupled Electron Transfer from Tyrosine in the Interior of a Protein: Mechanisms and Primary Proton Acceptor. *Journal of the American Chemical Society*, **2020**, 142, 11550-11559	16.4	6
232	Environmental Effects on Guanine-Thymine Mispair Tautomerization Explored with Quantum Mechanical/Molecular Mechanical Free Energy Simulations. *Journal of the American Chemical Society*, **2020**, 142, 11183-11191	16.4	10
231	Confronting Racism in Chemistry Journals. *ACS Applied Nano Materials*, **2020**, 3, 6131-6133	5.6	
230	Confronting Racism in Chemistry Journals. *ACS Applied Polymer Materials*, **2020**, 2, 2496-2498	4.3	
229	Confronting Racism in Chemistry Journals. *Organometallics*, **2020**, 39, 2331-2333	3.8	
228	Proton-coupled electron transfer across benzimidazole bridges in bioinspired proton wires. *Chemical Science*, **2020**, 11, 3820-3828	9.4	17
227	Development of nuclear basis sets for multicomponent quantum chemistry methods. *Journal of Chemical Physics*, **2020**, 152, 244123	3.9	23
226	Update to Our Reader, Reviewer, and Author Communities April 2020. *Energy & Fuels*, **2020**, 34, 5107-5108	4.1	

225	Conformational Motions and Water Networks at the Interface in Ribonucleotide Reductase. *Journal of the American Chemical Society*, **2020**, 142, 13768-13778	16.4	11
224	Modeling voltammetry curves for proton coupled electron transfer: The importance of nuclear quantum effects. *Journal of Chemical Physics*, **2020**, 152, 234108	3.9	6
223	Examining the Mechanism of Phosphite Dehydrogenase with Quantum Mechanical/Molecular Mechanical Free Energy Simulations. *Biochemistry*, **2020**, 59, 943-954	3.2	1
222	Inhomogeneity of Interfacial Electric Fields at Vibrational Probes on Electrode Surfaces. *ACS Central Science*, **2020**, 6, 304-311	16.8	25
221	Multicomponent Orbital-Optimized Perturbation Theory Methods: Approaching Coupled Cluster Accuracy at Lower Cost. *Journal of Physical Chemistry Letters*, **2020**, 11, 1578-1583	6.4	18
220	Multicomponent Quantum Chemistry: Integrating Electronic and Nuclear Quantum Effects via the Nuclear-Electronic Orbital Method. *Chemical Reviews*, **2020**, 120, 4222-4253	68.1	42
219	Update to Our Reader, Reviewer, and Author Communities April 2020. *Organometallics*, **2020**, 39, 1665-1666	3.8	
218	Confronting Racism in Chemistry Journals. *Journal of Chemical Health and Safety*, **2020**, 27, 198-200	1.7	
217	Theory of Electrochemical Proton-Coupled Electron Transfer in Diabatic Vibronic Representation: Application to Proton Discharge on Metal Electrodes in Alkaline Solution. *Journal of Physical Chemistry C*, **2020**, 124, 27309-27322	3.8	10
216	Nuclear-electronic orbital Ehrenfest dynamics. *Journal of Chemical Physics*, **2020**, 153, 224111	3.9	13
215	Mirror-image antiparallel sheets organize water molecules into superstructures of opposite chirality. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 32902-32909	11.5	7
214	Substituent Effects on Photochemistry of Anthracene-Phenol-Pyridine Triads Revealed by Multireference Calculations. *Journal of the American Chemical Society*, **2020**, 142, 487-494	16.4	4
213	Formation of an unusual glutamine tautomer in a blue light using flavin photocycle characterizes the light-adapted state. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 26626-26632	11.5	17
212	Theoretical Study of Shallow Distance Dependence of Proton-Coupled Electron Transfer in Oligoproline Peptides. *Journal of the American Chemical Society*, **2020**, 142, 13795-13804	16.4	1
211	Frequency and Time Domain Nuclear-Electronic Orbital Equation-of-Motion Coupled Cluster Methods: Combination Bands and Electronic-Protonic Double Excitations. *Journal of Physical Chemistry Letters*, **2020**, 11, 6435-6442	6.4	11
210	Nuclear-Electronic Orbital Multistate Density Functional Theory. *Journal of Physical Chemistry Letters*, **2020**, 11, 10106-10113	6.4	9
209	Interfacial Field-Driven Proton-Coupled Electron Transfer at Graphite-Conjugated Organic Acids. *Journal of the American Chemical Society*, **2020**, 142, 20855-20864	16.4	15
208	Excited State Molecular Dynamics of Photoinduced Proton-Coupled Electron Transfer in Anthracene-Phenol-Pyridine Triads. *Journal of Physical Chemistry Letters*, **2020**, 11, 7109-7115	6.4	2

207	Advances and challenges for experiment and theory for multi-electron multi-proton transfer at electrified solid-liquid interfaces. *Physical Chemistry Chemical Physics*, **2020**, 22, 19401-19442	3.6	18
206	Nonequilibrium Dynamics of Proton-Coupled Electron Transfer in Proton Wires: Concerted but Asynchronous Mechanisms. *ACS Central Science*, **2020**, 6, 1594-1601	16.8	12
205	Role of Intact Hydrogen-Bond Networks in Multiproton-Coupled Electron Transfer. *Journal of the American Chemical Society*, **2020**, 142, 21842-21851	16.4	12
204	Real-Time Time-Dependent Nuclear-Electronic Orbital Approach: Dynamics beyond the Born-Oppenheimer Approximation. *Journal of Physical Chemistry Letters*, **2020**, 11, 4052-4058	6.4	27
203	Kinetics of Proton Discharge on Metal Electrodes: Effects of Vibrational Nonadiabaticity and Solvent Dynamics. *Journal of Physical Chemistry Letters*, **2019**, 10, 5312-5317	6.4	17
202	Substrate-to-Product Conversion Facilitates Active Site Loop Opening in Yeast Enolase: A Molecular Dynamics Study. *ACS Catalysis*, **2019**, 9, 8985-8990	13.1	5
201	Strategies for Enhancing the Rate Constant of C-H Bond Cleavage by Concerted Proton-Coupled Electron Transfer. *Journal of the American Chemical Society*, **2019**, 141, 15183-15189	16.4	13
200	Multicomponent density functional theory: Including the density gradient in the electron-proton correlation functional for hydrogen and deuterium. *Journal of Chemical Physics*, **2019**, 151, 124102	3.9	19
199	Theoretical analysis of the inverted region in photoinduced proton-coupled electron transfer. *Faraday Discussions*, **2019**, 216, 363-378	3.6	10
198	Constructing Molecular Orbital Active Spaces for Multireference Calculations of Conjugated Systems. *Journal of Chemical Theory and Computation*, **2019**, 15, 1679-1689	6.4	20
197	Brønsted Acid Scaling Relationships Enable Control Over Product Selectivity from O Reduction with a Mononuclear Cobalt Porphyrin Catalyst. *ACS Central Science*, **2019**, 5, 1024-1034	16.8	32
196	Enhancing the applicability of multicomponent time-dependent density functional theory. *Journal of Chemical Physics*, **2019**, 150, 201101	3.9	25
195	Theory of Proton Discharge on Metal Electrodes: Electronically Adiabatic Model. *Journal of Physical Chemistry C*, **2019**, 123, 12335-12345	3.8	24
194	Modeling Electron Transfer in Diffusive Multidimensional Electrochemical Systems. *Journal of Physical Chemistry C*, **2019**, 123, 13304-13317	3.8	4
193	Multicomponent equation-of-motion coupled cluster singles and doubles: Theory and calculation of excitation energies for positronium hydride. *Journal of Chemical Physics*, **2019**, 150, 161102	3.9	21
192	Concerted proton-electron transfer reactions in the Marcus inverted region. *Science*, **2019**, 364, 471-475	33.3	63
191	Proton-Coupled Electron Transfer Drives Long-Range Proton Translocation in Bioinspired Systems. *Journal of the American Chemical Society*, **2019**, 141, 14057-14061	16.4	22
190	Multicomponent coupled cluster singles and doubles and Brueckner doubles methods: Proton densities and energies. *Journal of Chemical Physics*, **2019**, 151, 074104	3.9	17

189	Diagonal Born-Oppenheimer Corrections within the Nuclear-Electronic Orbital Framework. *Journal of Physical Chemistry Letters*, **2019**, 10, 4639-4643	6.4	4
188	Molecular Vibrational Frequencies with Multiple Quantum Protons within the Nuclear-Electronic Orbital Framework. *Journal of Chemical Theory and Computation*, **2019**, 15, 6840-6849	6.4	8
187	Emerging opportunities and future directions: general discussion. *Faraday Discussions*, **2019**, 221, 564-581	3.6	5
186	Spectroscopic signatures of quantum effects: general discussion. *Faraday Discussions*, **2019**, 221, 322-349	3.6	2
185	Zero-point energy and tunnelling: general discussion. *Faraday Discussions*, **2019**, 221, 478-500	3.6	4
184	Quantum effects in complex systems: summarizing remarks. *Faraday Discussions*, **2019**, 221, 582-588	3.6	8
183	Molecular Vibrational Frequencies within the Nuclear-Electronic Orbital Framework. *Journal of Physical Chemistry Letters*, **2019**, 10, 1167-1172	6.4	17
182	Early Photocycle of Slr1694 Blue-Light Using Flavin Photoreceptor Unraveled through Adiabatic Excited-State Quantum Mechanical/Molecular Mechanical Dynamics. *Journal of the American Chemical Society*, **2019**, 141, 20470-20479	16.4	16
181	Electron-Coupled Double Proton Transfer in the Slr1694 BLUF Photoreceptor: A Multireference Electronic Structure Study. *Journal of Physical Chemistry B*, **2019**, 123, 439-447	3.4	15
180	Proton Discharge on a Gold Electrode from Triethylammonium in Acetonitrile: Theoretical Modeling of Potential-Dependent Kinetic Isotope Effects. *Journal of the American Chemical Society*, **2019**, 141, 1084-1090	16.4	25
179	Multicomponent Coupled Cluster Singles and Doubles Theory within the Nuclear-Electronic Orbital Framework. *Journal of Chemical Theory and Computation*, **2019**, 15, 338-347	6.4	38
178	Fundamental Insights into Proton-Coupled Electron Transfer in Soybean Lipoxygenase from Quantum Mechanical/Molecular Mechanical Free Energy Simulations. *Journal of the American Chemical Society*, **2018**, 140, 3068-3076	16.4	30
177	Multicomponent Time-Dependent Density Functional Theory: Proton and Electron Excitation Energies. *Journal of Physical Chemistry Letters*, **2018**, 9, 1765-1770	6.4	35
176	Exploring the Role of the Third Active Site Metal Ion in DNA Polymerase with QM/MM Free Energy Simulations. *Journal of the American Chemical Society*, **2018**, 140, 8965-8969	16.4	26
175	Kinetic and Mechanistic Characterization of Low-Overpotential, HO-Selective Reduction of O Catalyzed by NO-Ligated Cobalt Complexes. *Journal of the American Chemical Society*, **2018**, 140, 10890-10899	16.4	31
174	Controlling Electrons and Protons through Theory: Molecular Electrocatalysts to Nanoparticles. *Accounts of Chemical Research*, **2018**, 51, 1975-1983	24.3	27
173	Propensity for Proton Relay and Electrostatic Impact of Protein Reorganization in Slr1694 BLUF Photoreceptor. *Journal of the American Chemical Society*, **2018**, 140, 15241-15251	16.4	11
172	Impact of Mutations on the Binding Pocket of Soybean Lipoxygenase: Implications for Proton-Coupled Electron Transfer. *Journal of Physical Chemistry Letters*, **2018**, 9, 6444-6449	6.4	7

171	Controlling Proton-Coupled Electron Transfer in Bioinspired Artificial Photosynthetic Relays. *Journal of the American Chemical Society*, **2018**, 140, 15450-15460	16.4	38
170	Theoretical Study of C-H Bond Cleavage via Concerted Proton-Coupled Electron Transfer in Fluorenyl-Benzoates. *Journal of the American Chemical Society*, **2018**, 140, 15641-15645	16.4	17
169	Alternative forms and transferability of electron-proton correlation functionals in nuclear-electronic orbital density functional theory. *Journal of Chemical Physics*, **2018**, 149, 044110	3.9	23
168	Stability conditions and local minima in multicomponent Hartree-Fock and density functional theory. *Journal of Chemical Physics*, **2018**, 149, 084105	3.9	6
167	A conundrum for density functional theory. *Science*, **2017**, 355, 28-29	33.3	56
166	Tuning the Ultrafast Dynamics of Photoinduced Proton-Coupled Electron Transfer in Energy Conversion Processes. *ACS Energy Letters*, **2017**, 2, 512-519	20.1	34
165	Role of active site conformational changes in photocycle activation of the AppA BLUF photoreceptor. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 1480-1485	11.5	28
164	C ENDOR Spectroscopy of Lipoxygenase-Substrate Complexes Reveals the Structural Basis for C-H Activation by Tunneling. *Journal of the American Chemical Society*, **2017**, 139, 1984-1997	16.4	32
163	Calculation of Positron Binding Energies and Electron-Positron Annihilation Rates for Atomic Systems with the Reduced Explicitly Correlated Hartree-Fock Method in the Nuclear-Electronic Orbital Framework. *Journal of Physical Chemistry A*, **2017**, 121, 515-522	2.8	9
162	Characterization of NiFe oxyhydroxide electrocatalysts by integrated electronic structure calculations and spectroelectrochemistry. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 3050-3055	11.5	119
161	The GlcN6P cofactor plays multiple catalytic roles in the glmS ribozyme. *Nature Chemical Biology*, **2017**, 13, 439-445	11.7	37
160	Enhanced Rigidification within a Double Mutant of Soybean Lipoxygenase Provides Experimental Support for Vibronically Nonadiabatic Proton-Coupled Electron Transfer Models. *ACS Catalysis*, **2017**, 7, 3569-3574	13.1	34
159	Concerted One-Electron Two-Proton Transfer Processes in Models Inspired by the Tyr-His Couple of Photosystem II. *ACS Central Science*, **2017**, 3, 372-380	16.8	67
158	Is the Accuracy of Density Functional Theory for Atomization Energies and Densities in Bonding Regions Correlated?. *Journal of Physical Chemistry Letters*, **2017**, 8, 2076-2081	6.4	51
157	Interplay between Terminal and Bridging Diiron Hydrides in Neutral and Oxidized States. *Organometallics*, **2017**, 36, 2245-2253	3.8	22
156	Communication: Density functional theory embedding with the orthogonality constrained basis set expansion procedure. *Journal of Chemical Physics*, **2017**, 146, 211101	3.9	32
155	Catalysts by Design: The Power of Theory. *Accounts of Chemical Research*, **2017**, 50, 561-566	24.3	51
154	Effects of Active Site Mutations on Specificity of Nucleobase Binding in Human DNA Polymerase *Journal of Physical Chemistry B*, **2017**, 121, 3667-3675	3.4	5

153	Development of a practical multicomponent density functional for electron-proton correlation to produce accurate proton densities. *Journal of Chemical Physics*, **2017**, 147, 114113	3.9	53
152	Theoretical Insights into Proton-Coupled Electron Transfer from a Photoreduced ZnO Nanocrystal to an Organic Radical. *Nano Letters*, **2017**, 17, 5762-5767	11.5	21
151	Role of Proton Diffusion in the Nonexponential Kinetics of Proton-Coupled Electron Transfer from Photoreduced ZnO Nanocrystals. *ACS Nano*, **2017**, 11, 10295-10302	16.7	5
150	Multicomponent Density Functional Theory: Impact of Nuclear Quantum Effects on Proton Affinities and Geometries. *Journal of Physical Chemistry Letters*, **2017**, 8, 3488-3493	6.4	60
149	Computational Insights into Five- versus Six-Coordinate Iron Center in Ferrous Soybean Lipoxygenase. *Journal of Physical Chemistry Letters*, **2016**, 7, 3429-33	6.4	3
148	Quinone 1 e and 2 e/2 H Reduction Potentials: Identification and Analysis of Deviations from Systematic Scaling Relationships. *Journal of the American Chemical Society*, **2016**, 138, 15903-15910	16.4	124
147	Proton-coupled electron transfer reactions: analytical rate constants and case study of kinetic isotope effects in lipoxygenase. *Faraday Discussions*, **2016**, 195, 171-189	3.6	27
146	Mechanism of H2 Production by Models for the [NiFe]-Hydrogenases: Role of Reduced Hydrides. *Journal of the American Chemical Society*, **2016**, 138, 9234-45	16.4	48
145	Electrochemical Electron Transfer and Proton-Coupled Electron Transfer: Effects of Double Layer and Ionic Environment on Solvent Reorganization Energies. *Journal of Chemical Theory and Computation*, **2016**, 12, 2917-25	6.4	24
144	Molecular Dynamics Study of Twister Ribozyme: Role of Mg(2+) Ions and the Hydrogen-Bonding Network in the Active Site. *Biochemistry*, **2016**, 55, 3834-46	3.2	24
143	Hydrogenase Enzymes and Their Synthetic Models: The Role of Metal Hydrides. *Chemical Reviews*, **2016**, 116, 8693-749	68.1	366
142	Effect of Protonation upon Electronic Coupling in the Mixed Valence and Mixed Protonated Complex, [Ni(2,3-pyrazinedithiol)2]. *Inorganic Chemistry*, **2016**, 55, 1433-45	5.1	20
141	Experimental and Computational Mechanistic Studies Guiding the Rational Design of Molecular Electrocatalysts for Production and Oxidation of Hydrogen. *Inorganic Chemistry*, **2016**, 55, 445-60	5.1	61
140	Nickel phlorin intermediate formed by proton-coupled electron transfer in hydrogen evolution mechanism. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 485-92	11.5	101
139	Proton Quantization and Vibrational Relaxation in Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer in a Solvated Phenol-Amine Complex. *Journal of Physical Chemistry B*, **2016**, 120, 2407-17	3.4	31
138	Co(salophen)-Catalyzed Aerobic Oxidation of p-Hydroquinone: Mechanism and Implications for Aerobic Oxidation Catalysis. *Journal of the American Chemical Society*, **2016**, 138, 4186-93	16.4	85
137	Computational Study of Fluorinated Diglyoxime-Iron Complexes: Tuning the Electrocatalytic Pathways for Hydrogen Evolution. *Inorganic Chemistry*, **2016**, 55, 2934-40	5.1	14
136	Multicomponent density functional theory embedding formulation. *Journal of Chemical Physics*, **2016**, 145, 044106	3.9	18

135	Assessing the Potential Effects of Active Site Mg Ions in the glmS Ribozyme-Cofactor Complex. *Journal of Physical Chemistry Letters*, **2016**, 7, 3984-3988	6.4	11
134	Proton-Coupled Electron Transfer: Moving Together and Charging Forward. *Journal of the American Chemical Society*, **2015**, 137, 8860-71	16.4	264
133	Inverse thio effects in the hepatitis delta virus ribozyme reveal that the reaction pathway is controlled by metal ion charge density. *Biochemistry*, **2015**, 54, 2160-75	3.2	40
132	Dependence of Vibronic Coupling on Molecular Geometry and Environment: Bridging Hydrogen Atom Transfer and Electron-Proton Transfer. *Journal of the American Chemical Society*, **2015**, 137, 13545-55	16.4	29
131	How large are nonadiabatic effects in atomic and diatomic systems?. *Journal of Chemical Physics*, **2015**, 143, 124308	3.9	13
130	Quantum treatment of protons with the reduced explicitly correlated Hartree-Fock approach. *Journal of Chemical Physics*, **2015**, 142, 214107	3.9	32
129	Nuclear-electronic orbital reduced explicitly correlated Hartree-Fock approach: Restricted basis sets and open-shell systems. *Journal of Chemical Physics*, **2015**, 142, 214108	3.9	21
128	Relative Binding Free Energies of Adenine and Guanine to Damaged and Undamaged DNA in Human DNA Polymerase Clues for Fidelity and Overall Efficiency. *Journal of the American Chemical Society*, **2015**, 137, 13240-3	16.4	13
127	Role of Solvent Dynamics in Photoinduced Proton-Coupled Electron Transfer in a Phenol-Amine Complex in Solution. *Journal of Physical Chemistry Letters*, **2015**, 6, 3515-20	6.4	25
126	Nonadiabatic rate constants for proton transfer and proton-coupled electron transfer reactions in solution: Effects of quadratic term in the vibronic coupling expansion. *Journal of Chemical Physics*, **2015**, 143, 194101	3.9	19
125	Comparative Molecular Dynamics Studies of Human DNA Polymerase *Journal of Chemical Information and Modeling*, **2015**, 55, 2672-81	6.1	9
124	Role of the active site guanine in the glmS ribozyme self-cleavage mechanism: quantum mechanical/molecular mechanical free energy simulations. *Journal of the American Chemical Society* , **2015**, 137, 784-98	16.4	48
123	Calculation of Electrochemical Reorganization Energies for Redox Molecules at Self-Assembled Monolayer Modified Electrodes. *Journal of Physical Chemistry Letters*, **2015**, 6, 1-5	6.4	11
122	Nonadiabatic dynamics of photoinduced proton-coupled electron transfer in a solvated phenol-amine complex. *Journal of Physical Chemistry B*, **2015**, 119, 2758-68	3.4	41
121	Hydrogen tunneling in enzymes and biomimetic models. *Chemical Reviews*, **2014**, 114, 3466-94	68.1	167
120	Protonation of nickel-iron hydrogenase models proceeds after isomerization at nickel. *Journal of the American Chemical Society*, **2014**, 136, 12385-95	16.4	25
119	Role of pendant proton relays and proton-coupled electron transfer on the hydrogen evolution reaction by nickel hangman porphyrins. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 15001-6	11.5	119
118	Probing Nonadiabaticity in the Proton-Coupled Electron Transfer Reaction Catalyzed by Soybean Lipoxygenase. *Journal of Physical Chemistry Letters*, **2014**, 5, 3274-3278	6.4	35

117	Quantum mechanical/molecular mechanical free energy simulations of the self-cleavage reaction in the hepatitis delta virus ribozyme. *Journal of the American Chemical Society*, **2014**, 136, 1483-96	16.4	57
116	Computational investigation of [FeFe]-hydrogenase models: characterization of singly and doubly protonated intermediates and mechanistic insights. *Inorganic Chemistry*, **2014**, 53, 10301-11	5.1	24
115	Proton-coupled electron transfer in molecular electrocatalysis: theoretical methods and design principles. *Inorganic Chemistry*, **2014**, 53, 6427-43	5.1	137
114	Probing the electrostatics of active site microenvironments along the catalytic cycle for Escherichia coli dihydrofolate reductase. *Journal of the American Chemical Society*, **2014**, 136, 10349-60	16.4	69
113	Electrochemical Solvent Reorganization Energies in the Framework of the Polarizable Continuum Model. *Journal of Chemical Theory and Computation*, **2014**, 10, 2091-102	6.4	32
112	Extremely elevated room-temperature kinetic isotope effects quantify the critical role of barrier width in enzymatic C-H activation. *Journal of the American Chemical Society*, **2014**, 136, 8157-60	16.4	66
111	Escherichia coli dihydrofolate reductase catalyzed proton and hydride transfers: temporal order and the roles of Asp27 and Tyr100. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 18231-6	11.5	44
110	Nonadiabatic dynamics of electron transfer in solution: explicit and implicit solvent treatments that include multiple relaxation time scales. *Journal of Chemical Physics*, **2014**, 140, 034113	3.9	30
109	Beyond the Born-Oppenheimer approximation with quantum Monte Carlo methods. *Physical Review A*, **2014**, 90,	2.6	26
108	Theoretical Analysis of Cobalt Hangman Porphyrins: Ligand Dearomatization and Mechanistic Implications for Hydrogen Evolution. *ACS Catalysis*, **2014**, 4, 4516-4526	13.1	76
107	Reduced explicitly correlated Hartree-Fock approach within the nuclear-electronic orbital framework: theoretical formulation. *Journal of Chemical Physics*, **2013**, 139, 034102	3.9	27
106	Reduced explicitly correlated Hartree-Fock approach within the nuclear-electronic orbital framework: applications to positronic molecular systems. *Journal of Chemical Physics*, **2013**, 139, 034103	3.9	19
105	Calculation of vibrational shifts of nitrile probes in the active site of ketosteroid isomerase upon ligand binding. *Journal of the American Chemical Society*, **2013**, 135, 717-25	16.4	46
104	Catalytic efficiency of enzymes: a theoretical analysis. *Biochemistry*, **2013**, 52, 2012-20	3.2	67
103	Theoretical Design of Molecular Electrocatalysts with Flexible Pendant Amines for Hydrogen Production and Oxidation. *Journal of Physical Chemistry Letters*, **2013**, 4, 542-6	6.4	29
102	pH-dependent reduction potentials and proton-coupled electron transfer mechanisms in hydrogen-producing nickel molecular electrocatalysts. *Inorganic Chemistry*, **2013**, 52, 3643-52	5.1	44
101	Effects of ligand modification and protonation on metal oxime hydrogen evolution electrocatalysts. *Inorganic Chemistry*, **2013**, 52, 6994-9	5.1	76
100	Nonadiabatic dynamics of photoinduced proton-coupled electron transfer: comparison of explicit and implicit solvent simulations. *Journal of Physical Chemistry B*, **2012**, 116, 7695-708	3.4	32

99	Multicomponent density functional theory study of the interplay between electron-electron and electron-proton correlation. *Journal of Chemical Physics*, **2012**, 136, 174114	3.9	30
98	Insights into proton-coupled electron transfer mechanisms of electrocatalytic H2 oxidation and production. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 15663-8	11.5	66
97	Theoretical Analysis of the Sequential Proton-Coupled Electron Transfer Mechanisms for H2 Oxidation and Production Pathways Catalyzed by Nickel Molecular Electrocatalysts. *Journal of Physical Chemistry C*, **2012**, 116, 3171-3180	3.8	49
96	Proton-coupled electron transfer: classification scheme and guide to theoretical methods. *Energy and Environmental Science*, **2012**, 5, 7696	35.4	125
95	Analysis of electron-positron wavefunctions in the nuclear-electronic orbital framework. *Journal of Chemical Physics*, **2012**, 136, 164105	3.9	16
94	Flexibility, diversity, and cooperativity: pillars of enzyme catalysis. *Biochemistry*, **2011**, 50, 10422-30	3.2	190
93	Theoretical analysis of proton relays in electrochemical proton-coupled electron transfer. *Journal of the American Chemical Society*, **2011**, 133, 8282-92	16.4	50
92	Proton-coupled electron transfer versus hydrogen atom transfer: generation of charge-localized diabatic states. *Journal of Physical Chemistry A*, **2011**, 115, 2367-77	2.8	123
91	Derivation of an Electron-Proton Correlation Functional for Multicomponent Density Functional Theory within the Nuclear-Electronic Orbital Approach. *Journal of Chemical Theory and Computation* , **2011**, 7, 2689-93	6.4	31
90	Diabatization Schemes for Generating Charge-Localized Electron-Proton Vibronic States in Proton-Coupled Electron Transfer Systems. *Journal of Chemical Theory and Computation*, **2011**, 7, 2831-41	6.4	34
89	Alternative wavefunction ansatz for including explicit electron-proton correlation in the nuclear-electronic orbital approach. *Journal of Chemical Physics*, **2011**, 135, 054106	3.9	19
88	Theoretical analysis of mechanistic pathways for hydrogen evolution catalyzed by cobaloximes. *Inorganic Chemistry*, **2011**, 50, 11252-62	5.1	183
87	Substituent effects on cobalt diglyoxime catalysts for hydrogen evolution. *Journal of the American Chemical Society*, **2011**, 133, 19036-9	16.4	123
86	Current Theoretical Challenges in Proton-Coupled Electron Transfer: Electron–Proton Nonadiabaticity, Proton Relays, and Ultrafast Dynamics. *Journal of Physical Chemistry Letters*, **2011**, 2, 1410-1416	6.4	53
85	Isotope Effects on the Nonequilibrium Dynamics of Ultrafast Photoinduced Proton-Coupled Electron Transfer Reactions in Solution. *Journal of Physical Chemistry Letters*, **2011**, 2, 36-40	6.4	35
84	When electrons and protons get excited. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 8531-2	11.5	22
83	Multidimensional treatment of stochastic solvent dynamics in photoinduced proton-coupled electron transfer processes: sequential, concerted, and complex branching mechanisms. *Journal of Chemical Physics*, **2011**, 135, 144115	3.9	29
82	Localized Hartree product treatment of multiple protons in the nuclear-electronic orbital framework. *Journal of Chemical Physics*, **2010**, 132, 084110	3.9	20

81	Role of solvent dynamics in ultrafast photoinduced proton-coupled electron transfer reactions in solution. *Journal of Physical Chemistry B*, **2010**, 114, 12319-32	3.4	55
80	Dynamics of Photoinduced Proton-Coupled Electron Transfer at Molecule−Semiconductor Interfaces: A Reduced Density Matrix Approach. *Journal of Physical Chemistry C*, **2010**, 114, 487-496	3.8	23
79	Electrochemical proton-coupled electron transfer of an osmium aquo complex: theoretical analysis of asymmetric tafel plots and transfer coefficients. *Journal of the American Chemical Society*, **2010**, 132, 1234-5	16.4	26
78	Impact of distal mutation on hydrogen transfer interface and substrate conformation in soybean lipoxygenase. *Journal of Physical Chemistry B*, **2010**, 114, 6653-60	3.4	41
77	Nuclear-Electronic Orbital Method within the Fragment Molecular Orbital Approach. *Journal of Physical Chemistry C*, **2010**, 114, 5582-5588	3.8	15
76	Theory of coupled electron and proton transfer reactions. *Chemical Reviews*, **2010**, 110, 6939-60	68.1	565
75	Combining the nuclear-electronic orbital approach with vibronic coupling theory: calculation of the tunneling splitting for malonaldehyde. *Journal of Chemical Physics*, **2009**, 130, 054108	3.9	24
74	Photoinduced homogeneous proton-coupled electron transfer: model study of isotope effects on reaction dynamics. *Journal of Chemical Physics*, **2009**, 131, 154502	3.9	20
73	Electrochemical proton-coupled electron transfer: beyond the golden rule. *Journal of Chemical Physics*, **2009**, 131, 024112	3.9	21
72	Analysis of kinetic isotope effects for proton-coupled electron transfer reactions. *Journal of Physical Chemistry A*, **2009**, 113, 2117-26	2.8	89
71	Driving force dependence of rates for nonadiabatic proton and proton-coupled electron transfer: conditions for inverted region behavior. *Journal of Physical Chemistry B*, **2009**, 113, 14545-8	3.4	28
70	Calculation of the positron annihilation rate in PsH with the positronic extension of the explicitly correlated nuclear-electronic orbital method. *Journal of Physical Chemistry A*, **2009**, 113, 4004-8	2.8	16
69	Theory of proton-coupled electron transfer in energy conversion processes. *Accounts of Chemical Research*, **2009**, 42, 1881-9	24.3	296
68	Properties of the exact universal functional in multicomponent density functional theory. *Journal of Chemical Physics*, **2009**, 131, 124115	3.9	35
67	Free-energy landscape of enzyme catalysis. *Biochemistry*, **2008**, 47, 3317-21	3.2	218
66	Proton-coupled electron transfer in solution, proteins, and electrochemistry. *Journal of Physical Chemistry B*, **2008**, 112, 14108-23	3.4	298
65	Modeling positrons in molecular electronic structure calculations with the nuclear-electronic orbital method. *Journal of Physical Chemistry A*, **2008**, 112, 1346-51	2.8	31
64	Model system-bath Hamiltonian and nonadiabatic rate constants for proton-coupled electron transfer at electrode-solution interfaces. *Journal of Chemical Physics*, **2008**, 128, 244712	3.9	36

63	Inclusion of explicit electron-proton correlation in the nuclear-electronic orbital approach using Gaussian-type geminal functions. *Journal of Chemical Physics*, **2008**, 129, 014101	3.9	66
62	Theoretical Formulation of Nonadiabatic Electrochemical Proton-Coupled Electron Transfer at Metal□Solution Interfaces. *Journal of Physical Chemistry C*, **2008**, 112, 12386-12397	3.8	57
61	Development of electron-proton density functionals for multicomponent density functional theory. *Physical Review Letters*, **2008**, 101, 153001	7.4	79
60	Theoretical Studies of Proton-Coupled Electron Transfer: Models and Concepts Relevant to Bioenergetics. *Coordination Chemistry Reviews*, **2008**, 252, 384-394	23.2	78
59	Buffer-assisted proton-coupled electron transfer in a model rhenium-tyrosine complex. *Journal of the American Chemical Society*, **2007**, 129, 11146-52	16.4	55
58	Proton-coupled electron transfer in soybean lipoxygenase: dynamical behavior and temperature dependence of kinetic isotope effects. *Journal of the American Chemical Society*, **2007**, 129, 187-96	16.4	145
57	Density functional theory treatment of electron correlation in the nuclear-electronic orbital approach. *Journal of Physical Chemistry A*, **2007**, 111, 4522-6	2.8	59
56	Hydrogen tunneling and protein motion in enzyme reactions. *FASEB Journal*, **2007**, 21, A151	0.9	2
55	Hydride transfer catalysed by Escherichia coli and Bacillus subtilis dihydrofolate reductase: coupled motions and distal mutations. *Philosophical Transactions of the Royal Society B: Biological Sciences*, **2006**, 361, 1365-73	5.8	26
54	Calculation of vibronic couplings for phenoxyl/phenol and benzyl/toluene self-exchange reactions: implications for proton-coupled electron transfer mechanisms. *Journal of the American Chemical Society*, **2006**, 128, 16655-63	16.4	121
53	Explicit dynamical electron-proton correlation in the nuclear-electronic orbital framework. *Journal of Physical Chemistry A*, **2006**, 110, 9983-7	2.8	86
52	Relating protein motion to catalysis. *Annual Review of Biochemistry*, **2006**, 75, 519-41	29.1	510
51	Hydrogen tunneling and protein motion in enzyme reactions. *Accounts of Chemical Research*, **2006**, 39, 93-100	24.3	204
50	Quantum and dynamical effects of proton donor-acceptor vibrational motion in nonadiabatic proton-coupled electron transfer reactions. *Journal of Chemical Physics*, **2005**, 122, 14505	3.9	109
49	Impact of nuclear quantum effects on the molecular structure of bihalides and the hydrogen fluoride dimer. *Journal of Physical Chemistry A*, **2005**, 109, 10410-7	2.8	45
48	Investigation of isotope effects with the nuclear-electronic orbital approach. *Journal of Chemical Physics*, **2005**, 123, 64104	3.9	60
47	Alternative formulation of many-body perturbation theory for electron□proton correlation. *Chemical Physics Letters*, **2005**, 404, 394-399	2.5	58
46	Nuclear-electronic orbital nonorthogonal configuration interaction approach. *Journal of Chemical Physics*, **2005**, 123, 134108	3.9	44

45	Analysis of the nuclear-electronic orbital method for model hydrogen transfer systems. *Journal of Chemical Physics*, **2005**, 123, 014303	3.9	24
44	Electron-proton correlation for hydrogen tunneling systems. *Physical Review Letters*, **2004**, 92, 103002	7.4	55
43	Quantum-classical simulation methods for hydrogen transfer in enzymes: a case study of dihydrofolate reductase. *Current Opinion in Structural Biology*, **2004**, 14, 192-201	8.1	63
42	Application of the nuclear–electronic orbital method to hydrogen transfer systems: multiple centers and multiconfigurational wavefunctions. *Chemical Physics*, **2004**, 304, 227-236	2.3	37
41	Proton-coupled electron transfer in soybean lipoxygenase. *Journal of the American Chemical Society* , **2004**, 126, 5763-75	16.4	195
40	Theoretical studies of proton-coupled electron transfer reactions. *Biochimica Et Biophysica Acta - Bioenergetics*, **2004**, 1655, 29-36	4.6	60
39	Proton-coupled electron transfer in a model for tyrosine oxidation in photosystem II. *Journal of the American Chemical Society*, **2003**, 125, 10429-36	16.4	97
38	A perspective on enzyme catalysis. *Science*, **2003**, 301, 1196-202	33.3	977
37	Molecular dynamics with quantum transitions for proton transfer: Quantum treatment of hydrogen and donor–acceptor motions. *Journal of Chemical Physics*, **2003**, 119, 4389-4398	3.9	64
36	Vibrational analysis for the nuclear–electronic orbital method. *Journal of Chemical Physics*, **2003**, 118, 9489-9496	3.9	47
35	Comparison of hydride, hydrogen atom, and proton-coupled electron transfer reactions. *ChemPhysChem*, **2002**, 3, 33-42	3.2	95
34	Impact of enzyme motion on activity. *Biochemistry*, **2002**, 41, 13335-43	3.2	143
33	Multiconfigurational nuclear-electronic orbital approach: Incorporation of nuclear quantum effects in electronic structure calculations. *Journal of Chemical Physics*, **2002**, 117, 4106-4118	3.9	217
32	Network of coupled promoting motions in enzyme catalysis. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 2794-9	11.5	409
31	Theoretical formulation for electron transfer coupled to multiple protons: Application to amidinium–carboxylate interfaces. *Journal of Chemical Physics*, **2001**, 115, 285-296	3.9	21
30	Theoretical perspectives on proton-coupled electron transfer reactions. *Accounts of Chemical Research*, **2001**, 34, 273-81	24.3	377
29	Hybrid approach for including electronic and nuclear quantum effects in molecular dynamics simulations of hydrogen transfer reactions in enzymes. *Journal of Chemical Physics*, **2001**, 114, 6925-6936	3.9	116
28	Theoretical study of electron, proton, and proton-coupled electron transfer in iron bi-imidazoline complexes. *Journal of the American Chemical Society*, **2001**, 123, 3723-33	16.4	70

27	Molecular Dynamics Simulation of Proton-Coupled Electron Transfer in Solution. *Journal of Physical Chemistry B*, **2001**, 105, 10435-10445	3.4	16
26	Derivation of rate expressions for nonadiabatic proton-coupled electron transfer reactions in solution. *Journal of Chemical Physics*, **2000**, 113, 2385-2396	3.9	172
25	Fourier grid Hamiltonian multiconfigurational self-consistent-field: A method to calculate multidimensional hydrogen vibrational wavefunctions. *Journal of Chemical Physics*, **2000**, 113, 5214	3.9	88
24	Computational Studies of the Mechanism for Proton and Hydride Transfer in Liver Alcohol Dehydrogenase. *Journal of the American Chemical Society*, **2000**, 122, 4803-4812	16.4	154
23	Combining Electronic Structure Methods with the Calculation of Hydrogen Vibrational Wavefunctions:Application to Hydride Transfer in Liver Alcohol Dehydrogenase. *Journal of Physical Chemistry B*, **2000**, 104, 8884-8894	3.4	50
22	Reaction Path Hamiltonian Analysis of Dynamical Solvent Effects for a Claisen Rearrangement and a Diels-Alder Reaction. *Journal of Physical Chemistry A*, **2000**, 104, 8058-8066	2.8	34
21	Model Proton-Coupled Electron Transfer Reactions in Solution: Predictions of Rates, Mechanisms, and Kinetic Isotope Effects. *Journal of Physical Chemistry A*, **2000**, 104, 9370-9384	2.8	96
20	Multistate continuum theory for multiple charge transfer reactions in solution. *Journal of Chemical Physics*, **1999**, 111, 4672-4687	3.9	123
19	Comparison of surface hopping and mean field approaches for model proton transfer reactions. *Journal of Chemical Physics*, **1999**, 110, 11166-11175	3.9	119
18	Theoretical Study of Photoinduced Proton-Coupled Electron Transfer through Asymmetric Salt Bridges. *Journal of the American Chemical Society*, **1999**, 121, 10598-10607	16.4	40
17	Improvement of the Internal Consistency in Trajectory Surface Hopping. *Journal of Physical Chemistry A*, **1999**, 103, 9399-9407	2.8	154
16	Solvation and Hydrogen-Bonding Effects on Proton Wires. *Journal of Physical Chemistry A*, **1999**, 103, 2891-2898	2.8	69
15	Effects of Model Protein Environments on the Dynamics of Proton Wires. *Israel Journal of Chemistry* , **1999**, 39, 397-407	3.4	15
14	Proton transport along water chains and NADH hydride transfer in solution. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1998**, 102, 533-543		6
13	Time-dependent self-consistent-field dynamics based on a reaction path Hamiltonian. II. Numerical tests. *Journal of Chemical Physics*, **1998**, 109, 7051-7063	3.9	6
12	Time-dependent self-consistent-field dynamics based on a reaction path Hamiltonian. I. Theory. *Journal of Chemical Physics*, **1998**, 108, 7085-7099	3.9	13
11	Mixed Quantum/Classical Dynamics of Hydrogen Transfer Reactions. *Journal of Physical Chemistry A* , **1998**, 102, 10443-10454	2.8	76
10	Proton transport along water chains in an electric field. *Journal of Chemical Physics*, **1998**, 108, 6799-6808	3.9	43

9	Nonadiabatic dynamics for processes involving multiple avoided curve crossings: Double proton transfer and proton-coupled electron transfer reactions. *Journal of Chemical Physics*, **1997**, 107, 8933-8939	3.9	70
8	An analytical derivation of MC-SCF vibrational wave functions for the quantum dynamical simulation of multiple proton transfer reactions: Initial application to protonated water chains. *Journal of Chemical Physics*, **1997**, 107, 363-374	3.9	40
7	Proton-coupled electron transfer reactions in solution: Molecular dynamics with quantum transitions for model systems. *Journal of Chemical Physics*, **1997**, 106, 8442-8454	3.9	70
6	Excited state dynamics with nonadiabatic transitions for model photoinduced proton-coupled electron transfer reactions. *Journal of Chemical Physics*, **1997**, 107, 5727-5739	3.9	40
5	Development of a Potential Surface for Simulation of Proton and Hydride Transfer Reactions in Solution: Application to NADH Hydride Transfer. *Journal of Physical Chemistry A*, **1997**, 101, 3977-3989	2.8	16
4	Proton-Coupled Electron Transfer: Theoretical Formulation and Applications479-502		1
3	Dihydrofolate Reductase: Hydrogen Tunneling and Protein Motion1439-1454		1
2	Understanding Hydrogen Atom and Hydride Transfer Processes during Electrochemical Alcohol and Aldehyde Oxidation. *ACS Catalysis*,15110-15124	13.1	6
1	Integration of theory and experiment in the modelling of heterogeneous electrocatalysis. *Nature Energy*,	62.3	14