Sharon Hammes-Schiffer

List of Publications by Citations

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	A perspective on enzyme catalysis. *Science*, **2003**, 301, 1196-202	33.3	977
259	Theory of coupled electron and proton transfer reactions. *Chemical Reviews*, **2010**, 110, 6939-60	68.1	565
258	Relating protein motion to catalysis. *Annual Review of Biochemistry*, **2006**, 75, 519-41	29.1	510
257	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
256	Theoretical perspectives on proton-coupled electron transfer reactions. *Accounts of Chemical Research*, **2001**, 34, 273-81	24.3	377
255	Hydrogenase Enzymes and Their Synthetic Models: The Role of Metal Hydrides. *Chemical Reviews*, **2016**, 116, 8693-749	68.1	366
254	Proton-coupled electron transfer in solution, proteins, and electrochemistry. *Journal of Physical Chemistry B*, **2008**, 112, 14108-23	3.4	298
253	Theory of proton-coupled electron transfer in energy conversion processes. *Accounts of Chemical Research*, **2009**, 42, 1881-9	24.3	296
252	Proton-Coupled Electron Transfer: Moving Together and Charging Forward. *Journal of the American Chemical Society*, **2015**, 137, 8860-71	16.4	264
251	Free-energy landscape of enzyme catalysis. *Biochemistry*, **2008**, 47, 3317-21	3.2	218
250	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
249	Hydrogen tunneling and protein motion in enzyme reactions. *Accounts of Chemical Research*, **2006**, 39, 93-100	24.3	204
248	Proton-coupled electron transfer in soybean lipoxygenase. *Journal of the American Chemical Society* , **2004**, 126, 5763-75	16.4	195
247	Flexibility, diversity, and cooperativity: pillars of enzyme catalysis. *Biochemistry*, **2011**, 50, 10422-30	3.2	190
246	Theoretical analysis of mechanistic pathways for hydrogen evolution catalyzed by cobaloximes. *Inorganic Chemistry*, **2011**, 50, 11252-62	5.1	183
245	Derivation of rate expressions for nonadiabatic proton-coupled electron transfer reactions in solution. *Journal of Chemical Physics*, **2000**, 113, 2385-2396	3.9	172
244	Hydrogen tunneling in enzymes and biomimetic models. *Chemical Reviews*, **2014**, 114, 3466-94	68.1	167

243	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
242	Improvement of the Internal Consistency in Trajectory Surface Hopping. *Journal of Physical Chemistry A*, **1999**, 103, 9399-9407	2.8	154
241	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
240	Impact of enzyme motion on activity. *Biochemistry*, **2002**, 41, 13335-43	3.2	143
239	Proton-coupled electron transfer in molecular electrocatalysis: theoretical methods and design principles. *Inorganic Chemistry*, **2014**, 53, 6427-43	5.1	137
238	Proton-coupled electron transfer: classification scheme and guide to theoretical methods. *Energy and Environmental Science*, **2012**, 5, 7696	35.4	125
237	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
236	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
235	Substituent effects on cobalt diglyoxime catalysts for hydrogen evolution. *Journal of the American Chemical Society*, **2011**, 133, 19036-9	16.4	123
234	Multistate continuum theory for multiple charge transfer reactions in solution. *Journal of Chemical Physics*, **1999**, 111, 4672-4687	3.9	123
233	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
232	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
231	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
230	Comparison of surface hopping and mean field approaches for model proton transfer reactions. *Journal of Chemical Physics*, **1999**, 110, 11166-11175	3.9	119
229	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
228	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
227	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
226	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

225	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
224	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
223	Comparison of hydride, hydrogen atom, and proton-coupled electron transfer reactions. *ChemPhysChem*, **2002**, 3, 33-42	3.2	95
222	Analysis of kinetic isotope effects for proton-coupled electron transfer reactions. *Journal of Physical Chemistry A*, **2009**, 113, 2117-26	2.8	89
221	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
220	Explicit dynamical electron-proton correlation in the nuclear-electronic orbital framework. *Journal of Physical Chemistry A*, **2006**, 110, 9983-7	2.8	86
219	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
218	Development of electron-proton density functionals for multicomponent density functional theory. *Physical Review Letters*, **2008**, 101, 153001	7.4	79
217	Theoretical Studies of Proton-Coupled Electron Transfer: Models and Concepts Relevant to Bioenergetics. *Coordination Chemistry Reviews*, **2008**, 252, 384-394	23.2	78
216	Theoretical Analysis of Cobalt Hangman Porphyrins: Ligand Dearomatization and Mechanistic Implications for Hydrogen Evolution. *ACS Catalysis*, **2014**, 4, 4516-4526	13.1	76
215	Effects of ligand modification and protonation on metal oxime hydrogen evolution electrocatalysts. *Inorganic Chemistry*, **2013**, 52, 6994-9	5.1	76
214	Mixed Quantum/Classical Dynamics of Hydrogen Transfer Reactions. *Journal of Physical Chemistry A* , **1998**, 102, 10443-10454	2.8	76
213	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
212	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
211	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
210	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
209	Solvation and Hydrogen-Bonding Effects on Proton Wires. *Journal of Physical Chemistry A*, **1999**, 103, 2891-2898	2.8	69
208	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

207	Catalytic efficiency of enzymes: a theoretical analysis. *Biochemistry*, **2013**, 52, 2012-20	3.2	67
206	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
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204	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
203	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
202	Concerted proton-electron transfer reactions in the Marcus inverted region. *Science*, **2019**, 364, 471-475	33.3	63
201	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
200	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
199	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
198	Investigation of isotope effects with the nuclear-electronic orbital approach. *Journal of Chemical Physics*, **2005**, 123, 64104	3.9	60
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196	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
195	Alternative formulation of many-body perturbation theory for electron–proton correlation. *Chemical Physics Letters*, **2005**, 404, 394-399	2.5	58
194	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
193	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
192	A conundrum for density functional theory. *Science*, **2017**, 355, 28-29	33.3	56
191	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
190	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

189	Electron-proton correlation for hydrogen tunneling systems. *Physical Review Letters*, **2004**, 92, 103002	7.4	55
188	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
187	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
186	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
185	Catalysts by Design: The Power of Theory. *Accounts of Chemical Research*, **2017**, 50, 561-566	24.3	51
184	Theoretical analysis of proton relays in electrochemical proton-coupled electron transfer. *Journal of the American Chemical Society*, **2011**, 133, 8282-92	16.4	50
183	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
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181	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
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179	Vibrational analysis for the nuclear–electronic orbital method. *Journal of Chemical Physics*, **2003**, 118, 9489-9496	3.9	47
178	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
177	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
176	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
175	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
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170	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
169	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
168	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
167	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
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165	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
164	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
163	Controlling Proton-Coupled Electron Transfer in Bioinspired Artificial Photosynthetic Relays. *Journal of the American Chemical Society*, **2018**, 140, 15450-15460	16.4	38
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161	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
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159	Multicomponent Time-Dependent Density Functional Theory: Proton and Electron Excitation Energies. *Journal of Physical Chemistry Letters*, **2018**, 9, 1765-1770	6.4	35
158	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
157	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
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153	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
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151	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
150	Communication: Density functional theory embedding with the orthogonality constrained basis set expansion procedure. *Journal of Chemical Physics*, **2017**, 146, 211101	3.9	32
149	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
148	Quantum treatment of protons with the reduced explicitly correlated Hartree-Fock approach. *Journal of Chemical Physics*, **2015**, 142, 214107	3.9	32
147	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
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144	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
143	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
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140	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
139	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
138	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
137	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
136	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

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133	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
132	Controlling Electrons and Protons through Theory: Molecular Electrocatalysts to Nanoparticles. *Accounts of Chemical Research*, **2018**, 51, 1975-1983	24.3	27
131	Reduced explicitly correlated Hartree-Fock approach within the nuclear-electronic orbital framework: theoretical formulation. *Journal of Chemical Physics*, **2013**, 139, 034102	3.9	27
130	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
129	Exploring the Role of the Third Active Site Metal Ion in DNA Polymerase β with QM/MM Free Energy Simulations. *Journal of the American Chemical Society*, **2018**, 140, 8965-8969	16.4	26
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123	Inhomogeneity of Interfacial Electric Fields at Vibrational Probes on Electrode Surfaces. *ACS Central Science*, **2020**, 6, 304-311	16.8	25
122	Protonation of nickel-iron hydrogenase models proceeds after isomerization at nickel. *Journal of the American Chemical Society*, **2014**, 136, 12385-95	16.4	25
121	Electrocatalysis in Alkaline Media and Alkaline Membrane-Based Energy Technologies.. *Chemical Reviews*, **2022**,	68.1	25
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117	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
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112	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
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