William H Green

List of Publications by Year in Descending Order

282	12,637	62	97
papers	citations	h-index	g-index
306	14,800	4.7	6.9
ext. papers	ext. citations	avg, IF	L-index

#	Paper	IF	Citations
282	Group Contribution and Machine Learning Approaches to Predict Abraham Solute Parameters, Solvation Free Energy, and Solvation Enthalpy.. *Journal of Chemical Information and Modeling*, **2022**,	6.1	6
281	Detailed Reaction Mechanism for 350–400 °C Pyrolysis of an Alkane, Aromatic, and Long-Chain Alkylaromatic Mixture. *Energy & Fuels*, **2022**, 36, 1635-1646	4.1	1
280	Multi-fidelity prediction of molecular optical peaks with deep learning.. *Chemical Science*, **2022**, 13, 1152-1162	9.1	2
279	Detailed Kinetic Modeling for the Pyrolysis of a Jet A Surrogate. *Energy & Fuels*, **2022**, 36, 1304-1315	4.1	2
278	Automatically generated model for light alkene combustion. *Combustion and Flame*, **2022**, 241, 112080	5.3	4
277	Chemistry of Simple Organic Peroxy Radicals under Atmospheric through Combustion Conditions: Role of Temperature, Pressure, and NO Level. *Journal of Physical Chemistry A*, **2021**, 125, 10303-10314	2.8	0
276	Effects of surface species and homogeneous reactions on rates and selectivity in ethane oxidation on oxide catalysts. *AICHE Journal*, **2021**, 67, e17483	3.6	0
275	Reaction Mechanism Generator v3.0: Advances in Automatic Mechanism Generation. *Journal of Chemical Information and Modeling*, **2021**, 61, 2686-2696	6.1	32
274	Predicting Infrared Spectra with Message Passing Neural Networks. *Journal of Chemical Information and Modeling*, **2021**, 61, 2594-2609	6.1	4
273	Oxidation and pyrolysis of methyl propyl ether. *International Journal of Chemical Kinetics*, **2021**, 53, 915-938	1.4	3
272	Kinetic Modeling of API Oxidation: (1) The AIBN/HO/CHOH Radical "Soup". *Molecular Pharmaceutics* , **2021**, 18, 3037-3049	5.6	5
271	Predicting polycyclic aromatic hydrocarbon formation with an automatically generated mechanism for acetylene pyrolysis. *International Journal of Chemical Kinetics*, **2021**, 53, 27-42	1.4	6
270	Transfer learning for solvation free energies: From quantum chemistry to experiments. *Chemical Engineering Journal*, **2021**, 418, 129307	14.7	16
269	Screening for New Pathways in Atmospheric Oxidation Chemistry with Automated Mechanism Generation. *Journal of Physical Chemistry A*, **2021**, 125, 6772-6788	2.8	2
268	EHreact: Extended Hasse Diagrams for the Extraction and Scoring of Enzymatic Reaction Templates. *Journal of Chemical Information and Modeling*, **2021**, 61, 4949-4961	6.1	1
267	CH polycyclic aromatic hydrocarbon formation by acetylene addition to naphthalenyl radicals observed. *Physical Chemistry Chemical Physics*, **2021**, 23, 14325-14339	3.6	2
266	Learning to Optimize Molecular Geometries Using Reinforcement Learning. *Journal of Chemical Theory and Computation*, **2021**, 17, 818-825	6.4	9

265	Temperature-dependent vapor□liquid equilibria and solvation free energy estimation from minimal data. *AICHE Journal*, **2020**, 66, e16976	3.6	5
264	Reactants, products, and transition states of elementary chemical reactions based on quantum chemistry. *Scientific Data*, **2020**, 7, 137	8.2	27
263	Deep Learning of Activation Energies. *Journal of Physical Chemistry Letters*, **2020**, 11, 2992-2997	6.4	37
262	Intramolecular 13C isotope distributions of butane from natural gases. *Chemical Geology*, **2020**, 541, 119571	4.2	8
261	Current and Future Roles of Artificial Intelligence in Medicinal Chemistry Synthesis. *Journal of Medicinal Chemistry*, **2020**, 63, 8667-8682	8.3	53
260	Evaluating Scalable Uncertainty Estimation Methods for Deep Learning-Based Molecular Property Prediction. *Journal of Chemical Information and Modeling*, **2020**, 60, 2697-2717	6.1	49
259	Direct Measurement of Radical-Catalyzed CH Formation from Acetylene and Validation of Theoretical Rate Coefficients for CH + CH and CH + CH Reactions. *Journal of Physical Chemistry A*, **2020**, 124, 2871-2884	2.8	5
258	Recharging systems and business operations to improve the economics of electrified taxi fleets. *Sustainable Cities and Society*, **2020**, 57, 102119	10.1	5
257	Transition to electric vehicles in China: Implications for private motorization rate and battery market. *Energy Policy*, **2020**, 144, 111654	7.2	19
256	Artificial Intelligence for Computer-Aided Synthesis In Flow: Analysis and Selection of Reaction Components. *Frontiers in Chemical Engineering*, **2020**, 2,	1	7
255	Thermochemistry Prediction and Automatic Reaction Mechanism Generation for Oxygenated Sulfur Systems: A Case Study of Dimethyl Sulfide Oxidation. *ChemSystemsChem*, **2020**, 2, e1900051	3.1	5
254	Direct Kinetics and Product Measurement of Phenyl Radical + Ethylene. *Journal of Physical Chemistry A*, **2020**, 124, 2352-2365	2.8	2
253	Uncertainty analysis of correlated parameters in automated reaction mechanism generation. *International Journal of Chemical Kinetics*, **2020**, 52, 266-282	1.4	9
252	Formation of Two-Ring Aromatics in Hexylbenzene Pyrolysis. *Energy & Fuels*, **2020**, 34, 1365-1377	4.1	2
251	Combining retrosynthesis and mixed-integer optimization for minimizing the chemical inventory needed to realize a WHO essential medicines list. *Reaction Chemistry and Engineering*, **2020**, 5, 367-376	4.9	3
250	Revealing the critical role of radical-involved pathways in high temperature cyclopentanone pyrolysis. *Combustion and Flame*, **2020**, 216, 280-292	5.3	8
249	Generating transition states of isomerization reactions with deep learning. *Physical Chemistry Chemical Physics*, **2020**, 22, 23618-23626	3.6	12
248	Moving from postdictive to predictive kinetics in reaction engineering. *AICHE Journal*, **2020**, 66, e17059	3.6	11

247	Pressure-dependent kinetics of peroxy radicals formed in isobutanol combustion. *Physical Chemistry Chemical Physics*, **2020**, 22, 19802-19815	3.6	3
246	Theoretical study on the HACA chemistry of naphthalenyl radicals and acetylene: The formation of C12H8, C14H8, and C14H10 species. *International Journal of Chemical Kinetics*, **2020**, 52, 752-768	1.4	6
245	Iterative experimental design based on active machine learning reduces the experimental burden associated with reaction screening. *Reaction Chemistry and Engineering*, **2020**, 5, 1963-1972	4.9	19
244	Regio-selectivity prediction with a machine-learned reaction representation and on-the-fly quantum mechanical descriptors. *Chemical Science*, **2020**, 12, 2198-2208	9.4	21
243	Detailed kinetic model for hexyl sulfide pyrolysis and its desulfurization by supercritical water. *Physical Chemistry Chemical Physics*, **2019**, 21, 10311-10324	3.6	9
242	Reaction Pathways, Thermodynamics, and Kinetics of Cyclopentanone Oxidation Intermediates: A Theoretical Approach. *Journal of Physical Chemistry A*, **2019**, 123, 9644-9657	2.8	4
241	A graph-convolutional neural network model for the prediction of chemical reactivity. *Chemical Science*, **2019**, 10, 370-377	9.4	237
240	Modeling of aromatics formation in fuel-rich methane oxy-combustion with an automatically generated pressure-dependent mechanism. *Physical Chemistry Chemical Physics*, **2019**, 21, 813-832	3.6	23
239	Learning only buys you so much: Practical limits on battery price reduction. *Applied Energy*, **2019**, 239, 218-224	10.7	54
238	Numerical investigation of strained extinction at engine-relevant pressures: Pressure dependence and sensitivity to chemical and physical parameters for methane-based flames. *Combustion and Flame*, **2019**, 202, 318-333	5.3	10
237	Accurate Thermochemistry with Small Data Sets: A Bond Additivity Correction and Transfer Learning Approach. *Journal of Physical Chemistry A*, **2019**, 123, 5826-5835	2.8	40
236	Automatic generation of reaction mechanisms. *Computer Aided Chemical Engineering*, **2019**, 259-294	0.6	8
235	RDChiral: An RDKit Wrapper for Handling Stereochemistry in Retrosynthetic Template Extraction and Application. *Journal of Chemical Information and Modeling*, **2019**, 59, 2529-2537	6.1	43
234	Large Intermediates in Hydrazine Decomposition: A Theoretical Study of the NH and NH Potential Energy Surfaces. *Journal of Physical Chemistry A*, **2019**, 123, 4679-4692	2.8	4
233	H2 Generation from H2O and H2S through an Iodine Cycle. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 7369-7377	8.3	4
232	Thermochemistry and Kinetics of Intermolecular Addition of Radicals to Toluene and Alkylaromatics. *Journal of Physical Chemistry A*, **2019**, 123, 3176-3184	2.8	4
231	Cooperative Co /Co Sites Stabilized by a Perovskite Matrix Enable Selective C-O and C-C bond Hydrogenolysis of Oxygenated Arenes. *ChemSusChem*, **2019**, 12, 2171-2175	8.3	9
230	Computer-generated isotope model achieves experimental accuracy of filiation for position-specific isotope analysis. *Chemical Geology*, **2019**, 514, 1-9	4.2	5

229	Thermochemistry and Group Additivity Values for Fused Two-Ring Species and Radicals. *Journal of Physical Chemistry A*, **2019**, 123, 3418-3428	2.8	9
228	Capturing aromaticity in automatic mechanism generation software. *Proceedings of the Combustion Institute*, **2019**, 37, 575-581	5.9	8
227	Automated computational thermochemistry for butane oxidation: A prelude to predictive automated combustion kinetics. *Proceedings of the Combustion Institute*, **2019**, 37, 363-371	5.9	37
226	An experimental, theoretical, and modeling study of the ignition behavior of cyclopentanone. *Proceedings of the Combustion Institute*, **2019**, 37, 657-665	5.9	13
225	A robotic platform for flow synthesis of organic compounds informed by AI planning. *Science*, **2019**, 365,	33.3	271
224	Automated chemical resonance generation and structure filtration for kinetic modeling. *International Journal of Chemical Kinetics*, **2019**, 51, 760-776	1.4	4
223	Kinetic analysis and reaction mechanism for anisole conversion over zirconia-supported molybdenum oxide. *Journal of Catalysis*, **2019**, 376, 248-257	7.3	25
222	Scalability strategies for automated reaction mechanism generation. *Computers and Chemical Engineering*, **2019**, 131, 106578	4	3
221	Correct Symmetry Treatment for X + X Reactions Prevents Large Errors in Predicted Isotope Enrichment. *Journal of Physical Chemistry A*, **2019**, 123, 2320-2324	2.8	3
220	Self-Evolving Machine: A Continuously Improving Model for Molecular Thermochemistry. *Journal of Physical Chemistry A*, **2019**, 123, 2142-2152	2.8	27
219	From benzene to naphthalene: direct measurement of reactions and intermediates of phenyl radicals and acetylene. *Physical Chemistry Chemical Physics*, **2019**, 21, 22248-22258	3.6	10
218	An apparatus-independent extinction strain rate in counterflow flames. *Proceedings of the Combustion Institute*, **2019**, 37, 1979-1987	5.9	5
217	Detailed Experimental and Kinetic Modeling Study of Cyclopentadiene Pyrolysis in the Presence of Ethene. *Energy & Fuels*, **2018**, 32, 3920-3934	4.1	15
216	Chemistry of Alkylaromatics Reconsidered. *Energy & Fuels*, **2018**, 32, 5489-5500	4.1	10
215	Perspective on Mechanism Development and Structure-Activity Relationships for Gas-Phase Atmospheric Chemistry. *International Journal of Chemical Kinetics*, **2018**, 50, 435-469	1.4	34
214	Phenyl radical + propene: a prototypical reaction surface for aromatic-catalyzed 1,2-hydrogen-migration and subsequent resonance-stabilized radical formation. *Physical Chemistry Chemical Physics*, **2018**, 20, 13191-13214	3.6	14
213	Automated Reaction Mechanism Generation Including Nitrogen as a Heteroatom. *International Journal of Chemical Kinetics*, **2018**, 50, 243-258	1.4	14
212	An Extended Group Additivity Method for Polycyclic Thermochemistry Estimation. *International Journal of Chemical Kinetics*, **2018**, 50, 294-303	1.4	26

211	Unimolecular Reaction Pathways of a -Ketohydroperoxide from Combined Application of Automated Reaction Discovery Methods. *Journal of the American Chemical Society*, **2018**, 140, 1035-1048	16.4	50
210	SCScore: Synthetic Complexity Learned from a Reaction Corpus. *Journal of Chemical Information and Modeling*, **2018**, 58, 252-261	6.1	90
209	Modeling study of the anti-knock tendency of substituted phenols as additives: an application of the reaction mechanism generator (RMG). *Physical Chemistry Chemical Physics*, **2018**, 20, 10637-10649	3.6	25
208	Machine Learning in Computer-Aided Synthesis Planning. *Accounts of Chemical Research*, **2018**, 51, 1281-1289	24.3	255
207	An experimental and modeling study of vacuum residue upgrading in supercritical water. *AICHE Journal*, **2018**, 64, 1732-1743	3.6	20
206	Order out of Randomness: Self-Organization Processes in Astrophysics. *Space Science Reviews*, **2018**, 214, 1	7.5	25
205	Pressure dependent kinetic analysis of pathways to naphthalene from cyclopentadienyl recombination. *Combustion and Flame*, **2018**, 187, 247-256	5.3	42
204	A combined photoionization time-of-flight mass spectrometry and laser absorption spectrometry flash photolysis apparatus for simultaneous determination of reaction rates and product branching. *Review of Scientific Instruments*, **2018**, 89, 074102	1.7	11
203	Modeling Study of High Temperature Pyrolysis of Natural Gas. *Industrial & Engineering Chemistry Research*, **2018**, 57, 7404-7420	3.9	9
202	Using Machine Learning To Predict Suitable Conditions for Organic Reactions. *ACS Central Science*, **2018**, 4, 1465-1476	16.8	131
201	Incorporating Multiple Uncertainties into Projections of Chinese Private Car Sales and Stock. *Transportation Research Record*, **2018**, 2672, 182-193	1.7	9
200	Kinetics of Intramolecular Phenyl Migration and Fused Ring Formation in Hexylbenzene Radicals. *Journal of Physical Chemistry A*, **2018**, 122, 9778-9791	2.8	3
199	A Fragment-Based Mechanistic Kinetic Modeling Framework for Complex Systems. *Industrial & Engineering Chemistry Research*, **2018**, 57, 14022-14030	3.9	6
198	Experimental and modeling study of the mutual oxidation of N-pentane and nitrogen dioxide at low and high temperatures in a jet stirred reactor. *Energy*, **2018**, 165, 727-738	7.9	29
197	Ember: An open-source, transient solver for 1D reacting flow using large kinetic models, applied to strained extinction. *Combustion and Flame*, **2018**, 195, 105-116	5.3	10
196	Thermochemical production of hydrogen from hydrogen sulfide with iodine thermochemical cycles. *International Journal of Hydrogen Energy*, **2018**, 43, 12939-12947	6.7	24
195	Automated Generation of Chemical Mechanisms for Predicting Extinction Strain Rates with Applications in Flame Stabilization and Combustion Instabilitie **2017**,		4
194	Steam methane reforming on a Ni-based bimetallic catalyst: density functional theory and experimental studies of the catalytic consequence of surface alloying of Ni with Ag. *Catalysis Science and Technology*, **2017**, 7, 1713-1725	5.5	39

193	Minimizing E-factor in the continuous-flow synthesis of diazepam and atropine. *Bioorganic and Medicinal Chemistry*, **2017**, 25, 6233-6241	3.4	41
192	On-the-fly pruning for rate-based reaction mechanism generation. *Computers and Chemical Engineering*, **2017**, 100, 1-8	4	10
191	Prediction of Organic Reaction Outcomes Using Machine Learning. *ACS Central Science*, **2017**, 3, 434-443	16.8	325
190	Structural Properties and Reactivity Trends of Molybdenum Oxide Catalysts Supported on Zirconia for the Hydrodeoxygenation of Anisole. *ACS Sustainable Chemistry and Engineering*, **2017**, 5, 5293-5301	8.3	55
189	Convolutional Embedding of Attributed Molecular Graphs for Physical Property Prediction. *Journal of Chemical Information and Modeling*, **2017**, 57, 1757-1772	6.1	191
188	Computational Investigation on Hydrodeoxygenation (HDO) of Acetone to Propylene on □MoO3(010) Surface. *Journal of Physical Chemistry C*, **2017**, 121, 17848-17855	3.8	21
187	Computer-Assisted Retrosynthesis Based on Molecular Similarity. *ACS Central Science*, **2017**, 3, 1237-1245	16.8	112
186	Combustion of Synthetic Jet Fuel: Chemical Kinetic Modeling and Uncertainty Analysis. *Journal of Propulsion and Power*, **2017**, 33, 350-359	1.8	3
185	Automatic mechanism generation for pyrolysis of di-tert-butyl sulfide. *Physical Chemistry Chemical Physics*, **2016**, 18, 21651-8	3.6	19
184	Methanol formation from the treatment of glycerol in supercritical water and with ethylsulfide. *Journal of Supercritical Fluids*, **2016**, 117, 80-88	4.2	8
183	Reaction Mechanism Generator: Automatic construction of chemical kinetic mechanisms. *Computer Physics Communications*, **2016**, 203, 212-225	4.2	335
182	Temperature- and Pressure-Dependent Kinetics of CH2OO + CH3COCH3 and CH2OO + CH3CHO: Direct Measurements and Theoretical Analysis. *International Journal of Chemical Kinetics*, **2016**, 48, 474-488	1.4	22
181	Micro-syngas technology options for GtL. *Canadian Journal of Chemical Engineering*, **2016**, 94, 613-622	2.3	16
180	The engine reformer: Syngas production in an engine for compact gas-to-liquids synthesis. *Canadian Journal of Chemical Engineering*, **2016**, 94, 623-635	2.3	18
179	A detailed combined experimental and theoretical study on dimethyl ether/propane blended oxidation. *Combustion and Flame*, **2016**, 168, 310-330	5.3	60
178	The Effect of Alcohol and Carbonyl Functional Groups on the Competition between Unimolecular Decomposition and Isomerization in C4 and C5 Alkoxy Radicals. *International Journal of Chemical Kinetics*, **2016**, 48, 544-555	1.4	1
177	JP-10 combustion studied with shock tube experiments and modeled with automatic reaction mechanism generation. *Combustion and Flame*, **2015**, 162, 3115-3129	5.3	57
176	Automated Discovery of Elementary Chemical Reaction Steps Using Freezing String and Berny Optimization Methods. *Journal of Chemical Theory and Computation*, **2015**, 11, 4248-59	6.4	86

175	Kinetics and Products of Vinyl + 1,3-Butadiene, a Potential Route to Benzene. *Journal of Physical Chemistry A*, **2015**, 119, 7325-38	2.8	17
174	Rule-based ab initio kinetic model for alkyl sulfide pyrolysis. *Chemical Engineering Journal*, **2015**, 278, 385-393	14.7	22
173	A kinetic and thermochemical database for organic sulfur and oxygen compounds. *Physical Chemistry Chemical Physics*, **2015**, 17, 13625-39	3.6	14
172	Supercritical Water Treatment of Crude Oil and Hexylbenzene: An Experimental and Mechanistic Study on Alkylbenzene Decomposition. *Energy & Fuels*, **2015**, 29, 5290-5302	4.1	18
171	Understanding low-temperature first-stage ignition delay: Propane. *Combustion and Flame*, **2015**, 162, 3658-3673	5.3	101
170	Reactivity and stability investigation of supported molybdenum oxide catalysts for the hydrodeoxygenation (HDO) of m-cresol. *Journal of Catalysis*, **2015**, 331, 86-97	7.3	159
169	Upgrading and desulfurization of heavy oils by supercritical water. *Journal of Supercritical Fluids*, **2015**, 96, 114-123	4.2	86
168	Natural Gas and Cellulosic Biomass: A Clean Fuel Combination? Determining the Natural Gas Blending Wall in Biofuel Production. *Environmental Science & Technology*, **2015**, 49, 8183-92	10.3	12
167	Influence of the double bond position on the oxidation of decene isomers at high pressures and temperatures. *Proceedings of the Combustion Institute*, **2015**, 35, 333-340	5.9	24
166	Continuous Thermal Oxidation of Alkenes with Nitrous Oxide in a Packed Bed Reactor. *Industrial & Engineering Chemistry Research*, **2015**, 54, 4166-4173	3.9	12
165	Kinetic Modeling of Jet Propellant-10 Pyrolysis. *Energy & Fuels*, **2015**, 29, 413-427	4.1	37
164	Cleavage of Side Chains on Thiophenic Compounds by Supercritical Water Treatment of Crude Oil Quantified by Two-Dimensional Gas Chromatography with Sulfur Chemiluminescence Detection. *Energy & Fuels*, **2014**, 28, 6589-6595	4.1	17
163	Combining experiment and theory to elucidate the role of supercritical water in sulfide decomposition. *Physical Chemistry Chemical Physics*, **2014**, 16, 9220-8	3.6	48
162	Theoretical kinetics study of the O(□P) + CH□CD□ hydrogen abstraction reaction: the role of anharmonicity, recrossing effects, and quantum mechanical tunneling. *Journal of Physical Chemistry A*, **2014**, 118, 3243-52	2.8	46
161	Quantum rate coefficients and kinetic isotope effect for the reaction Cl + CH4 -> HCl + CH3 from ring polymer molecular dynamics. *Journal of Physical Chemistry A*, **2014**, 118, 1989-96	2.8	47
160	A Signature of Roaming Dynamics in the Thermal Decomposition of Ethyl Nitrite: Chirped-Pulse Rotational Spectroscopy and Kinetic Modeling. *Journal of Physical Chemistry Letters*, **2014**, 5, 3641-8	6.4	26
159	Analysis of Adsorbent-Based Warm CO2 Capture Technology for Integrated Gasification Combined Cycle (IGCC) Power Plants. *Industrial & Engineering Chemistry Research*, **2014**, 53, 11145-11158	3.9	20
158	Direct Determination of the Simplest Criegee Intermediate (CH2OO) Self Reaction Rate. *Journal of Physical Chemistry Letters*, **2014**, 5, 2224-8	6.4	63

157	Direct kinetic measurements of reactions between the simplest Criegee intermediate CH2OO and alkenes. *Journal of Physical Chemistry A*, **2014**, 118, 1997-2006	2.8	73
156	Experimental and Modeling Study on the Thermal Decomposition of Jet Propellant-10. *Energy & Fuels*, **2014**, 28, 4976-4985	4.1	36
155	Response of Different Types of Sulfur Compounds to Oxidative Desulfurization of Jet Fuel. *Energy & Fuels*, **2014**, 28, 2977-2983	4.1	29
154	Economic and environmental benefits of higher-octane gasoline. *Environmental Science & Technology*, **2014**, 48, 6561-8	10.3	44
153	The role of catalyst in supercritical water desulfurization. *Applied Catalysis B: Environmental*, **2014**, 147, 144-155	21.8	51
152	Ring-polymer molecular dynamics: rate coefficient calculations for energetically symmetric (near thermoneutral) insertion reactions (X + H2) -> HX + H(X = C(1D), S(1D)). *Journal of Chemical Physics*, **2014**, 141, 244103	3.9	43
151	System and Market Analysis of Methanol Production Using Compact Engine Reformers **2014**,		1
150	Stress Test for Quantum Dynamics Approximations: Deep Tunneling in the Muonium Exchange Reaction D + HMu -> DMu + H. *Journal of Physical Chemistry Letters*, **2014**, 5, 4219-24	6.4	54
149	A coordinated investigation of the combustion chemistry of diisopropyl ketone, a prototype for biofuels produced by endophytic fungi. *Combustion and Flame*, **2014**, 161, 711-724	5.3	45
148	New pathways for formation of acids and carbonyl products in low-temperature oxidation: the Korcek decomposition of □-ketohydroperoxides. *Journal of the American Chemical Society*, **2013**, 135, 11100-14	16.4	124
147	Dehydration of isobutanol and the elimination of water from fuel alcohols. *Journal of Physical Chemistry A*, **2013**, 117, 6724-36	2.8	14
146	Ring Polymer Molecular Dynamics Calculations of Thermal Rate Constants for the O((3)P) + CH4 -> OH + CH3 Reaction: Contributions of Quantum Effects. *Journal of Physical Chemistry Letters*, **2013**, 4, 48-52	6.4	63
145	Supercritical Water Desulfurization of Organic Sulfides Is Consistent with Free-Radical Kinetics. *Energy & Fuels*, **2013**, 27, 6108-6117	4.1	71
144	RPMDrate: Bimolecular chemical reaction rates from ring polymer molecular dynamics. *Computer Physics Communications*, **2013**, 184, 833-840	4.2	84
143	Communication: full dimensional quantum rate coefficients and kinetic isotope effects from ring polymer molecular dynamics for a seven-atom reaction OH + CH4 -> CH3 + H2O. *Journal of Chemical Physics*, **2013**, 138, 221103	3.9	62
142	The predictive capability of an automatically generated combustion chemistry mechanism: Chemical structures of premixed iso-butanol flames. *Combustion and Flame*, **2013**, 160, 2343-2351	5.3	42
141	Chemically activated formation of organic acids in reactions of the Criegee intermediate with aldehydes and ketones. *Physical Chemistry Chemical Physics*, **2013**, 15, 16841-52	3.6	44
140	Experimental Investigation of Sorbent for Warm CO2 Capture by Pressure Swing Adsorption. *Industrial & Engineering Chemistry Research*, **2013**, 52, 9665-9673	3.9	21

139	Which Ab Initio Wave Function Methods Are Adequate for Quantitative Calculations of the Energies of Biradicals? The Performance of Coupled-Cluster and Multi-Reference Methods Along a Single-Bond Dissociation Coordinate. *Journal of Chemical Theory and Computation*, **2013**, 9, 418-31	6.4	31
138	Design and implementation of a next-generation software interface for on-the-fly quantum and force field calculations in automated reaction mechanism generation. *Computers and Chemical Engineering*, **2013**, 52, 35-45	4	42
137	An extensible framework for capturing solvent effects in computer generated kinetic models. *Journal of Physical Chemistry B*, **2013**, 117, 2955-70	3.4	23
136	Combustion and pyrolysis of iso-butanol: Experimental and chemical kinetic modeling study. *Combustion and Flame*, **2013**, 160, 1907-1929	5.3	61
135	Rate coefficients and kinetic isotope effects of the X + CH4 -> CH3 + HX (X = H, D, Mu) reactions from ring polymer molecular dynamics. *Journal of Chemical Physics*, **2013**, 138, 094307	3.9	66
134	Balanced Splitting and Rebalanced Splitting. *SIAM Journal on Numerical Analysis*, **2013**, 51, 3084-3105	2.4	23
133	Automatic Generation of Detailed Mechanisms. *Green Energy and Technology*, **2013**, 59-92	0.6	14
132	Detailed chemical kinetic modeling of JP-10 (exo-tetrahydrodicyclopentadiene) high-temperature oxidation: Exploring the role of biradical species in initial decomposition steps. *International Journal of Chemical Kinetics*, **2012**, 44, 179-193	1.4	38
131	Oxidative Desulfurization of Middle-Distillate Fuels Using Activated Carbon and Power Ultrasound. *Energy & Fuels*, **2012**, 26, 5164-5176	4.1	46
130	Crossed beam reaction of phenyl and D5-phenyl radicals with propene and deuterated counterparts--competing atomic hydrogen and methyl loss pathways. *Physical Chemistry Chemical Physics*, **2012**, 14, 720-9	3.6	23
129	Reaction of phenyl radical with propylene as a possible source of indene and other polycyclic aromatic hydrocarbons: an ab initio/RRKM-ME study. *Journal of Physical Chemistry A*, **2012**, 116, 4176-91	2.8	35
128	Role of O2 + QOOH in low-temperature ignition of propane. 1. Temperature and pressure dependent rate coefficients. *Journal of Physical Chemistry A*, **2012**, 116, 3325-46	2.8	188
127	Screening of binary alloys for warm temperature capture of elemental mercury using density functional theory. *Chemical Engineering Science*, **2012**, 80, 128-133	4.4	5
126	Automatic estimation of pressure-dependent rate coefficients. *Physical Chemistry Chemical Physics*, **2012**, 14, 1131-55	3.6	76
125	Analysis of Hydroxide Sorbents for CO2 Capture from Warm Syngas. *Industrial & Engineering Chemistry Research*, **2012**, 51, 13473-13481	3.9	10
124	Database of small molecule thermochemistry for combustion. *Journal of Physical Chemistry A*, **2012**, 116, 9033-57	2.8	133
123	Reply to comment on "Automatic estimation of pressure-dependent rate coefficients" [J. W. Allen, C. F. Goldsmith, and W. H. Green, Phys. Chem. Chem. Phys., 2011, 14, 1131–1155). *Physical Chemistry Chemical Physics*, **2012**, 14, 8434	3.6	2
122	Investigating the techno-economic trade-offs of hydrogen source using a response surface model of drop-in biofuel production via bio-oil upgrading. *Biofuels, Bioproducts and Biorefining*, **2012**, 6, 503-520	5.3	26

121	Screening of metal oxides and metal sulfides as sorbents for elemental mercury at elevated temperatures. *Fuel*, **2012**, 97, 783-795	7.1	24
120	An Exact-Steady-state Adaptive Chemistry method for combustion simulations: Combining the efficiency of reduced models and the accuracy of the full model. *Combustion and Flame*, **2012**, 159, 2352-2362	5.3	8
119	Accelerating multi-dimensional combustion simulations using GPU and hybrid explicit/implicit ODE integration. *Combustion and Flame*, **2012**, 159, 2388-2397	5.3	43
118	Analysis of Membrane and Adsorbent Processes for Warm Syngas Cleanup in Integrated Gasification Combined-Cycle Power with CO2Capture and Sequestration. *Industrial & Engineering Chemistry Research*, **2011**, 50, 11313-11336	3.9	22
117	Computational Investigation of the Thermochemistry and Kinetics of Steam Methane Reforming Over a Multi-Faceted Nickel Catalyst. *Topics in Catalysis*, **2011**, 54, 828-844	2.3	73
116	Comprehensive reaction mechanism for n-butanol pyrolysis and combustion. *Combustion and Flame* , **2011**, 158, 16-41	5.3	210
115	Theoretical rate coefficients for allyl+HO2 and allyloxy decomposition. *Proceedings of the Combustion Institute*, **2011**, 33, 273-282	5.9	64
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