Peter C St John

List of Publications by Year
in descending order

45 papers	2,131 citations	304743 22 h-index	243625 44 g-index
53 all docs	53 docs citations	53 times ranked	3091 citing authors

#	Article	IF	Citations
1	Identification of Small Molecule Activators of Cryptochrome. Science, 2012, 337, 1094-1097.	12.6	408
2	Modification of silk fibroin using diazonium coupling chemistry and the effects on hMSC proliferation and differentiation. Biomaterials, 2008, 29, 2829-2838.	11.4	243
3	Innovative Chemicals and Materials from Bacterial Aromatic Catabolic Pathways. Joule, 2019, 3, 1523-1537.	24.0	142
4	Prediction of organic homolytic bond dissociation enthalpies at near chemical accuracy with sub-second computational cost. Nature Communications, 2020, 11, 2328.	12.8	128
5	Measuring and predicting sooting tendencies of oxygenates, alkanes, alkenes, cycloalkanes, and aromatics on a unified scale. Combustion and Flame, 2018, 190, 349-364.	5.2	122
6	Amplitude Metrics for Cellular Circadian Bioluminescence Reporters. Biophysical Journal, 2014, 107, 2712-2722.	0.5	106
7	Functional network inference of the suprachiasmatic nucleus. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 4512-4517.	7.1	64
8	Succinic acid production from lignocellulosic hydrolysate by Basfia succiniciproducens. Bioresource Technology, 2016, 214, 558-566.	9.6	63
9	Message-passing neural networks for high-throughput polymer screening. Journal of Chemical Physics, 2019, 150, 234111.	3.0	63
10	Spatiotemporal separation of PER and CRY posttranslational regulation in the mammalian circadian clock. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 2040-2045.	7.1	55
11	Real-time prediction of ¹H and ¹³C chemical shifts with DFT accuracy using a 3D graph neural network. Chemical Science, 2021, 12, 12012-12026.	7.4	50
12	Quantum chemical calculations for over 200,000 organic radical species and 40,000 associated closed-shell molecules. Scientific Data, 2020, 7, 244.	5.3	49
13	Metabolic Engineering of Actinobacillus succinogenes Provides Insights into Succinic Acid Biosynthesis. Applied and Environmental Microbiology, 2017, 83, .	3.1	47
14	Importance of Engineered and Learned Molecular Representations in Predicting Organic Reactivity, Selectivity, and Chemical Properties. Accounts of Chemical Research, 2021, 54, 827-836.	15.6	47
15	A Quantitative Model for the Prediction of Sooting Tendency from Molecular Structure. Energy & Fuels, 2017, 31, 9983-9990.	5.1	42
16	Prediction of Hydroxymethylfurfural Yield in Glucose Conversion through Investigation of Lewis Acid and Organic Solvent Effects. ACS Catalysis, 2020, 10, 14707-14721.	11.2	41
17	Sooting tendencies of co-optima test gasolines and their surrogates. Proceedings of the Combustion Institute, 2019, 37, 961-968.	3.9	39
18	Performance-advantaged ether diesel bioblendstock production by a priori design. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 26421-26430.	7.1	39

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19	Impact of ethanol blending into gasoline on aromatic compound evaporation and particle emissions from a gasoline direct injection engine. Applied Energy, 2019, 250, 1618-1631.	10.1	35
20	A quantitative metric for organic radical stability and persistence using thermodynamic and kinetic features. Chemical Science, 2021, 12, 13158-13166.	7.4	30
21	Bayesian inference of metabolic kinetics from genome-scale multiomics data. PLoS Computational Biology, 2019, 15, e1007424.	3.2	29
22	Tailoring diesel bioblendstock from integrated catalytic upgrading of carboxylic acids: a â€œfuel property firstâ€•approach. Green Chemistry, 2019, 21, 5813-5827.	9.0	25
23	A perspective on biomass-derived biofuels: From catalyst design principles to fuel properties. Journal of Hazardous Materials, 2020, 400, 123198.	12.4	23
24	Advances in integrative structural biology: Towards understanding protein complexes in their cellular context. Computational and Structural Biotechnology Journal, 2021, 19, 214-225.	4.1	23
25	Property predictions demonstrate that structural diversity can improve the performance of polyoxymethylene ethers as potential bio-based diesel fuels. Fuel, 2021, 295, 120509.	6.4	21
26	Approaches to Computational Strain Design in the Multiomics Era. Frontiers in Microbiology, 2019, 10, 597.	3.5	17
27	A comparison of computational models for predicting yield sooting index. Proceedings of the Combustion Institute, 2021, 38, 1385-1393.	3.9	17
28	Towards quantitative prediction of ignition-delay-time sensitivity on fuel-to-air equivalence ratio. Combustion and Flame, 2020, 214, 103-115.	5.2	16
29	Predicting energy and stability of known and hypothetical crystals using graph neural network. Patterns, 2021, 2, 100361.	5.9	16
30	Quantifying Stochastic Noise in Cultured Circadian Reporter Cells. PLoS Computational Biology, 2015, 11, e1004451.	3.2	14
31	Experimental and theoretical insight into the soot tendencies of the methylcyclohexene isomers. Proceedings of the Combustion Institute, 2019, 37, 1083-1090.	3.9	13
32	Prediction of reaction knockouts to maximize succinate production by Actinobacillus succinogenes. PLoS ONE, 2018, 13, e0189144.	2.5	12
33	Efficient estimation of the maximum metabolic productivity of batch systems. Biotechnology for Biofuels, 2017, 10, 28.	6.2	11
34	Estimating confidence intervals in predicted responses for oscillatory biological models. BMC Systems Biology, 2013, 7, 71.	3.0	10
35	Investigation of structural effects of aromatic compounds on sooting tendency with mechanistic insight into ethylphenol isomers. Proceedings of the Combustion Institute, 2021, 38, 1143-1151.	3.9	10
36	Biochemical Production with Purified Cell-Free Systems. Biochemical Engineering Journal, 2021, 166, 107002.	3.6	7

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37	Elucidating the chemical pathways responsible for the sooting tendency of 1 and 2-phenylethanol. Proceedings of the Combustion Institute, 2021, 38, 1327-1334.	3.9	7
38	Understanding how chemical structure affects ignition-delay-time <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.svg"><mml:mi>Ï•</mml:mi></mml:math>-sensitivity. Combustion and Flame, 2021, 225, 377-387.	5.2	7
39	A Coupled Stochastic Model Explains Differences in Cry Knockout Behavior. IEEE Life Sciences Letters, 2015, 1, 3-6.	1.2	6
40	Bayesian Inference for Integrating Yarrowia lipolytica Multiomics Datasets with Metabolic Modeling. ACS Synthetic Biology, 2021, 10, 2968-2981.	3.8	4
41	Systems Biology. , 2014, , 159-187.		3
42	Thermodynamic and Kinetic Modeling of Co-utilization of Glucose and Xylose for 2,3-BDO Production by Zymomonas mobilis. Frontiers in Bioengineering and Biotechnology, 2021, 9, 707749.	4.1	3
43	Development of a Data-Derived Sooting Index Including Oxygen-Containing Fuel Components. Energy & Fuels, 2019, 33, 10290-10296.	5.1	2
44	Estimation of the Maximum Theoretical Productivity of Fed-Batch Bioreactors * *This work was funded by the US Department of Energyâ€™s Bioen-ergy Technologies Office (DOE-BETO), Contract No. DE-AC36-08GO28308 with the National Renewable Energy Laboratory. IFAC-PapersOnLine, 2017, 50, 9883-9888.	0.9	0
45	Software and Methods for Computational Flux Balance Analysis. Methods in Molecular Biology, 2020, 2096, 165-177.	0.9	0