# Peter C St John

List of Publications by Year
in descending order



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|---|---|---|---|
| 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 | Biochemical Production with Purified Cell-Free Systems. Biochemical Engineering Journal, 2021, 166, 107002. | 3.6 | 7 |
| 2 | 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 |
| 3 | Understanding how chemical structure affects ignition-delay-time <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.svg"><mml:mi>İ</mml:mi></mml:math>-sensitivity. Combustion and Flame, 2021, 225, 377-387. | 5.2 | 7 |
| 4 | A comparison of computational models for predicting yield sooting index. Proceedings of the Combustion Institute, 2021, 38, 1385-1393. | 3.9 | 17 |
| 5 | 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 |
| 6 | Real-time prediction of <sup>1</sup>H and <sup>13</sup>C chemical shifts with DFT accuracy using a 3D graph neural network. Chemical Science, 2021, 12, 12012-12026. | 7.4 | 50 |
| 7 | 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 |
| 8 | 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 |
| 9 | 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 |
| 10 | 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 |
| 11 | Predicting energy and stability of known and hypothetical crystals using graph neural network. Patterns, 2021, 2, 100361. | 5.9 | 16 |
| 12 | A quantitative metric for organic radical stability and persistence using thermodynamic and kinetic features. Chemical Science, 2021, 12, 13158-13166. | 7.4 | 30 |
| 13 | Bayesian Inference for Integrating Yarrowia lipolytica Multiomics Datasets with Metabolic Modeling. ACS Synthetic Biology, 2021, 10, 2968-2981. | 3.8 | 4 |
| 14 | 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 |
| 15 | 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 |
| 16 | Towards quantitative prediction of ignition-delay-time sensitivity on fuel-to-air equivalence ratio. Combustion and Flame, 2020, 214, 103-115. | 5.2 | 16 |
| 17 | Prediction of organic homolytic bond dissociation enthalpies at near chemical accuracy with sub-second computational cost. Nature Communications, 2020, 11, 2328. | 12.8 | 128 |
| 18 | A perspective on biomass-derived biofuels: From catalyst design principles to fuel properties. Journal of Hazardous Materials, 2020, 400, 123198. | 12.4 | 23 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Software and Methods for Computational Flux Balance Analysis. Methods in Molecular Biology, 2020, 2096, 165-177. | 0.9 | 0 |
| 20 | Sooting tendencies of co-optima test gasolines and their surrogates. Proceedings of the Combustion Institute, 2019, 37, 961-968. | 3.9 | 39 |
| 21 | Experimental and theoretical insight into the soot tendencies of the methylcyclohexene isomers. Proceedings of the Combustion Institute, 2019, 37, 1083-1090. | 3.9 | 13 |
| 22 | Bayesian inference of metabolic kinetics from genome-scale multiomics data. PLoS Computational Biology, 2019, 15, e1007424. | 3.2 | 29 |
| 23 | 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 |
| 24 | Development of a Data-Derived Sooting Index Including Oxygen-Containing Fuel Components. Energy & Fuels, 2019, 33, 10290-10296. | 5.1 | 2 |
| 25 | Message-passing neural networks for high-throughput polymer screening. Journal of Chemical Physics, 2019, 150, 234111. | 3.0 | 63 |
| 26 | 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 |
| 27 | Innovative Chemicals and Materials from Bacterial Aromatic Catabolic Pathways. Joule, 2019, 3, 1523-1537. | 24.0 | 142 |
| 28 | Approaches to Computational Strain Design in the Multiomics Era. Frontiers in Microbiology, 2019, 10, 597. | 3.5 | 17 |
| 29 | 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 |
| 30 | 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 |
| 31 | Prediction of reaction knockouts to maximize succinate production by Actinobacillus succinogenes. PLoS ONE, 2018, 13, e0189144. | 2.5 | 12 |
| 32 | Metabolic Engineering of Actinobacillus succinogenes Provides Insights into Succinic Acid Biosynthesis. Applied and Environmental Microbiology, 2017, 83, . | 3.1 | 47 |
| 33 | 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 |
| 34 | Efficient estimation of the maximum metabolic productivity of batch systems. Biotechnology for Biofuels, 2017, 10, 28. | 6.2 | 11 |
| 35 | A Quantitative Model for the Prediction of Sooting Tendency from Molecular Structure. Energy & Fuels, 2017, 31, 9983-9990. | 5.1 | 42 |
| 36 | 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 |

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|---|---|---|---|
| 37 | Succinic acid production from lignocellulosic hydrolysate by Basfia succiniciproducens. Bioresource Technology, 2016, 214, 558-566. | 9.6 | 63 |
| 38 | Quantifying Stochastic Noise in Cultured Circadian Reporter Cells. PLoS Computational Biology, 2015, 11, e1004451. | 3.2 | 14 |
| 39 | A Coupled Stochastic Model Explains Differences in Cry Knockout Behavior. IEEE Life Sciences Letters, 2015, 1, 3-6. | 1.2 | 6 |
| 40 | Systems Biology. , 2014, , 159-187. | | 3 |
| 41 | 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 |
| 42 | Amplitude Metrics for Cellular Circadian Bioluminescence Reporters. Biophysical Journal, 2014, 107, 2712-2722. | 0.5 | 106 |
| 43 | Estimating confidence intervals in predicted responses for oscillatory biological models. BMC Systems Biology, 2013, 7, 71. | 3.0 | 10 |
| 44 | Identification of Small Molecule Activators of Cryptochrome. Science, 2012, 337, 1094-1097. | 12.6 | 408 |
| 45 | Modification of silk fibroin using diazonium coupling chemistry and the effects on hMSC proliferation and differentiation. Biomaterials, 2008, 29, 2829-2838. | 11.4 | 243 |