Liam Wilbraham

List of Publications by Year
in descending order

32 papers	2,242 citations	331670 21 h-index	377865 34 g-index
61 all docs	61 docs citations	61 times ranked	2646 citing authors

#	Article	IF	Citations
1	The potential scarcity, or not, of polymeric overall water splitting photocatalysts. Sustainable Energy and Fuels, 2022, 6, 2233-2242.	4.9	2
2	Using high-throughput virtual screening to explore the optoelectronic property space of organic dyes; finding diketopyrrolopyrrole dyes for dye-sensitized water splitting and solar cells. Sustainable Energy and Fuels, 2021, 5, 704-719.	4.9	15
3	Modeling UVâ€“Vis spectra of low dimensional materials using electrostatic embedding: The case of CdSe. Journal of Computational Chemistry, 2021, 42, 1212-1224.	3.3	3
4	Exploring and mapping chemical space with molecular assembly trees. Science Advances, 2021, 7, eabj2465.	10.3	13
5	Photocatalytic polymers of intrinsic microporosity for hydrogen production from water. Journal of Materials Chemistry A, 2021, 9, 19958-19964.	10.3	36
6	Structureâ€“activity relationships in well-defined conjugated oligomer photocatalysts for hydrogen production from water. Chemical Science, 2020, 11, 8744-8756.	7.4	41
7	Side-chain tuning in conjugated polymer photocatalysts for improved hydrogen production from water. Energy and Environmental Science, 2020, 13, 1843-1855.	30.8	92
8	Photocatalytic proton reduction by a computationally identified, molecular hydrogen-bonded framework. Journal of Materials Chemistry A, 2020, 8, 7158-7170.	10.3	45
9	Hydrogen evolution from water using heteroatom substituted fluorene conjugated co-polymers. Journal of Materials Chemistry A, 2020, 8, 8700-8705.	10.3	47
10	Electron Storage System Based on a Two-Way Inversion of Redox Potentials. Journal of the American Chemical Society, 2020, 142, 5162-5176.	13.7	17
11	Mapping the optoelectronic property space of small aromatic molecules. Communications Chemistry, 2020, 3, .	4.5	14
12	Insight into the self-assembly of water-soluble perylene bisimide derivatives through a combined computational and experimental approach. Nanoscale, 2019, 11, 15917-15928.	5.6	13
13	Current understanding and challenges of solar-driven hydrogen generation using polymeric photocatalysts. Nature Energy, 2019, 4, 746-760.	39.5	638
14	Computational high-throughput screening of polymeric photocatalysts: exploring the effect of composition, sequence isomerism and conformational degrees of freedom. Faraday Discussions, 2019, 215, 98-110.	3.2	17
15	Photocatalytically active ladder polymers. Faraday Discussions, 2019, 215, 84-97.	3.2	20
16	Accelerated Discovery of Organic Polymer Photocatalysts for Hydrogen Evolution from Water through the Integration of Experiment and Theory. Journal of the American Chemical Society, 2019, 141, 9063-9071.	13.7	264
17	Mapping binary copolymer property space with neural networks. Chemical Science, 2019, 10, 4973-4984.	7.4	36
18	Photocatalytic Hydrogen Evolution from Water Using Fluorene and Dibenzothiophene Sulfone-Conjugated Microporous and Linear Polymers. Chemistry of Materials, 2019, 31, 305-313.	6.7	173

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19	Communication: Evaluating non-empirical double hybrid functionals for spin-state energetics in transition-metal complexes. Journal of Chemical Physics, 2018, 148, 041103.	3.0	28
20	Emissive Azobenzenes Delivered on a Silver Coordination Polymer. Inorganic Chemistry, 2018, 57, 15009-15022.	4.0	14
21	Revealing the Origins of Mechanically Induced Fluorescence Changes in Organic Molecular Crystals. Advanced Materials, 2018, 30, e1800817.	21.0	82
22	High-Throughput Screening Approach for the Optoelectronic Properties of Conjugated Polymers. Journal of Chemical Information and Modeling, 2018, 58, 2450-2459.	5.4	57
23	Nitrogen Containing Linear Poly(phenylene) Derivatives for Photo-catalytic Hydrogen Evolution from Water. Chemistry of Materials, 2018, 30, 5733-5742.	6.7	88
24	Maximising the hydrogen evolution activity in organic photocatalysts by co-polymerisation. Journal of Materials Chemistry A, 2018, 6, 11994-12003.	10.3	93
25	Understanding Aggregation-Induced Emission in Molecular Crystals: Insights from Theory. Journal of Physical Chemistry C, 2017, 121, 5747-5752.	3.1	52
26	Comparison of structural dynamics and coherence of dâ€“d and MLCT light-induced spin state trapping. Chemical Science, 2017, 8, 4978-4986.	7.4	43
27	Multiconfiguration Pair-Density Functional Theory Predicts Spin-State Ordering in Iron Complexes with the Same Accuracy as Complete Active Space Second-Order Perturbation Theory at a Significantly Reduced Computational Cost. Journal of Physical Chemistry Letters, 2017, 8, 2026-2030.	4.6	57
28	Electrostatic Embedding To Model the Impact of Environment on Photophysical Properties of Molecular Crystals: A Self-Consistent Charge Adjustment Procedure. Journal of Chemical Theory and Computation, 2016, 12, 3316-3324.	5.3	28
29	Modelling photophysical properties of metalâ€“organic frameworks: a density functional theory based approach. Physical Chemistry Chemical Physics, 2016, 18, 25176-25182.	2.8	27
30	Solvent tuned single molecule dual emission in protic solvents: effect of polarity and H-bonding. Faraday Discussions, 2015, 185, 285-297.	3.2	21
31	Exploring excited states using Time Dependent Density Functional Theory and density-based indexes. Coordination Chemistry Reviews, 2015, 304-305, 166-178.	18.8	118
32	Describing Excited State Intramolecular Proton Transfer in Dual Emissive Systems: A Density Functional Theory Based Analysis. Journal of Physical Chemistry B, 2015, 119, 2459-2466.	2.6	38