Lauren Takahashi

List of Publications by Year
in descending order

32 papers	638 citations	566801 15 h-index	580395 25 g-index
32 all docs	32 docs citations	32 times ranked	775 citing authors

#	Article	IF	Citations
1	Designing transformer oil immersion cooling servers for machine learning and first principle calculations. PLoS ONE, 2022, 17, e0266880.	1.1	2
2	Direct design of active catalysts for low temperature oxidative coupling of methane via machine learning and data mining. Catalysis Science and Technology, 2021, 11, 524-530.	2.1	17
3	Constructing catalyst knowledge networks from catalyst big data in oxidative coupling of methane for designing catalysts. Chemical Science, 2021, 12, 12546-12555.	3.7	13
4	Representing Catalytic and Processing Space in Methane Oxidation Reaction via Multioutput Machine Learning. Journal of Physical Chemistry Letters, 2021, 12, 808-814.	2.1	9
5	Unveiling gasâ€phase oxidative coupling of methane via data analysis. Journal of Computational Chemistry, 2021, 42, 1447-1451.	1.5	4
6	Extraction of Catalyst Design Heuristics from Random Catalyst Dataset and their Utilization in Catalyst Development for Oxidative Coupling of Methane. ChemCatChem, 2021, 13, 3262-3269.	1.8	14
7	Catalysis Gene Expression Profiling: Sequencing and Designing Catalysts. Journal of Physical Chemistry Letters, 2021, 12, 7335-7341.	2.1	8
8	Learning Catalyst Design Based on Bias-Free Data Set for Oxidative Coupling of Methane. ACS Catalysis, 2021, 11, 1797-1809.	5.5	31
9	Representing the Methane Oxidation Reaction via Linking First-Principles Calculations and Experiment with Graph Theory. Journal of Physical Chemistry Letters, 2021, 12, 558-568.	2.1	7
10	High-Throughput Experimentation and Catalyst Informatics for Oxidative Coupling of Methane. ACS Catalysis, 2020, 10, 921-932.	5.5	117
11	Multidimensional Classification of Catalysts in Oxidative Coupling of Methane through Machine Learning and High-Throughput Data. Journal of Physical Chemistry Letters, 2020, 11, 6819-6826.	2.1	18
12	Data-Driven Identification of the Reaction Network in Oxidative Coupling of the Methane Reaction via Experimental Data. Journal of Physical Chemistry Letters, 2020, 11, 787-795.	2.1	18
13	Catalyst Acquisition by Data Science (CADS): a web-based catalyst informatics platform for discovering catalysts. Reaction Chemistry and Engineering, 2020, 5, 903-911.	1.9	26
14	Data Driven Determination in Growth of Silver from Clusters to Nanoparticles and Bulk. Journal of Physical Chemistry Letters, 2019, 10, 4063-4068.	2.1	15
15	Visualizing Scientistsâ€™ Cognitive Representation of Materials Data through the Application of Ontology. Journal of Physical Chemistry Letters, 2019, 10, 7482-7491.	2.1	16
16	Automatic oxidation threshold recognition of XAFS data using supervised machine learning. Molecular Systems Design and Engineering, 2019, 4, 1014-1018.	1.7	25
17	The Rise of Catalyst Informatics: Towards Catalyst Genomics. ChemCatChem, 2019, 11, 1146-1152.	1.8	72
18	Functionalized Single-Atom-Embedded Bilayer Graphene and Hexagonal Boron Nitride. ACS Applied Electronic Materials, 2019, 1, 2-6.	2.0	1

#	Article	IF	Citations
19	Creating Machine Learning-Driven Material Recipes Based on Crystal Structure. Journal of Physical Chemistry Letters, 2019, 10, 283-288.	2.1	37
20	Tuning the Electronic Structure of an Aluminum Phosphide Nanotube through Configuration of the Lattice Geometry. ACS Applied Nano Materials, 2018, 1, 501-504.	2.4	1
21	Searching for Hidden Perovskite Materials for Photovoltaic Systems by Combining Data Science and First Principle Calculations. ACS Photonics, 2018, 5, 771-775.	3.2	70
22	Electronic structure of octagonal boron nitride nanotubes. International Journal of Quantum Chemistry, 2018, 118, e25542.	1.0	1
23	Redesigning the Materials and Catalysts Database Construction Process Using Ontologies. Journal of Chemical Information and Modeling, 2018, 58, 1742-1754.	2.5	22
24	Designing Mg7 cluster-assembled two dimensional crystal. FlatChem, 2017, 1, 57-59.	2.8	4
25	Structural stability and electronic properties of an octagonal allotrope of two dimensional boron nitride. Dalton Transactions, 2017, 46, 4259-4264.	1.6	15
26	Descriptors for predicting the lattice constant of body centered cubic crystal. Journal of Chemical Physics, 2017, 146, 204104.	1.2	22
27	Reactivity of Two-Dimensional Au₉, Pt₉, and Au₁₈Pt₁₈ against Common Molecules. Inorganic Chemistry, 2016, 55, 9410-9416.	1.9	2
28	Prediction of the dopant activity of chemical compounds against ammonia borane with key descriptors: electronegativity and crystal structures. New Journal of Chemistry, 2016, 40, 7303-7306.	1.4	1
29	Hydrophobic and antioxidant effects in In, Sn, and Sb based two dimensional materials. Dalton Transactions, 2016, 45, 3244-3246.	1.6	5
30	Designing Square Two-Dimensional Gold and Platinum. Crystal Growth and Design, 2016, 16, 1746-1750.	1.4	15
31	Low temperature pollutant trapping and dissociation over two-dimensional tin. Physical Chemistry Chemical Physics, 2015, 17, 21394-21396.	1.3	28
32	Data in Materials and Catalysts Informatics. ACS Symposium Series, 0, , 239-246.	0.5	2