Wen-Cong Lu

List of Publications by Year
in descending order

80 papers	2,391 citations	201674 27 h-index	223800 46 g-index
81 all docs	81 docs citations	81 times ranked	2696 citing authors

#	Article	IF	Citations
1	Application of Machine Learning Methods for the Development of Antidiabetic Drugs. Current Pharmaceutical Design, 2022, 28, 260-271.	1.9	5
2	Search for ABO_3 Type Ferroelectric Perovskites with Targeted Multi-Properties by Machine Learning Strategies. Journal of Chemical Information and Modeling, 2022, 62, 5038-5049.	5.4	29
3	A machine learning-based alloy design system to facilitate the rational design of high entropy alloys with enhanced hardness. Acta Materialia, 2022, 222, 117431.	7.9	112
4	Theoretical exploration of diverse electron-deficient core and terminal groups in A–DA′D–A type non-fullerene acceptors for organic solar cells. New Journal of Chemistry, 2022, 46, 3370-3382.	2.8	12
5	New Opportunity: Machine Learning for Polymer Materials Design and Discovery. Advanced Theory and Simulations, 2022, 5, .	2.8	44
6	Predicting Experimental Formability of Hybrid Organic–Inorganic Perovskites via Imbalanced Learning. Journal of Physical Chemistry Letters, 2022, 13, 3032-3038.	4.6	9
7	Machine Learning-Assisted Design of Yttria-Stabilized Zirconia Thermal Barrier Coatings with High Bonding Strength. ACS Omega, 2022, 7, 21052-21061.	3.5	9
8	Material machine learning for alloys: Applications, challenges and perspectives. Journal of Alloys and Compounds, 2022, 921, 165984.	5.5	39
9	Inverse Design of Hybrid Organic–Inorganic Perovskites with Suitable Bandgaps via Proactive Searching Progress. ACS Omega, 2022, 7, 21583-21594.	3.5	14
10	Machine Learning Aided Design of Polymer with Targeted Band Gap Based on DFT Computation. Journal of Physical Chemistry B, 2021, 125, 601-611.	2.6	20
11	Identifying the Immunological Gene Signatures of Immune Cell Subtypes. BioMed Research International, 2021, 2021, 1-10.	1.9	1
12	Machine Learning Model for High-Throughput Screening of Perovskite Manganites with the Highest Néel Temperature. Journal of Superconductivity and Novel Magnetism, 2021, 34, 1961-1969.	1.8	3
13	Accelerated discovery of boron-dipyrromethene sensitizer for solar cells by integrating data mining and first principle. Journal of Materiomics, 2021, 7, 790-801.	5.7	7
14	Predicting the Formability of Hybrid Organic–Inorganic Perovskites via an Interpretable Machine Learning Strategy. Journal of Physical Chemistry Letters, 2021, 12, 7423-7430.	4.6	36
15	Rapid discovery of narrow bandgap oxide double perovskites using machine learning. Computational Materials Science, 2021, 196, 110528.	3.0	33
16	Physics-Based Feature Makes Machine Learning Cognizing Crystal Properties Simple. Journal of Physical Chemistry Letters, 2021, 12, 8521-8527.	4.6	3
17	Multiobjective Stepwise Design Strategy-Assisted Design of High-Performance Perovskite Oxide Photocatalysts. Journal of Physical Chemistry C, 2021, 125, 21141-21150.	3.1	9
18	A Property–Driven Stepwise Design Strategy for Multiple Low–Melting Alloys via Machine Learning. Advanced Engineering Materials, 2021, 23, 2100612.	3.5	7

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19	Machine learning aided design of perovskite oxide materials for photocatalytic water splitting. Journal of Energy Chemistry, 2021, 60, 351-359.	12.9	68
20	Studies on the regularity of perovskite formation via machine learning. Computational Materials Science, 2021, 199, 110712.	3.0	17
21	Machine learning for perovskite materials design and discovery. Npj Computational Materials, 2021, 7, .	8.7	189
22	Rational design of SM315-based porphyrin sensitizers for highly efficient dye-sensitized solar cells: A theoretical study. Journal of Molecular Structure, 2020, 1205, 127567.	3.6	5
23	Prediction of photoelectric properties, especially power conversion efficiency of cells, of IQ1 and derivative dyes in high-efficiency dye-sensitized solar cells. Solar Energy, 2020, 195, 82-88.	6.1	25
24	First-principles screening and design of C275-based organic dyes for highly efficient dye-sensitized solar cells. Solar Energy, 2020, 207, 759-766.	6.1	3
25	Active learning for the power factor prediction in diamond-like thermoelectric materials. Npj Computational Materials, 2020, 6, .	8.7	43
26	Fuel Ratio Optimization of Blast Furnace Based on Data Mining. ISIJ International, 2020, 60, 2471-2476.	1.4	13
27	Inferring novel genes related to colorectal cancer via random walk with restart algorithm. Gene Therapy, 2019, 26, 373-385.	4.5	3
28	Novel composite BiFeO3/ZrO2 and its high photocatalytic performance under white LED visible-light irradiation. Materials Research Bulletin, 2019, 120, 110605.	5.2	36
29	Deep Neural Network Classifier for Virtual Screening Inhibitors of (S)-Adenosyl-L-Methionine (SAM)-Dependent Methyltransferase Family. Frontiers in Chemistry, 2019, 7, 324.	3.6	10
30	Easily recyclable photocatalyst Bi2WO6/MOF/PVDF composite film for efficient degradation of aqueous refractory organic pollutants under visible-light irradiation. Journal of Materials Science, 2019, 54, 6238-6257.	3.7	37
31	Theoretical study of high-efficiency organic dyes with the introduction of different auxiliary heterocyclic acceptors based on IQ1 toward dye-sensitized solar cells. Journal of Molecular Graphics and Modelling, 2019, 86, 170-178.	2.4	19
32	Machine-learning-assisted prediction of surgical outcomes in patients undergoing gastrectomy. Chinese Journal of Cancer Research: Official Journal of China Anti-Cancer Association, Beijing Institute for Cancer Research, 2019, 31, 797-805.	2.2	12
33	Predicting specific surface areas of layered double hydroxides based on support vector regression integrated with a residual bootstrapping method. Journal of Mathematical Chemistry, 2018, 56, 1744-1758.	1.5	4
34	Material data mining in Nianyi Chen's scientific family. Journal of Chemometrics, 2018, 32, e3022.	1.3	2
35	OCPMDM: Online computation platform for materials data mining. Chemometrics and Intelligent Laboratory Systems, 2018, 177, 26-34.	3.5	28
36	Discovery of 1,8-acridinedione derivatives as novel GCN5 inhibitors via high throughput screening. European Journal of Medicinal Chemistry, 2018, 151, 740-751.	5.5	29

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37	Characterization of Tobacco Leaves by Near-Infrared Reflectance Spectroscopy and Electronic Nose with Support Vector Machine. Analytical Letters, 2018, 51, 1935-1943.	1.8	5
38	Theoretical screening and design of SM315-based porphyrin dyes for highly efficient dye-sensitized solar cells with near-IR light harvesting. Dyes and Pigments, 2018, 155, 292-299.	3.7	41
39	Prediction of potential drivers connecting different dysfunctional levels in lung adenocarcinoma via a protein–protein interaction network. Biochimica Et Biophysica Acta - Molecular Basis of Disease, 2018, 1864, 2284-2293.	3.8	18
40	Using Data Mining To Search for Perovskite Materials with Higher Specific Surface Area. Journal of Chemical Information and Modeling, 2018, 58, 2420-2427.	5.4	28
41	Accelerated search for perovskite materials with higher Curie temperature based on the machine learning methods. Computational Materials Science, 2018, 151, 41-48.	3.0	49
42	Data mining assisted materials design of layered double hydroxide with desired specific surface area. Computational Materials Science, 2017, 136, 29-35.	3.0	18
43	Prediction and synthesis of novel layered double hydroxide with desired basal spacing based on relevance vector machine. Materials Research Bulletin, 2017, 93, 123-129.	5.2	11
44	Electrolyte-controlled discharge product distribution of Na–O$_2$ batteries: a combined computational and experimental study. Physical Chemistry Chemical Physics, 2017, 19, 2940-2949.	2.8	14
45	Data mining-aided materials discovery and optimization. Journal of Materiomics, 2017, 3, 191-201.	5.7	65
46	Prediction of the aquatic toxicity of aromatic compounds to tetrahymena pyriformis through support vector regression. Oncotarget, 2017, 8, 49359-49369.	1.8	53
47	A Cancer Gene Selection Algorithm Based on the K-S Test and CFS. BioMed Research International, 2017, 2017, 1-6.	1.9	24
48	Mining for genes related to choroidal neovascularization based on the shortest path algorithm and protein interaction information. Biochimica Et Biophysica Acta - General Subjects, 2016, 1860, 2740-2749.	2.4	6
49	DFT study on addition reaction mechanism of guanine-cytosine base pair with OH radical. Journal of Physical Organic Chemistry, 2015, 28, 437-444.	1.9	10
50	Materials design and control synthesis of the layered double hydroxide with the desired basal spacing. Chemometrics and Intelligent Laboratory Systems, 2015, 144, 11-16.	3.5	12
51	Theoretical Study of WS-9-Based Organic Sensitizers for Unusual Vis/NIR Absorption and Highly Efficient Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2015, 119, 9782-9790.	3.1	121
52	Theoretical Study of Acene-Bridged Dyes for Dye-Sensitized Solar Cells. Journal of Physical Chemistry A, 2015, 119, 3299-3309.	2.5	48
53	Discovery and Optimization of Novel, Selective Histone Methyltransferase SET7 Inhibitors by Pharmacophore- and Docking-Based Virtual Screening. Journal of Medicinal Chemistry, 2015, 58, 8166-8181.	6.4	59
54	DFT study of adenine–uracil base pair damage by OH radical. Journal of Physical Organic Chemistry, 2015, 28, 645-651.	1.9	6

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55	Solvothermal synthesis of Co_3O_4/Al_2O_3 hollow core–shell microspheres for the catalytic oxidation of CO. CrystEngComm, 2014, 16, 6126-6134.	2.6	6
56	Core–Shell Al2O3-Supported Ni for High-Performance Catalytic Reforming of Toluene as a Model Compound of Tar. Arabian Journal for Science and Engineering, 2014, 39, 6671-6678.	1.1	9
57	Size-Controlled Synthesis of BiPO4 Nanostructures and Their Photocatalytic Performances. Arabian Journal for Science and Engineering, 2014, 39, 6721-6725.	1.1	6
58	A DFT study on reaction of eupatilin with hydroxyl radical in solution. International Journal of Quantum Chemistry, 2013, 113, 966-974.	2.0	32
59	Novel three-dimensional Co3O4 dendritic superstructures: hydrothermal synthesis, formation mechanism and magnetic properties. CrystEngComm, 2013, 15, 1389.	2.6	73
60	Using support vector machine for materials design. Advances in Manufacturing, 2013, 1, 151-159.	6.1	44
61	QSAR studies on pyrrolidine amides derivatives as DPP-IV inhibitors for type 2 diabetes. Medicinal Chemistry Research, 2013, 22, 5274-5283.	2.4	14
62	Thermal-reforming of toluene over core-shell $Ni/\gamma-Al_2O_3$ catalysts. , 2013, , .		0
63	Particle swarm optimization-based support vector regression and Bayesian networks applied to the toxicity of organic compounds to tadpoles (Rana japonica). , 2011, , .		0
64	DFT Study on Molecular Structures and ROS Scavenging Mechanisms of Novel Antioxidants from *Lespedeza Virgata*. Chinese Journal of Chemical Physics, 2011, 24, 173-180.	1.3	8
65	Predicting Functions of Proteins in Mouse Based on Weighted Protein-Protein Interaction Network and Protein Hybrid Properties. PLoS ONE, 2011, 6, e14556.	2.5	144
66	Classification of the Toxicity of Some Organic Compounds to Tadpoles (*Rana Temporaria*) Through Integrating Multiple Classifiers. Molecular Informatics, 2011, 30, 672-675.	2.5	7
67	QSPR Study of *n*–Octanol/Water Partition Coefficient of Some Aromatic Compounds Using Support Vector Regression. QSAR and Combinatorial Science, 2009, 28, 175-182.	1.4	21
68	Classification of Src Kinase Inhibitors Based on Support Vector Machine. QSAR and Combinatorial Science, 2009, 28, 719-727.	1.4	15
69	Low-Temperature Synthesis of Monodisperse 3D Manganese Oxide Nanoflowers and Their Pseudocapacitance Properties. Journal of Physical Chemistry C, 2009, 113, 54-60.	3.1	119
70	Synthesis of Three-Dimensional Hierarchical Dendrites of NdOHCO3 via a Facile Hydrothermal Method. Crystal Growth and Design, 2009, 9, 1415-1420.	3.0	27
71	Template-Free Synthesis and Self-Assembly of CeO_2 Nanospheres Fabricated with Foursquare Nanoflakes. Journal of Physical Chemistry C, 2009, 113, 21520-21525.	3.1	35
72	One-Step Synthesis of Hierarchical Cantaloupe-like AlOOH Superstructures via a Hydrothermal Route. Crystal Growth and Design, 2008, 8, 1426-1429.	3.0	122

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73	Support vector machine for SAR/QSAR of phenethyl-amines. Acta Pharmacologica Sinica, 2007, 28, 1075-1086.	6.1	31
74	Support vector classification for structure-activity-relationship of 1-(1H-1,2,4-triazole-1-yl)-2-(2,4-difluorophenyl)-3-substituted-2-propanols. Journal of Shanghai University, 2007, 11, 521-526.	0.1	0
75	Support vector classification for SAR of 5-HT3 receptor antagonists. Journal of Shanghai University, 2006, 10, 366-370.	0.1	0
76	Morphological characterization of A12O3 membrane fabricated by sol-gel dip-coating method. Journal of Shanghai University, 2006, 10, 553-557.	0.1	0
77	Using support vector regression for the prediction of the band gap and melting point of binary and ternary compound semiconductors. Solid State Sciences, 2006, 8, 129-136.	3.2	62
78	Predicting Anti-HIV-1 Activities of HEPT-analog Compounds by Using Support Vector Classification. QSAR and Combinatorial Science, 2005, 24, 1021-1025.	1.4	12
79	Semiempirical Quantum Chemical Method and Artificial Neural Networks Applied for λmaxComputation of Some Azo Dyes. Journal of Chemical Information and Computer Sciences, 2004, 44, 2047-2050.	2.8	24
80	Regularities of formation of ternary alloy phases between non-transition metals. Science in China Series D: Earth Sciences, 2000, 43, 199-205.	0.9	3