Wen-Cong Lu

List of Publications by Year
in descending order

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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	Machine learning for perovskite materials design and discovery. Npj Computational Materials, 2021, 7, .	8.7	189
2	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
3	One-Step Synthesis of Hierarchical Cantaloupe-like AlOOH Superstructures via a Hydrothermal Route. Crystal Growth and Design, 2008, 8, 1426-1429.	3.0	122
4	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
5	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
6	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
7	Novel three-dimensional Co3O4 dendritic superstructures: hydrothermal synthesis, formation mechanism and magnetic properties. CrystEngComm, 2013, 15, 1389.	2.6	73
8	Machine learning aided design of perovskite oxide materials for photocatalytic water splitting. Journal of Energy Chemistry, 2021, 60, 351-359.	12.9	68
9	Data mining-aided materials discovery and optimization. Journal of Materiomics, 2017, 3, 191-201.	5.7	65
10	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
11	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
12	Prediction of the aquatic toxicity of aromatic compounds to tetrahymena pyriformis through support vector regression. Oncotarget, 2017, 8, 49359-49369.	1.8	53
13	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
14	Theoretical Study of Acene-Bridged Dyes for Dye-Sensitized Solar Cells. Journal of Physical Chemistry A, 2015, 119, 3299-3309.	2.5	48
15	Using support vector machine for materials design. Advances in Manufacturing, 2013, 1, 151-159.	6.1	44
16	New Opportunity: Machine Learning for Polymer Materials Design and Discovery. Advanced Theory and Simulations, 2022, 5, .	2.8	44
17	Active learning for the power factor prediction in diamond-like thermoelectric materials. Npj Computational Materials, 2020, 6, .	8.7	43
18	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

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19	Material machine learning for alloys: Applications, challenges and perspectives. Journal of Alloys and Compounds, 2022, 921, 165984.	5.5	39
20	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
21	Novel composite BiFeO3/ZrO2 and its high photocatalytic performance under white LED visible-light irradiation. Materials Research Bulletin, 2019, 120, 110605.	5.2	36
22	Predicting the Formability of Hybrid Organicâ€“Inorganic Perovskites via an Interpretable Machine Learning Strategy. Journal of Physical Chemistry Letters, 2021, 12, 7423-7430.	4.6	36
23	Template-Free Synthesis and Self-Assembly of CeO₂ Nanospheres Fabricated with Foursquare Nanoflakes. Journal of Physical Chemistry C, 2009, 113, 21520-21525.	3.1	35
24	Rapid discovery of narrow bandgap oxide double perovskites using machine learning. Computational Materials Science, 2021, 196, 110528.	3.0	33
25	A DFT study on reaction of eupatilin with hydroxyl radical in solution. International Journal of Quantum Chemistry, 2013, 113, 966-974.	2.0	32
26	Support vector machine for SAR/QSAR of phenethyl-amines. Acta Pharmacologica Sinica, 2007, 28, 1075-1086.	6.1	31
27	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
28	Search for ABO₃ Type Ferroelectric Perovskites with Targeted Multi-Properties by Machine Learning Strategies. Journal of Chemical Information and Modeling, 2022, 62, 5038-5049.	5.4	29
29	OCPMDM: Online computation platform for materials data mining. Chemometrics and Intelligent Laboratory Systems, 2018, 177, 26-34.	3.5	28
30	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
31	Synthesis of Three-Dimensional Hierarchical Dendrites of NdOHCO3 via a Facile Hydrothermal Method. Crystal Growth and Design, 2009, 9, 1415-1420.	3.0	27
32	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
33	Semiempirical Quantum Chemical Method and Artificial Neural Networks Applied for Î»maxComputation of Some Azo Dyes. Journal of Chemical Information and Computer Sciences, 2004, 44, 2047-2050.	2.8	24
34	A Cancer Gene Selection Algorithm Based on the K-S Test and CFS. BioMed Research International, 2017, 2017, 1-6.	1.9	24
35	QSPR Study of nâ€Octanol/Water Partition Coefficient of Some Aromatic Compounds Using Support Vector Regression. QSAR and Combinatorial Science, 2009, 28, 175-182.	1.4	21
36	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

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37	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
38	Data mining assisted materials design of layered double hydroxide with desired specific surface area. Computational Materials Science, 2017, 136, 29-35.	3.0	18
39	Prediction of potential drivers connecting different dysfunctional levels in lung adenocarcinoma via a proteinâ€“protein interaction network. Biochimica Et Biophysica Acta - Molecular Basis of Disease, 2018, 1864, 2284-2293.	3.8	18
40	Studies on the regularity of perovskite formation via machine learning. Computational Materials Science, 2021, 199, 110712.	3.0	17
41	Classification of Src Kinase Inhibitors Based on Support Vector Machine. QSAR and Combinatorial Science, 2009, 28, 719-727.	1.4	15
42	QSAR studies on pyrrolidine amides derivatives as DPP-IV inhibitors for type 2 diabetes. Medicinal Chemistry Research, 2013, 22, 5274-5283.	2.4	14
43	Electrolyte-controlled discharge product distribution of Naâ€“O₂batteries: a combined computational and experimental study. Physical Chemistry Chemical Physics, 2017, 19, 2940-2949.	2.8	14
44	Inverse Design of Hybrid Organicâ€“Inorganic Perovskites with Suitable Bandgaps via Proactive Searching Progress. ACS Omega, 2022, 7, 21583-21594.	3.5	14
45	Fuel Ratio Optimization of Blast Furnace Based on Data Mining. ISIJ International, 2020, 60, 2471-2476.	1.4	13
46	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
47	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
48	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
49	Theoretical exploration of diverse electron-deficient core and terminal groups in Aâ€“DAâ€²Dâ€“A type non-fullerene acceptors for organic solar cells. New Journal of Chemistry, 2022, 46, 3370-3382.	2.8	12
50	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
51	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
52	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
53	Coreâ€“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
54	Multiobjective Stepwise Design Strategy-Assisted Design of High-Performance Perovskite Oxide Photocatalysts. Journal of Physical Chemistry C, 2021, 125, 21141-21150.	3.1	9

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55	Predicting Experimental Formability of Hybrid Organicâ€“Inorganic Perovskites via Imbalanced Learning. Journal of Physical Chemistry Letters, 2022, 13, 3032-3038.	4.6	9
56	Machine Learning-Assisted Design of Yttria-Stabilized Zirconia Thermal Barrier Coatings with High Bonding Strength. ACS Omega, 2022, 7, 21052-21061.	3.5	9
57	DFT Study on Molecular Structures and ROS Scavenging Mechanisms of Novel Antioxidants fromLespedeza Virgata. Chinese Journal of Chemical Physics, 2011, 24, 173-180.	1.3	8
58	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
59	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
60	A Propertyâ€Đriven Stepwise Design Strategy for Multiple Lowâ€Melting Alloys via Machine Learning. Advanced Engineering Materials, 2021, 23, 2100612.	3.5	7
61	Solvothermal synthesis of Co₃O₄/Al₂O₃ hollow coreâ€“shell microspheres for the catalytic oxidation of CO. CrystEngComm, 2014, 16, 6126-6134.	2.6	6
62	Size-Controlled Synthesis of BiPO4 Nanostructures and Their Photocatalytic Performances. Arabian Journal for Science and Engineering, 2014, 39, 6721-6725.	1.1	6
63	DFT study of adenineâ€•uracil base pair damage by OH radical. Journal of Physical Organic Chemistry, 2015, 28, 645-651.	1.9	6
64	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
65	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
66	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
67	Application of Machine Learning Methods for the Development of Antidiabetic Drugs. Current Pharmaceutical Design, 2022, 28, 260-271.	1.9	5
68	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
69	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
70	Inferring novel genes related to colorectal cancer via random walk with restart algorithm. Gene Therapy, 2019, 26, 373-385.	4.5	3
71	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
72	Machine Learning Model for High-Throughput Screening of Perovskite Manganites with the Highest NÃ©el Temperature. Journal of Superconductivity and Novel Magnetism, 2021, 34, 1961-1969.	1.8	3

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73	Physics-Based Feature Makes Machine Learning Cognizing Crystal Properties Simple. Journal of Physical Chemistry Letters, 2021, 12, 8521-8527.	4.6	3
74	Material data mining in Nianyi Chen's scientific family. Journal of Chemometrics, 2018, 32, e3022.	1.3	2
75	Identifying the Immunological Gene Signatures of Immune Cell Subtypes. BioMed Research International, 2021, 2021, 1-10.	1.9	1
76	Support vector classification for SAR of 5-HT3 receptor antagonists. Journal of Shanghai University, 2006, 10, 366-370.	0.1	0
77	Morphological characterization of A12O3 membrane fabricated by sol-gel dip-coating method. Journal of Shanghai University, 2006, 10, 553-557.	0.1	0
78	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
79	Particle swarm optimization-based support vector regression and Bayesian networks applied to the toxicity of organic compounds to tadpoles (Rana japonica). , 2011, , .		0
80	Thermal-reforming of toluene over core-shell Ni/γ-Al<inf>2</inf>O<inf>3</inf> catalysts. , 2013, , .		0