

Hao Li

List of Publications by Year in descending order

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120
papers

10,619
citations

36203

51
h-index

32761

100
g-index

121
all docs

121
docs citations

121
times ranked

9800
citing authors

#	ARTICLE	IF	CITATIONS
1	Gold boosts nitrate reduction and deactivation resistance to indium-promoted palladium catalysts. <i>Applied Catalysis B: Environmental</i> , 2022, 305, 121048.	10.8	29
2	Tracking the redox reaction-induced reconstruction of NiAu nanoparticles <i>via</i> environmental scanning transmission electron microscopy. <i>Nanoscale</i> , 2022, 14, 4089-4097.	2.8	2
3	Design of 3d transition metal anchored B ₅ N ₃ catalysts for electrochemical CO ₂ reduction to methane. <i>Journal of Materials Chemistry A</i> , 2022, 10, 9737-9745.	5.2	31
4	Exploring the Effects of Ionic Defects on the Stability of CsPbI ₃ with a Deep Learning Potential. <i>ChemPhysChem</i> , 2022, 23, e202100841.	1.0	8
5	Opportunities and Challenges in Electrolytic Propylene Epoxidation. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 2057-2063.	2.1	15
6	Stability and Activity of Cobalt Antimonate for Oxygen Reduction in Strong Acid. <i>ACS Energy Letters</i> , 2022, 7, 993-1000.	8.8	21
7	Threeâ€”One Alkylamineâ€”Tuned MoO _x for Labâ€”Scale to Realâ€”Life Aqueous Supercapacitors. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	18
8	Electrocatalytic ammonia synthesis catalyzed by mesoporous nickel oxide nanosheets loaded with Pt nanoparticles. <i>Chinese Journal of Catalysis</i> , 2022, 43, 1371-1378.	6.9	18
9	Layer structured materials for ambient nitrogen fixation. <i>Coordination Chemistry Reviews</i> , 2022, 460, 214468.	9.5	28
10	Design strategy of bifunctional catalysts for CO oxidation. <i>Fuel</i> , 2022, 320, 123909.	3.4	10
11	Direct In Situ Vertical Growth of Interlaced Mesoporous NiO Nanosheets on Carbon Felt for Electrocatalytic Ammonia Synthesis. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	13
12	MgH ₂ /single-atom heterojunctions: effective hydrogen storage materials with facile dehydrogenation. <i>Journal of Materials Chemistry A</i> , 2022, 10, 19839-19851.	5.2	23
13	Understanding trends in the mercury oxidation activity of single-atom catalysts. <i>Environmental Science: Nano</i> , 2022, 9, 2041-2050.	2.2	13
14	Integrating Covalent Organic Framework with Transition Metal Phosphide for Nobleâ€”Metalâ€”Free Visibleâ€”Lightâ€”Driven Photocatalytic H ₂ Evolution. <i>Small</i> , 2022, 18, .	5.2	33
15	A WS ₂ /sepiolite composite with highly dispersed WS ₂ nanosheets for photocatalytic wastewater treatment. <i>Applied Clay Science</i> , 2022, 228, 106576.	2.6	7
16	Performance Prediction and Optimization of Solar Water Heater via a Knowledge-Based Machine Learning Method. , 2022, , 714-733.		0
17	Rareâ€”Earth Singleâ€”Atom Catalysts: A New Frontier in Photo/Electrocatalysis. <i>Small Methods</i> , 2022, 6, .	4.6	63
18	Hydrogen generation during the purification of metallurgical-grade silicon. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 23406-23416.	3.8	12

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19	One-Dimensional van der Waals Heterostructures as Efficient Metal-Free Oxygen Electrocatalysts. ACS Nano, 2021, 15, 3309-3319.	7.3	79
20	Emulsion-template synthesis of mesoporous nickel oxide nanoflowers composed of crossed nanosheets for effective nitrogen reduction. Dalton Transactions, 2021, 50, 5835-5844.	1.6	24
21	Electrochemical behavior of a Ni ₃ N OER precatalyst in Fe-purified alkaline media: the impact of self-oxidation and Fe incorporation. Materials Advances, 2021, 2, 2299-2309.	2.6	28
22	Origin of the hydrophobicity of sulfur-containing iron surfaces. Physical Chemistry Chemical Physics, 2021, 23, 13971-13976.	1.3	38
23	A small change in the local atomic environment for a big improvement in single-atom catalysis. Journal of Materials Chemistry A, 2021, 9, 4184-4192.	5.2	44
24	Properties and reactivity of sulfidized nanoscale zero-valent iron prepared with different borohydride amounts. Environmental Science: Nano, 2021, 8, 2607-2617.	2.2	24
25	Li ⁺ /Zn Overlayer to Facilitate Uniform Lithium Deposition for Lithium Metal Batteries. ACS Applied Materials & Interfaces, 2021, 13, 9985-9993.	4.0	19
26	Unveiling the Role of Sulfur in Rapid Defluorination of Florfenicol by Sulfidized Nanoscale Zero-Valent Iron in Water under Ambient Conditions. Environmental Science & Technology, 2021, 55, 2628-2638.	4.6	98
27	3d Transition-Metal-Mediated Columbite Nanocatalysts for Decentralized Electrosynthesis of Hydrogen Peroxide. Small, 2021, 17, e2007249.	5.2	35
28	An electro-activated bimetallic zinc-nickel hydroxide cathode for supercapacitor with super-long 140,000 cycle durability. Nano Energy, 2021, 82, 105727.	8.2	68
29	Calculations of Hydrogen Associative Desorption on Mono- and Bimetallic Catalysts. Journal of Physical Chemistry C, 2021, 125, 12028-12037.	1.5	12
30	Higher photocatalytic removal of organic pollutants using pangolin-like composites made of 3 rd atomic layers of MoS ₂ nanosheets deposited on tourmaline. Environmental Chemistry Letters, 2021, 19, 3573-3582.	8.3	37
31	Analysis of the limitations in the oxygen reduction activity of transition metal oxide surfaces. Nature Catalysis, 2021, 4, 463-468.	16.1	156
32	Sulfidized Nanoscale Zero-Valent Iron: Tuning the Properties of This Complex Material for Efficient Groundwater Remediation. Accounts of Materials Research, 2021, 2, 420-431.	5.9	96
33	Factors that influence hydrogen binding at metal-atop sites. Journal of Chemical Physics, 2021, 155, 024703.	1.2	7
34	Scalable Synthesis of Tungsten Disulfide Nanosheets for Alkali ⁺ -Acid Electrocatalytic Sulfion Recycling and H ₂ Generation. Angewandte Chemie - International Edition, 2021, 60, 21550-21557.	7.2	82
35	New insights on CO and CO ₂ hydrogenation for methanol synthesis: The key role of adsorbate-adsorbate interactions on Cu and the highly active MgO-Cu interface. Journal of Catalysis, 2021, 400, 325-331.	3.1	32
36	Scalable Synthesis of Tungsten Disulfide Nanosheets for Alkali ⁺ -Acid Electrocatalytic Sulfion Recycling and H ₂ Generation. Angewandte Chemie, 2021, 133, 21720-21727.	1.6	4

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37	Understanding Trends in Ethylene Epoxidation on Group IB Metals. ACS Catalysis, 2021, 11, 12052-12057.	5.5	19
38	Iminodiacetonitrile induce-synthesis of two-dimensional PdNi/Ni@carbon nanosheets with uniform dispersion and strong interface bonding as an effective bifunctional electrocatalyst in air-cathode. Energy Storage Materials, 2021, 42, 118-128.	9.5	64
39	Co-Fe-Cr (oxy)Hydroxides as Efficient Oxygen Evolution Reaction Catalysts. Advanced Energy Materials, 2021, 11, 2003412.	10.2	94
40	Gd-induced electronic structure engineering of a NiFe-layered double hydroxide for efficient oxygen evolution. Journal of Materials Chemistry A, 2021, 9, 2999-3006.	5.2	133
41	Relations between Surface Oxygen Vacancies and Activity of Methanol Formation from CO ₂ Hydrogenation over In ₂ O ₃ Surfaces. ACS Catalysis, 2021, 11, 1780-1786.	5.5	88
42	Methane activation on dual-atom catalysts supported on graphene. Chemical Communications, 2021, 57, 12127-12130.	2.2	6
43	Tuning the Catalytic Preference of Ruthenium Catalysts for Nitrogen Reduction by Atomic Dispersion. Advanced Functional Materials, 2020, 30, 1905665.	7.8	159
44	Thiocyanate-Modified Silver Nanofoam for Efficient CO ₂ Reduction to CO. ACS Catalysis, 2020, 10, 1444-1453.	5.5	51
45	New insights into the solid-state hydrogen storage of nanostructured LiBH ₄ -MgH ₂ system. Chemical Engineering Journal, 2020, 385, 123856.	6.6	119
46	Dechlorination and defluorination capability of sulfidized nanoscale zerovalent iron with suppressed water reactivity. Chemical Engineering Journal, 2020, 400, 125900.	6.6	61
47	Octahedral Coordinated Trivalent Cobalt Enriched Multimetal Oxygen Evolution Catalysts. Advanced Energy Materials, 2020, 10, 2002593.	10.2	47
48	Iron and Sulfur Precursors Affect Crystalline Structure, Speciation, and Reactivity of Sulfidized Nanoscale Zerovalent Iron. Environmental Science & Technology, 2020, 54, 13294-13303.	4.6	128
49	Electrical and Structural Dual Function of Oxygen Vacancies for Promoting Electrochemical Capacitance in Tungsten Oxide. Small, 2020, 16, e2004709.	5.2	24
50	Computational design of (100) alloy surfaces for the hydrogen evolution reaction. Journal of Materials Chemistry A, 2020, 8, 17987-17997.	5.2	47
51	Effects of a conductive support on the bonding of oxygen containing molecules to transition metal oxide surfaces. Physical Chemistry Chemical Physics, 2020, 22, 26216-26222.	1.3	7
52	Mechanism of hydrogen storage on Fe ₃ B. Chemical Communications, 2020, 56, 14235-14238.	2.2	13
53	Co ₃ O ₄ Nanocrystals with an Oxygen Vacancy-Rich and Highly Reactive (222) Facet on Carbon Nitride Scaffolds for Efficient Photocatalytic Oxygen Evolution. ACS Applied Materials & Interfaces, 2020, 12, 44608-44616.	4.0	43
54	Evaluation of a V ₈ C ₇ Anode for Oxygen Evolution in Alkaline Media: Unusual Morphological Behavior. ACS Sustainable Chemistry and Engineering, 2020, 8, 14101-14108.	3.2	6

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55	Intrinsic Activity of Metal Centers in Metal-Nitrogen-Carbon Single-Atom Catalysts for Hydrogen Peroxide Synthesis. <i>Journal of the American Chemical Society</i> , 2020, 142, 21861-21871.	6.6	163
56	Hydrogen coverage dependent C-C hydrogenation activity on Rh(111). <i>Chemical Physics Letters</i> , 2020, 746, 137287.	1.2	3
57	Catalytic activity atlas of ternary Co-Fe-V metal oxides for the oxygen evolution reaction. <i>Journal of Materials Chemistry A</i> , 2020, 8, 15951-15961.	5.2	43
58	Nitrogen-doped phosphorene for electrocatalytic ammonia synthesis. <i>Journal of Materials Chemistry A</i> , 2020, 8, 15875-15883.	5.2	88
59	Identify Zr Promotion Effects in Atomic Scale for Co-Based Catalysts in Fischer-Tropsch Synthesis. <i>ACS Catalysis</i> , 2020, 10, 7894-7906.	5.5	57
60	Pair-distribution-function guided optimization of fingerprints for atom-centered neural network potentials. <i>Journal of Chemical Physics</i> , 2020, 152, 224102.	1.2	8
61	Coupling N ₂ and CO ₂ in H ₂ O to synthesize urea under ambient conditions. <i>Nature Chemistry</i> , 2020, 12, 717-724.	6.6	485
62	Dual Single-Atomic Ni ₄ and Fe ₄ Sites Constructing Janus Hollow Graphene for Selective Oxygen Electrocatalysis. <i>Advanced Materials</i> , 2020, 32, e2003134.	11.1	376
63	PdAg Alloy Nanocatalysts: Toward Economically Viable Nitrite Reduction in Drinking Water. <i>ACS Catalysis</i> , 2020, 10, 7979-7989.	5.5	64
64	Cu _x Ir _{1-x} Nanoalloy Catalysts Achieve Near 100% Selectivity for Aqueous Nitrite Reduction to NH ₃ . <i>ACS Catalysis</i> , 2020, 10, 7915-7921.	5.5	69
65	Recent advances in carbon dioxide utilization. <i>Renewable and Sustainable Energy Reviews</i> , 2020, 125, 109799.	8.2	369
66	Sulfur Loading and Speciation Control the Hydrophobicity, Electron Transfer, Reactivity, and Selectivity of Sulfidized Nanoscale Zerovalent Iron. <i>Advanced Materials</i> , 2020, 32, e1906910.	11.1	204
67	Correlating surface chemistry and hydrophobicity of sulfidized nanoscale zerovalent iron with its reactivity and selectivity for denitration and dechlorination. <i>Chemical Engineering Journal</i> , 2020, 394, 124876.	6.6	79
68	Testing the predictive power of theory for Pd _x Ir _(100-x) alloy nanoparticles for the oxygen reduction reaction. <i>Journal of Materials Chemistry A</i> , 2020, 8, 8421-8429.	5.2	9
69	Design of a Pd-Au Nitrite Reduction Catalyst by Identifying and Optimizing Active Ensembles. <i>ACS Catalysis</i> , 2019, 9, 7957-7966.	5.5	160
70	Rational Design of Rhodium-Iridium Alloy Nanoparticles as Highly Active Catalysts for Acidic Oxygen Evolution. <i>ACS Nano</i> , 2019, 13, 13225-13234.	7.3	151
71	The adsorption and activation of oxygen molecule on nickel clusters doped graphene-based support by DFT. <i>Molecular Catalysis</i> , 2019, 477, 110547.	1.0	12
72	Non-Monotonic Trends of Hydrogen Adsorption on Single Atom Doped g-C ₃ N ₄ . <i>Catalysts</i> , 2019, 9, 84.	1.6	19

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73	Selectivity for ethanol partial oxidation: the unique chemistry of single-atom alloy catalysts on Au, Ag, and Cu(111). <i>Journal of Materials Chemistry A</i> , 2019, 7, 23868-23877.	5.2	80
74	Data-Mining for Processes in Chemistry, Materials, and Engineering. <i>Processes</i> , 2019, 7, 151.	1.3	36
75	Prediction of CO ₂ absorption by physical solvents using a chemoinformatics-based machine learning model. <i>Environmental Chemistry Letters</i> , 2019, 17, 1397-1404.	8.3	42
76	Sea-urchin-structure g-C ₃ N ₄ with narrow bandgap (E _g = 2.0 eV) for efficient overall water splitting under visible light irradiation. <i>Applied Catalysis B: Environmental</i> , 2019, 249, 275-281.	10.8	110
77	Oxidative Cross-Esterification and Related Pathways of Co-Adsorbed Oxygen and Ethanol on Pd@Au. <i>ACS Catalysis</i> , 2019, 9, 4516-4525.	5.5	28
78	Big to Small: Ultrafine Mo ₂ C Particles Derived from Giant Polyoxomolybdate Clusters for Hydrogen Evolution Reaction. <i>Small</i> , 2019, 15, e1900358.	5.2	53
79	Stabilizer-Free Cu ₂ Alloy Nanoparticle Catalysts. <i>Chemistry of Materials</i> , 2019, 31, 10225-10235.	3.2	16
80	Photoelectrochemical Synthesis of Ammonia on the Aerophilic-Hydrophilic Heterostructure with 37.8% Efficiency. <i>Chem</i> , 2019, 5, 617-633.	5.8	241
81	Defect Engineering Strategies for Nitrogen Reduction Reactions under Ambient Conditions. <i>Small Methods</i> , 2019, 3, 1800331.	4.6	199
82	A computational study of supported Cu-based bimetallic nanoclusters for CO oxidation. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 7508-7513.	1.3	17
83	Oxygen Reduction Reaction on Classically Immiscible Bimetallics: A Case Study of RhAu. <i>Journal of Physical Chemistry C</i> , 2018, 122, 2712-2716.	1.5	123
84	Oxygen Vacancy-Mediated Photocatalysis of BiOCl: Reactivity, Selectivity, and Perspectives. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 122-138.	7.2	871
85	Rapid Synthesis of Rhodium-Palladium Alloy Nanocatalysts. <i>ChemCatChem</i> , 2018, 10, 329-333.	1.8	19
86	Progress in enhancement of CO ₂ absorption by nanofluids: A mini review of mechanisms and current status. <i>Renewable Energy</i> , 2018, 118, 527-535.	4.3	252
87	Exploring the potential relationship between indoor air quality and the concentration of airborne culturable fungi: a combined experimental and neural network modeling study. <i>Environmental Science and Pollution Research</i> , 2018, 25, 3510-3517.	2.7	77
88	Effects of ensembles, ligand, and strain on adsorbate binding to alloy surfaces. <i>Journal of Chemical Physics</i> , 2018, 149, 174705.	1.2	193
89	Microwave-Assisted Synthesis of Classically Immiscible Ag-Ir Alloy Nanoparticle Catalysts. <i>ACS Catalysis</i> , 2018, 8, 11386-11397.	5.5	57
90	Ethanol Decomposition on Pd@Au Alloy Catalysts. <i>Journal of Physical Chemistry C</i> , 2018, 122, 22024-22032.	1.5	77

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91	Mining the intrinsic trends of CO ₂ solubility in blended solutions. <i>Journal of CO₂ Utilization</i> , 2018, 26, 496-502.	3.3	55
92	Machine learning predictive framework for CO ₂ thermodynamic properties in solution. <i>Journal of CO₂ Utilization</i> , 2018, 26, 152-159.	3.3	54
93	Functional Group Effects on the HOMO-LUMO Gap of g-C ₃ N ₄ . <i>Nanomaterials</i> , 2018, 8, 589.	1.9	42
94	Performance Prediction and Optimization of Solar Water Heater via a Knowledge-Based Machine Learning Method. <i>Advances in Computer and Electrical Engineering Book Series</i> , 2018, , 55-74.	0.2	4
95	PdAu Alloy Nanoparticle Catalysts: Effective Candidates for Nitrite Reduction in Water. <i>ACS Catalysis</i> , 2017, 7, 3268-3276.	5.5	89
96	Tunability of the Adsorbate Binding on Bimetallic Alloy Nanoparticles for the Optimization of Catalytic Hydrogenation. <i>Journal of the American Chemical Society</i> , 2017, 139, 5538-5546.	6.6	96
97	Solar Water Splitting and Nitrogen Fixation with Layered Bismuth Oxyhalides. <i>Accounts of Chemical Research</i> , 2017, 50, 112-121.	7.6	554
98	Design of high-performance water-in-glass evacuated tube solar water heaters by a high-throughput screening based on machine learning: A combined modeling and experimental study. <i>Solar Energy</i> , 2017, 142, 61-67.	2.9	137
99	Mechanistic insights on ethanol dehydrogenation on Pd-Au model catalysts: a combined experimental and DFT study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 30578-30589.	1.3	57
100	Computationally Assisted STEM and EXAFS Characterization of Tunable Rh/Au and Rh/Ag Bimetallic Nanoparticle Catalysts. <i>Microscopy and Microanalysis</i> , 2017, 23, 2030-2031.	0.2	10
101	Dehydrogenation Selectivity of Ethanol on Close-Packed Transition Metal Surfaces: A Computational Study of Monometallic, Pd/Au, and Rh/Au Catalysts. <i>Journal of Physical Chemistry C</i> , 2017, 121, 27504-27510.	1.5	96
102	Application of Artificial Neural Networks for Catalysis: A Review. <i>Catalysts</i> , 2017, 7, 306.	1.6	167
103	Quick Estimation Model for the Concentration of Indoor Airborne Culturable Bacteria: An Application of Machine Learning. <i>International Journal of Environmental Research and Public Health</i> , 2017, 14, 857.	1.2	37
104	Predictive Power of Machine Learning for Optimizing Solar Water Heater Performance: The Potential Application of High-Throughput Screening. <i>International Journal of Photoenergy</i> , 2017, 2017, 1-10.	1.4	49
105	Comparative Study on Theoretical and Machine Learning Methods for Acquiring Compressed Liquid Densities of 1,1,1,2,3,3,3-Heptafluoropropane (R227ea) via Song and Mason Equation, Support Vector Machine, and Artificial Neural Networks. <i>Applied Sciences (Switzerland)</i> , 2016, 6, 25.	1.3	25
106	Prediction of the physicochemical properties of woody biomass using linear prediction and artificial neural networks. <i>Energy Sources, Part A: Recovery, Utilization and Environmental Effects</i> , 2016, 38, 1569-1573.	1.2	9
107	Extreme learning machine: a new alternative for measuring heat collection rate and heat loss coefficient of water-in-glass evacuated tube solar water heaters. <i>SpringerPlus</i> , 2016, 5, 626.	1.2	8
108	Microwave-Assisted Synthesis of Pd ₁₀₀ -Au Alloy Nanoparticles: A Combined Experimental and Theoretical Assessment of Synthetic and Compositional Effects upon Catalytic Reactivity. <i>ACS Catalysis</i> , 2016, 6, 4882-4893.	5.5	54

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109	Facet-dependent solar ammonia synthesis of BiOCl nanosheets via a proton-assisted electron transfer pathway. <i>Nanoscale</i> , 2016, 8, 1986-1993.	2.8	242
110	Novel Method for Measuring the Heat Collection Rate and Heat Loss Coefficient of Water-in-Glass Evacuated Tube Solar Water Heaters Based on Artificial Neural Networks and Support Vector Machine. <i>Energies</i> , 2015, 8, 8814-8834.	1.6	32
111	Artificial Neural Networks-Based Software for Measuring Heat Collection Rate and Heat Loss Coefficient of Water-in-Glass Evacuated Tube Solar Water Heaters. <i>PLoS ONE</i> , 2015, 10, e0143624.	1.1	13
112	Artificial Neural Network Analysis of Xinhui Pericarpium & Citri Reticulatae Using Gas Chromatography - Mass Spectrometer - Automated Mass Spectral Deconvolution and Identification System. <i>Tropical Journal of Pharmaceutical Research</i> , 2015, 14, 2071.	0.2	5
113	User-friendly optimization approach of fed-batch fermentation conditions for the production of iturin A using artificial neural networks and support vector machine. <i>Electronic Journal of Biotechnology</i> , 2015, 18, 273-280.	1.2	35
114	Investigation of dust loading and culturable microorganisms of HVAC systems in 24 office buildings in Beijing. <i>Energy and Buildings</i> , 2015, 103, 166-174.	3.1	40
115	Probing the reactivity of microhydrated I^{\pm} nucleophile in the anionic gas phase $\text{S}_{\text{N}}2$ reaction. <i>Journal of Computational Chemistry</i> , 2015, 36, 844-852.	1.5	13
116	Efficient Visible Light Nitrogen Fixation with BiOBr Nanosheets of Oxygen Vacancies on the Exposed {001} Facets. <i>Journal of the American Chemical Society</i> , 2015, 137, 6393-6399.	6.6	1,468
117	Evaluation Models for Soil Nutrient Based on Support Vector Machine and Artificial Neural Networks. <i>Scientific World Journal</i> , The, 2014, 2014, 1-7.	0.8	25
118	Infrared Spectroscopic Study on the Modified Mechanism of Aluminum-Impregnated Bone Charcoal. <i>Journal of Spectroscopy</i> , 2014, 2014, 1-7.	0.6	5
119	Analysis of the Oil Content of Rapeseed Using Artificial Neural Networks Based on Near Infrared Spectral Data. <i>Journal of Spectroscopy</i> , 2014, 2014, 1-5.	0.6	9
120	Application of Artificial Neural Networks in predicting abrasion resistance of solution polymerized styrene-butadiene rubber based composites. , 2014, , .		3