

Kai Li

List of Publications by Year in descending order

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106
papers

6,516
citations

53794

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66911

78
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all docs

110
docs citations

110
times ranked

7176
citing authors

#	ARTICLE	IF	CITATIONS
1	Deciphering a Nanocarbon-Based Artificial Peroxidase: Chemical Identification of the Catalytically Active and Substrate-Binding Sites on Graphene Quantum Dots. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 7176-7180.	13.8	380
2	Synergistic Effect between Metal-Nitrogen-Carbon Sheets and NiO Nanoparticles for Enhanced Electrochemical Water Oxidation Performance. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 10530-10534.	13.8	301
3	Recent development in phosphors with different emitting colors via energy transfer. <i>Journal of Materials Chemistry C</i> , 2016, 4, 5507-5530.	5.5	269
4	A Hollow-Structured CuS@Cu ₂ S@Au Nanohybrid: Synergistically Enhanced Photothermal Efficiency and Photoswitchable Targeting Effect for Cancer Theranostics. <i>Advanced Materials</i> , 2017, 29, 1701266.	21.0	252
5	A novel greenish yellow-orange red Ba ₃ Y ₄ O ₉ :Bi ³⁺ ,Eu ³⁺ phosphor with efficient energy transfer for UV-LEDs. <i>Dalton Transactions</i> , 2015, 44, 20542-20550.	3.3	250
6	Sr ₂ Y ₈ (SiO ₄) ₆ O ₂ :Bi ³⁺ /Eu ³⁺ : a single-component white-emitting phosphor via energy transfer for UV w-LEDs. <i>Journal of Materials Chemistry C</i> , 2015, 3, 9989-9998.	5.5	199
7	In situ anchoring of Co ₉ S ₈ nanoparticles on N and S co-doped porous carbon tube as bifunctional oxygen electrocatalysts. <i>NPG Asia Materials</i> , 2016, 8, e308-e308.	7.9	164
8	Host-Sensitized Luminescence Properties in CaNb ₂ O ₆ :Ln ³⁺ (Ln ³⁺ = Eu ³⁺ /Tb ³⁺ /Dy ³⁺ /Sm ³⁺) Phosphors with Abundant Colors. <i>Inorganic Chemistry</i> , 2015, 54, 323-333.	4.0	157
9	Study of the Active Sites in Porous Nickel Oxide Nanosheets by Manganese Modulation for Enhanced Oxygen Evolution Catalysis. <i>ACS Energy Letters</i> , 2018, 3, 2150-2158.	17.4	131
10	Engineering Ultrathin C ₃ N ₄ Quantum Dots on Graphene as a Metal-Free Water Reduction Electrocatalyst. <i>ACS Catalysis</i> , 2018, 8, 3965-3970.	11.2	130
11	Site occupancy and photoluminescence properties of a novel deep-red-emitting phosphor NaMgGdTeO ₆ :Mn ⁴⁺ with perovskite structure for w-LEDs. <i>Journal of Luminescence</i> , 2018, 198, 155-162.	3.1	126
12	Deep red MGe ₄ O ₉ :Mn ⁴⁺ (M = Sr, Ba) phosphors: structure, luminescence properties and application in warm white light emitting diodes. <i>Journal of Materials Chemistry C</i> , 2016, 4, 6409-6416.	5.5	117
13	In Situ Designing a Gradient Li ⁺ Capture and Quasi-Spontaneous Diffusion Anode Protection Layer toward Long-Life Li ⁺ O ₂ Batteries. <i>Advanced Materials</i> , 2020, 32, e2004157.	21.0	114
14	A Solid Dual-Ions Transformation Route to S,N Co-Doped Carbon Nanotubes as Highly Efficient Metal-Free Catalysts for Organic Reactions. <i>Advanced Materials</i> , 2016, 28, 10679-10683.	21.0	107
15	A far-red-emitting NaMgLaTeO ₆ :Mn ⁴⁺ phosphor with perovskite structure for indoor plant growth. <i>Dyes and Pigments</i> , 2019, 162, 214-221.	3.7	107
16	Host-sensitized luminescence in LaNbO ₄ :Ln ³⁺ (Ln ³⁺ = Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 14 Chemistry Chemical Physics, 2015, 17, 4283-4292.	2.8	106
17	Photoluminescence and energy transfer properties of a novel molybdate KBaY(MoO ₄) ₃ :Ln ³⁺ (Ln ³⁺ = Tb ³⁺ ,) Tj ETQq1 1 0.784314 rgBT /Overlock Transactions, 2018, 47, 6995-7004.	3.3	103
18	Tunable luminescence and energy transfer properties in Ca ₈ MgLu(PO ₄) ₇ :Ce ³⁺ ,Tb ³⁺ ,Mn ²⁺ phosphors. <i>Journal of Materials Chemistry C</i> , 2015, 3, 4471-4481.	5.5	102

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19	The oxygen reduction reaction on Pt(111) and Pt(100) surfaces substituted by subsurface Cu: a theoretical perspective. <i>Journal of Materials Chemistry A</i> , 2015, 3, 11444-11452.	10.3	102
20	Rational Design of Multifunctional Fe ₂ O ₃ @TiO ₂ Nanocomposites with Enhanced Magnetic and Photoconversion Effects for Wide Applications: From Photocatalysis to Imaging-Guided Photothermal Cancer Therapy. <i>Advanced Materials</i> , 2018, 30, e1706747.	21.0	102
21	Photoluminescence properties of single-component white-emitting Ca ₉ Bi(PO ₄) ₇ :Ce ³⁺ , Tb ³⁺ , Mn ²⁺ phosphors for UV LEDs. <i>Journal of Materials Chemistry C</i> , 2015, 3, 7096-7104.		99
22	Sulfur-Doped Nickel Phosphide Nanoplates Arrays: A Monolithic Electrocatalyst for Efficient Hydrogen Evolution Reactions. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 26303-26311.	8.0	97
23	A novel deep red-emitting phosphor KMgLaTeO ₆ :Mn ⁴⁺ with high thermal stability and quantum yield for w-LEDs: structure, site occupancy and photoluminescence properties. <i>Dalton Transactions</i> , 2018, 47, 2501-2505.	3.3	91
24	An efficient rare-earth free deep red emitting phosphor for improving the color rendering of white light-emitting diodes. <i>Journal of Materials Chemistry C</i> , 2017, 5, 2927-2935.	5.5	88
25	Up-conversion luminescence and optical temperature sensing properties in novel KBaY(MoO ₄) ₃ :Yb ³⁺ , Er ³⁺ materials for temperature sensors. <i>Journal of Alloys and Compounds</i> , 2020, 816, 152554.	5.5	88
26	Resonance Emission Enhancement (REE) for Narrow Band Red-Emitting A ₂ GeF ₆ :Mn ⁴⁺ (A = Na, K, Rb, Cs) Phosphors Synthesized via a Precipitation-Cation Exchange Route. <i>Inorganic Chemistry</i> , 2017, 56, 11900-11910.	4.0	86
27	Site-Bi ³⁺ and Eu ³⁺ dual emissions in color-tunable Ca ₂ Y ₈ (SiO ₄) ₆ O ₂ :Bi ³⁺ , Eu ³⁺ phosphors prepared via sol-gel synthesis for potentially ratiometric temperature sensing. <i>Journal of Alloys and Compounds</i> , 2019, 787, 86-95.	5.5	82
28	Mechanistic Analysis-Guided Pd-Based Catalysts for Efficient Hydrogen Production from Formic Acid Dehydrogenation. <i>ACS Catalysis</i> , 2020, 10, 3921-3932.	11.2	82
29	Epitaxial Growth of CsPbX ₃ (X = Cl, Br, I) Perovskite Quantum Dots via Surface Chemical Conversion of Cs ₂ GeF ₆ Double Perovskites: A Novel Strategy for the Formation of Leadless Hybrid Perovskite Phosphors with Enhanced Stability. <i>Advanced Materials</i> , 2019, 31, e1807592.	21.0	81
30	Synthesis, Luminescence, and Energy-Transfer Properties of $\text{Na}_2\text{Ca}_4(\text{PO}_4)_2(\text{SiO}_4)_2\text{A}$ (A = Tl, Pb, Bi, Ba, Sr, Ca, Mg, Zn, Cd, Hg, Pb, Bi, Tl, Cs, Rb, K, Na, Li) Phosphors. <i>Inorganic Chemistry</i> , 2014, 53, 6743-6751.	4.0	79
31	Improved Doping and Emission Efficiencies of Mn-Doped CsPbCl ₃ Perovskite Nanocrystals via Nickel Chloride. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 4177-4184.	4.6	79
32	Achieving the Trade-Off between Selectivity and Activity in Semihydrogenation of Alkynes by Fabrication of (Asymmetrical Pd@Ag Core)@(CeO ₂) ₂ Shell Nanocatalysts via Auto-redox Reaction. <i>Advanced Materials</i> , 2017, 29, 1605332.	21.0	73
33	Photoluminescence and Energy Transfer Properties with Y ³⁺ /SiO ₄ Substituting Ba ²⁺ /PO ₄ in Ba ₃ Y(PO ₄) ₃ :Ce ³⁺ /Tb ³⁺ , Tb ³⁺ /Eu ³⁺ Phosphors for w-LEDs. <i>Inorganic Chemistry</i> , 2016, 55, 7593-7604.	4.0	69
34	Photoluminescence Properties of Efficient Blue-Emitting Phosphor $\text{Ca}_{1.65}\text{Sr}_{0.35}\text{SiO}_4\text{:Ce}^{3+}$: Color Tuning via the Substitutions of Si by Al/Ga/B. <i>Inorganic Chemistry</i> , 2015, 54, 7992-8002.	4.0	66
35	Tunable green to yellowish-orange phosphor Na ₃ LuSi ₂ O ₇ :Eu ²⁺ , Mn ²⁺ via energy transfer for UV-LEDs. <i>Journal of Materials Chemistry C</i> , 2015, 3, 11618-11628.	5.5	64
36	BaLu ₆ (Si ₂ O ₇) ₂ (Si ₃ O ₁₀):Ce ³⁺ , Tb ³⁺ : A novel blue-green emission phosphor via energy transfer for UV LEDs. <i>Dyes and Pigments</i> , 2017, 139, 701-707.	3.7	64

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37	Ce ³⁺ and Tb ³⁺ -doped lutetium-containing silicate phosphors: synthesis, structure refinement and photoluminescence properties. <i>Journal of Materials Chemistry C</i> , 2016, 4, 3443-3453.	5.5	60
38	Tunable blue-green emission and energy transfer properties in $\text{Ca}_3(\text{PO}_4)_2:\text{Eu}^{2+}$, Tb ³⁺ phosphors with high quantum efficiencies for UV-LEDs. <i>Dalton Transactions</i> , 2015, 44, 4683-4692.	3.3	56
39	Eu ³⁺ /Sm ³⁺ -doped Na ₂ BiMg ₂ (VO ₄) ₃ from substitution of Ca ²⁺ by Na ⁺ and Bi ³⁺ in Ca ₂ NaMg ₂ (VO) ₄ . <i>Dyes and Pigments</i> , 2018, 155, 258-264.	3.7	56
40	Improved Oxygen Reduction Activity in Heteronuclear FeCo-Codoped Graphene: A Theoretical Study. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 17273-17281.	6.7	56
41	Unravel the Catalytic Effect of Two-Dimensional Metal Sulfides on Polysulfide Conversions for Lithium-Sulfur Batteries. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 43560-43567.	8.0	52
42	Tunable-Color Luminescence via Energy Transfer in NaCa _{13/18} Mg _{5/18} PO ₄ :A (A =) Tj ETQq0 0 0 rgt /Overlock 10 Tf 50 542 Td (Eu ²⁺) Lighting. <i>Inorganic Chemistry</i> , 2014, 53, 12141-12150.	4.0	51
43	Photoluminescence properties and crystal field analysis of a novel red-emitting phosphor K ₂ BaGe ₈ O ₁₈ :Mn ⁴⁺ . <i>Dyes and Pigments</i> , 2017, 142, 69-76.	3.7	48
44	Light-Driven CO ₂ Reduction over Prussian Blue Analogues as Heterogeneous Catalysts. <i>ACS Catalysis</i> , 2022, 12, 89-100.	11.2	47
45	Design of broadband near-infrared Y _{0.57} La _{0.72} Sc _{2.71} (BO ₃) ₄ :Cr ³⁺ phosphors based on one-site occupation and their application in NIR light-emitting diodes. <i>Journal of Materials Chemistry C</i> , 2021, 9, 11761-11771.	5.5	46
46	Realizing a novel dazzling far-red-emitting phosphor NaLaCaTeO ₆ :Mn ⁴⁺ with high quantum yield and luminescence thermal stability via the ionic couple substitution of Na ⁺ +La ³⁺ for 2Ca ²⁺ in Ca ₃ TeO ₆ :Mn ⁴⁺ for indoor plant cultivation LEDs. <i>Chemical Communications</i> , 2019, 2019, 11095-11097.	4.1	45
47	Exceptional low-temperature CO sensing properties in novel KBaY(MoO ₄) ₃ :Yb ³⁺ , Ho ³⁺ materials based on FIR of Ho ³⁺ transitions ⁵ F ₅₍₁₎ → ⁵ I ₈ . <i>Journal of Materials Chemistry C</i> , 2022, 10, 6603-6610.	5.5	45
48	Rhodium and Nitrogen Codoped Graphene as a Bifunctional Electrocatalyst for the Oxygen Reduction Reaction and CO ₂ Reduction Reaction: Mechanism Insights. <i>Journal of Physical Chemistry C</i> , 2019, 123, 5176-5187.	3.1	44
49	Color Tuning from Greenish-Yellow to Orange-Red in Thermal-Stable KBaY(MoO ₄) ₃ :Dy ³⁺ , Eu ³⁺ Phosphors via Energy Transfer for UV W-LEDs. <i>ACS Applied Electronic Materials</i> , 2020, 2, 1735-1744.	4.3	43
50	First-Principles Study on Nitrobenzene-Doped Graphene as a Metal-Free Electrocatalyst for Oxygen Reduction Reaction. <i>Journal of Physical Chemistry C</i> , 2016, 120, 8804-8812.	3.1	42
51	CoN ₃ embedded graphene, a potential catalyst for the oxygen reduction reaction from a theoretical perspective. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 17670-17676.	2.8	41
52	A density functional study on the oxygen reduction reaction mechanism on FeN ₂ -doped graphene. <i>New Journal of Chemistry</i> , 2018, 42, 6873-6879.	2.8	41
53	Ultrathin g-C ₃ N ₄ Nanosheets Coupled with AgI ₃ as Highly Efficient Heterostructured Photocatalysts for Enhanced Visible-Light Photocatalytic Activity. <i>Chemistry - A European Journal</i> , 2015, 21, 17739-17747.	3.3	40
54	Deciphering a Nanocarbon-Based Artificial Peroxidase: Chemical Identification of the Catalytically Active and Substrate-Binding Sites on Graphene Quantum Dots. <i>Angewandte Chemie</i> , 2015, 127, 7282-7286.	2.0	39

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55	Dual-Site Single-Atom Catalysts with High Performance for Three-Way Catalysis. <i>Advanced Materials</i> , 2022, 34, e2201859.	21.0	39
56	An efficient green-emitting $\text{Ca}_{1.65}\text{Sr}_{0.35}\text{SiO}_4\text{:Eu}^{2+}$ phosphor for UV/n-UV w-LEDs: synthesis, luminescence and thermal properties. <i>Journal of Materials Chemistry C</i> , 2015, 3, 6341-6349.	5.5	37
57	Low-Temperature Solid-State Synthesis and Upconversion Luminescence Properties in $(\text{Na/Li})\text{Bi}(\text{MoO}_4)_2\text{:Yb}^{3+},\text{Er}^{3+}$ and Color Tuning in $(\text{Na/Li})\text{Bi}(\text{MoO}_4)_2\text{:Yb}^{3+},\text{Ho}^{3+},\text{Ce}^{3+}$ Phosphors. <i>Inorganic Chemistry</i> , 2019, 58, 6821-6831.	4.0	36
58	Crystalline Ni ₃ C as both carbon source and catalyst for graphene nucleation: a QM/MD study. <i>Scientific Reports</i> , 2015, 5, 12091.	3.3	35
59	Insight of Enhanced Redox Chemistry for Porous MoO ₂ Carbon-Derived Framework as Polysulfide Reservoir in Lithium-Sulfur Batteries. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 42286-42293.	8.0	35
60	Mutual energy transfer luminescent properties in novel CsGd(MoO ₄) ₂ :Yb ³⁺ ,Er ³⁺ /Ho ³⁺ phosphors for solid-state lighting and solar cells. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 4746-4754.	2.8	35
61	Achieving Efficient Red-Emitting Sr ₂ CaWO ₆ :Ln ³⁺ WO ₆ :Mn ⁴⁺ (Ln = La, Gd, Y, Lu, $\hat{\Gamma}$) Tj ETQq1 1 0.784314 Application via Facile Ion Substitution in Luminescence-Ignorable Sr ₂ (Ln,Ca)WO ₆ :Mn ⁴⁺ . <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 771-776.	1.0	35
62	A direct four-electron process on Fe ^N -doped graphene for the oxygen reduction reaction: a theoretical perspective. <i>RSC Advances</i> , 2017, 7, 23812-23819.	3.6	33
63	Synthesis of porous and metallic CoB nanosheets towards a highly efficient electrocatalyst for rechargeable Na-O ₂ batteries. <i>Energy and Environmental Science</i> , 2018, 11, 2833-2838.	30.8	33
64	Novel Intense Emission-Tunable Li _{1.5} La _{1.5} WO ₆ :Mn ⁴⁺ ,Nd ³⁺ ,Yb ³⁺ Material with Good Luminescence Thermal Stability for Potential Applications in c-Si Solar Cells and Plant-Cultivation Far-Red-NIR LEDs. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 16284-16294.	6.7	33
65	A highly active (102) surface-induced rapid degradation of a CuS nanotheranostic platform for <i>in situ</i> T ₁ -weighted magnetic resonance imaging-guided synergistic therapy. <i>Nanoscale</i> , 2019, 11, 12853-12857.	5.6	33
66	Wide-Band Excited YTiTaO ₆ : Eu ³⁺ /Er ³⁺ Phosphors: Structure Refinement, Luminescence Properties, and Energy Transfer Mechanisms. <i>Journal of Physical Chemistry C</i> , 2014, 118, 17983-17991.	3.1	31
67	Enhancing the energy transfer from Mn ⁴⁺ to Yb ³⁺ via a Nd ³⁺ bridge role in Ca ₃ La ₂ W ₂ O ₁₂ :Mn ⁴⁺ ,Nd ³⁺ ,Yb ³⁺ phosphors for spectral conversion of c-Si solar cells. <i>Dyes and Pigments</i> , 2019, 162, 990-997.	3.7	31
68	Interplay between local environments and photoluminescence of Eu ²⁺ in Ba ₂ Zr ₂ Si ₃ O ₁₂ : blue shift emission, optimal bond valence and luminescence mechanisms. <i>Journal of Materials Chemistry C</i> , 2015, 3, 3294-3303.	5.5	29
69	Ru ₄ Doped Graphene Oxide, a Highly Efficient Bifunctional Catalyst for Oxygen Reduction and CO ₂ Reduction from Computational Study. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 8136-8144.	6.7	29
70	MnO ₂ @ Graphene-oxide-scroll@TiO ₂ composite catalyst for low-temperature NH ₃ -SCR of NO with good steam and SO ₂ resistance obtained by low-temperature carbon-coating and selective atomic layer deposition. <i>Catalysis Science and Technology</i> , 2019, 9, 1602-1608.	4.1	28
71	Obtaining Efficiently Tunable Red Emission in Ca ₃ LnWO ₆ :Mn ⁴⁺ (Ln = La, Gd, Y, Lu, $\hat{\Gamma}$ = 0.1) Phosphors Derived from Nearly Nonluminescent Ca ₃ WO ₆ :Mn ⁴⁺ via Ionic Substitution Engineering for Solid-State Lighting. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 7256-7261.	6.7	28
72	The oxygen reduction reaction mechanism on Sn doped graphene as an electrocatalyst in fuel cells: a DFT study. <i>RSC Advances</i> , 2017, 7, 729-734.	3.6	27

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73	Synthesis and luminescence properties of a novel dazzling red-emitting phosphor NaSr ₃ SbO ₆ :Mn ⁴⁺ for UV/n-UV w-LEDs. Dalton Transactions, 2019, 48, 3187-3192.	3.3	27
74	Cr ³⁺ -doped borate phosphors for broadband near-infrared LED applications. Inorganic Chemistry Frontiers, 2022, 9, 2240-2251.	6.0	27
75	Ca ₃ La ₂ Te ₂ O ₁₂ :Mn ⁴⁺ ,Nd ³⁺ ,Yb ³⁺ : an efficient thermally-stable UV/visible far red/NIR broadband spectral converter for c-Si solar cells and plant-growth LEDs. Materials Chemistry Frontiers, 2019, 3, 403-413.	5.9	26
76	Synthesis and up-conversion luminescence properties of a novel Yb ³⁺ , Er ³⁺ co-doped Ca ₅ Mg ₄ (VO ₄) ₆ phosphor. Journal of Alloys and Compounds, 2018, 737, 767-773.	5.5	23
77	A Single-Atom Manipulation Approach for Synthesis of Atomically Mixed Nanoalloys as Efficient Catalysts. Angewandte Chemie - International Edition, 2020, 59, 13568-13574.	13.8	23
78	Theoretical insight into the catalytic activities of oxygen reduction reaction on transition metal N ₄ doped graphene. New Journal of Chemistry, 2018, 42, 9620-9625.	2.8	21
79	Near-Infrared Persistent Luminescence and Trap Reshuffling in Mn ⁴⁺ Doped Alkali Earth Metal Tungstates. Advanced Optical Materials, 2022, 10, 2101714.	7.3	20
80	DFT Study on the Methane Synthesis from Syngas on a Cerium-Doped Ni(111) Surface. Journal of Physical Chemistry C, 2016, 120, 23030-23043.	3.1	19
81	Effectively realizing broadband spectral conversion of UV/visible to near-infrared emission in (Na,K)Mg(La,Gd)TeO ₆ :Mn ⁴⁺ ,Nd ³⁺ ,Yb ³⁺ materials for c-Si solar cells via efficient energy transfer. Journal of Materials Chemistry C, 2018, 6, 7302-7310.	5.5	19
82	Phase Transformation and Thermal Decomposition Kinetics of a Mixed Rare Earth Concentrate. ACS Omega, 2018, 3, 17036-17041.	3.5	15
83	Lanthanide-centered luminescence evolution and potential anti-counterfeiting application of Tb ³⁺ /Eu ³⁺ grafted melamine cyanurate hydrogen-bonded triazine frameworks. Materials Chemistry Frontiers, 2019, 3, 579-586.	5.9	15
84	Color-Tunable Luminescence of Y ₄ Si ₂ N ₂ O ₇ :Ce ³⁺ , Tb ³⁺ , Dy ³⁺ Phosphors Prepared by the Soft-Chemical Ammonolysis Method. European Journal of Inorganic Chemistry, 2014, 2014, 1955-1964.	2.0	12
85	Insight into emission-tuning and luminescence thermal quenching investigations in NaLa _{1-x} Gd _x Ca ₄ W ₂ O ₁₂ :Mn ⁴⁺ phosphors via the ionic couple substitution of Na ⁺ + Ln ³⁺ (Ln = La, Gd) for 2Ca ²⁺ in Ca ₆ W ₂ O ₁₂ :Mn ⁴⁺ for plant-cultivation LED applications. Dalton Transactions, 2019, 48, 15936-15941.	3.3	12
86	Fe-porphyrin carbon matrix as a bifunctional catalyst for oxygen reduction and CO ₂ reduction from theoretical perspective. Molecular Physics, 2019, 117, 1805-1812.	1.7	12
87	Achievement of safer palladium nanocrystals by enlargement of {100} crystallographic facets. Nanotoxicology, 2017, 11, 907-922.	3.0	11
88	The reaction pathways of the oxygen reduction reaction on IrN ₄ doped divacancy graphene: A theoretical study. Journal of Molecular Graphics and Modelling, 2018, 80, 293-298.	2.4	11
89	Theoretical study of two-dimensional bis(iminothiolato)metal monolayers as promising electrocatalysts for carbon dioxide reduction. New Journal of Chemistry, 2020, 44, 12299-12306.	2.8	11
90	Ligand centered electrocatalytic efficient CO ₂ reduction reaction at low overpotential on single-atom Ni regulated molecular catalyst. Nano Research, 2022, 15, 5816-5823.	10.4	11

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91	Theoretical Investigation on the Reaction Pathways of the Oxygen Reduction Reaction on Graphene Codoped with Manganese and Phosphorus as a Potential Nonprecious Metal Catalyst. <i>ChemCatChem</i> , 2016, 8, 3353-3360.	3.7	10
92	A Density Functional Theory Study of the Two-Dimensional Bis(iminothiolato)metal Monolayers as Efficient Electrocatalysts for Oxygen Reduction Reaction. <i>Journal of Physical Chemistry C</i> , 2020, 124, 7803-7811.	3.1	10
93	A density functional theory study on 3d metal/graphene for the removal of CO from H ₂ feed gas in hydrogen fuel cells. <i>RSC Advances</i> , 2015, 5, 16394-16399.	3.6	9
94	Methylammonium cation deficient surface for enhanced binding stability at TiO ₂ /CH ₃ NH ₃ PbI ₃ interface. <i>Nano Research</i> , 2017, 10, 483-490.	10.4	8
95	Thermal Decomposition of CdS Nanowires Assisted by ZIF-67 to Induce the Formation of Co ₉ S ₈ -Based Carbon Nanomaterials with High Lithium-Storage Abilities. <i>ACS Applied Energy Materials</i> , 2018, 1, 6242-6249.	5.1	8
96	A Single-Atom Manipulation Approach for Synthesis of Atomically Mixed Nanoalloys as Efficient Catalysts. <i>Angewandte Chemie</i> , 2020, 132, 13670-13676.	2.0	8
97	FeRh and Nitrogen Codoped Graphene, a Highly Efficient Bifunctional Catalyst toward Oxygen Reduction and Oxygen Evolution Reactions. <i>Journal of Physical Chemistry C</i> , 2020, 124, 9142-9150.	3.1	8
98	Engineering Gadolinium-Integrated Tellurium Nanorods for Theory-Oriented Photonic Hyperthermia in the NIR-II Biowindow. <i>Small</i> , 2020, 16, 2003508.	10.0	7
99	Sinter-resistant and high-efficient Pt/CeO ₂ /NiAl ₂ O ₄ /Al ₂ O ₃ @SiO ₂ model catalysts with ϵ -composite energy traps. <i>Science China Chemistry</i> , 2020, 63, 519-525.	8.2	6
100	Theoretical insights on the oxygen-reduction reaction mechanism of LaN ₄ -embedded graphene. <i>Journal of Molecular Modeling</i> , 2018, 24, 14.	1.8	5
101	Selenium Vacancy Engineering Using Bi ₂ Se ₃ Nanodots for Boosting Highly Efficient Photonic Hyperthermia. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 48378-48385.	8.0	5
102	Searching for highly efficient multifunctional electrocatalysts based on the single metal doped graphitic carbon nitride. <i>Molecular Physics</i> , 2021, 119, .	1.7	3
103	Regulation of the electronic structure of perovskites to improve the electrocatalytic performance for the nitrogen-reduction reaction. <i>Journal of Materials Chemistry A</i> , 2022, 10, 2819-2825.	10.3	3
104	InnenrÄ¼cktitelbild: Deciphering a Nanocarbon-Based Artificial Peroxidase: Chemical Identification of the Catalytically Active and Substrate-Binding Sites on Graphene Quantum Dots (<i>Angew. Chem.</i> 24/2015). <i>Angewandte Chemie</i> , 2015, 127, 7305-7305.	2.0	2
105	Theoretical study on the two-dimensional bis(iminothiolato)rhodium as oxygen reduction reaction catalyst. <i>Molecular Physics</i> , 2021, 119, e1817593.	1.7	0
106	Density functional study on formic acid decomposition on Pd(111) surface: a revisit and comparison with other density functional methods. <i>Journal of Molecular Modeling</i> , 2021, 27, 285.	1.8	0