De-en Jiang

List of Publications by Year in descending order

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344 papers	27,102 citations	4120 87 h-index	8599 146 g-index
386 all docs	386 docs citations	386 times ranked	24198 citing authors

#	Article	IF	Citations
1	Sodium storage in triazine-based molecular organic electrodes: The importance of hydroxyl substituents. Chemical Engineering Journal, 2022, 430, 133055.	6.6	16
2	Newâ€Generation Carbonâ€Capture Ionic Liquids Regulated by Metalâ€Ion Coordination. ChemSusChem, 2022, 15, .	3.6	8
3	Ammonia synthesis on BaTiO_{2.5}H_{0.5}: computational insights into the role of hydrides. Physical Chemistry Chemical Physics, 2022, 24, 1496-1502.	1.3	4
4	Taâ€“TiOx nanoparticles as radical scavengers to improve the durability of Feâ€“Nâ€“C oxygen reduction catalysts. Nature Energy, 2022, 7, 281-289.	19.8	93
5	Mechanism for Acetone and Crotonaldehyde Production during Steam Reforming of Ethanol over La_{0.7}Sr_{0.3}MnO_{3â€“x} Perovskite: Evidence for a Shared C4 Aldol Addition Intermediate. ACS Catalysis, 2022, 12, 4358-4374.	5.5	3
6	Single Atoms Anchored in Hexagonal Boron Nitride for Propane Dehydrogenation from First Principles. ChemCatChem, 2022, 14, .	1.8	6
7	A Heteroleptic Gold Hydride Nanocluster for Efficient and Selective Electrocatalytic Reduction of CO₂ to CO. Journal of the American Chemical Society, 2022, 144, 5258-5262.	6.6	87
8	Adding MgCl₂ to Molten NaClâ^'UCl_n (n=3, 4): Insights from Firstâ€Principles Molecular Dynamics. ChemPhysChem, 2022, 23, .	1.0	2
9	Structural transformation and catalytic hydrogenation activity of amidinate-protected copper hydride clusters. Nature Communications, 2022, 13, 2082.	5.8	35
10	Ionic liquids for carbon capture. MRS Bulletin, 2022, 47, 395-404.	1.7	11
11	Defect-Regulated Frustrated-Lewis-Pair Behavior of Boron Nitride in Ambient Pressure Hydrogen Activation. Journal of the American Chemical Society, 2022, 144, 10688-10693.	6.6	17
12	How Water Attacks MXene. Chemistry of Materials, 2022, 34, 4975-4982.	3.2	44
13	Advancing Rare-Earth Separation by Machine Learning. Jacs Au, 2022, 2, 1428-1434.	3.6	16
14	Uncovering the Nature of Band Gap Engineering of Adsorption Energy by Elucidating an Adsorbate Bonding Mechanism on Two-Dimensional TiO₂(110). Journal of Physical Chemistry C, 2022, 126, 10677-10685.	1.5	3
15	Defect Engineering of Ceria Nanocrystals for Enhanced Catalysis via a High-Entropy Oxide Strategy. ACS Central Science, 2022, 8, 1081-1090.	5.3	25
16	Atomistic Insights into Structure and Dynamics of Neodymium(III) Complexation with a Bis-lactam Phenanthroline Ligand in the Organic Phase. ACS Omega, 2022, 7, 21317-21324.	1.6	5
17	Measuring and directing charge transfer in heterogenous catalysts. Nature Communications, 2022, 13, .	5.8	19
18	Theoretical Advances in Understanding and Designing the Active Sites for Hydrogen Evolution Reaction. ACS Catalysis, 2022, 12, 8404-8433.	5.5	72

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19	Atomically Precise Au₄₂ Nanorods with Longitudinal Excitons for an Intense Photothermal Effect. Journal of the American Chemical Society, 2022, 144, 12381-12389.	6.6	36
20	In Situ Strong Metalâ€“Support Interaction (SMSI) Affects Catalytic Alcohol Conversion. ACS Catalysis, 2021, 11, 1938-1945.	5.5	50
21	Understanding Superatomic Ag Nanohydrides. Small, 2021, 17, e2004808.	5.2	4
22	Band Gap as a Novel Descriptor for the Reactivity of 2D Titanium Dioxide and its Supported Pt Single Atom for Methane Activation. Journal of Physical Chemistry Letters, 2021, 12, 2484-2488.	2.1	8
23	Electrocatalytic synthesis of heterocycles from biomass-derived furfuryl alcohols. Nature Communications, 2021, 12, 1868.	5.8	28
24	Deep Learning Accelerated Determination of Hydride Locations in Metal Nanoclusters. Angewandte Chemie - International Edition, 2021, 60, 12289-12292.	7.2	23
25	Deep Learning Accelerated Determination of Hydride Locations in Metal Nanoclusters. Angewandte Chemie, 2021, 133, 12397-12400.	1.6	0
26	Benzene Ring Knitting Achieved by Ambientâ€Temperature Dehalogenation via Mechanochemical Ullmannâ€Type Reductive Coupling. Advanced Materials, 2021, 33, e2008685.	11.1	27
27	Facile Cr³⁺-Doping Strategy Dramatically Promoting Ru/CeO₂ for Low-Temperature CO₂ Methanation: Unraveling the Roles of Surface Oxygen Vacancies and Hydroxyl Groups. ACS Catalysis, 2021, 11, 5762-5775.	5.5	105
28	Design of Graphene/Ionic Liquid Composites for Carbon Capture. ACS Applied Materials & Interfaces, 2021, 13, 17511-17516.	4.0	17
29	Fabrication of Ionic Covalent Triazine Framework-Linked Membranes via a Facile Solâ€“Gel Approach. Chemistry of Materials, 2021, 33, 3386-3393.	3.2	20
30	Synthesis and Characterization of Macrocyclic Ionic Liquids for CO₂ Separation. Industrial & Engineering Chemistry Research, 2021, 60, 8218-8226.	1.8	6
31	Revealing the etching process of water-soluble Au25 nanoclusters at the molecular level. Nature Communications, 2021, 12, 3212.	5.8	32
32	Optimal Linear Water Density for Proton Transport in Tunnel Oxides. Journal of Physical Chemistry C, 2021, 125, 11508-11512.	1.5	2
33	Interfacial charge transfer and interaction in the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mrow><mml:mi>MXene</mml:mi><mml:mo>/</mml:mo><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> heterostructures. Physical Review Materials, 2021, 5, .	3.1	14
34	CO₂ Chemisorption Behavior of Coordinationâ€Derived Phenolate Sorbents. ChemSusChem, 2021, 14, 2854-2859.	3.6	9
35	Molecular Dynamics Simulations of Complexation of Am(III) with a Preorganized Dicationic Ligand in an Ionic Liquid. Journal of Physical Chemistry B, 2021, 125, 8532-8538.	1.2	7
36	Understanding the interaction between carboxylates and coinage metals from first principles. Journal of Chemical Physics, 2021, 155, 034301.	1.2	3

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37	CO 2 Chemisorption Behavior of Coordinationâ€Derived Phenolate Sorbents. ChemSusChem, 2021, 14, 2784-2784.	3.6	2
38	Fundamental Flaw in the Current Construction of the TiO₂ Electron Transport Layer of Perovskite Solar Cells and Its Elimination. ACS Applied Materials & Interfaces, 2021, 13, 39371-39378.	4.0	11
39	Titanium Carbide MXene Shows an Electrochemical Anomaly in Water-in-Salt Electrolytes. ACS Nano, 2021, 15, 15274-15284.	7.3	56
40	Molecular dynamics simulations of a dicationic ionic liquid for CO2 capture. Journal of Molecular Liquids, 2021, 335, 116163.	2.3	7
41	Effects of interlayer confinement and hydration on capacitive charge storage in birnessite. Nature Materials, 2021, 20, 1689-1694.	13.3	119
42	Locating Hydrides in Ligand-Protected Copper Nanoclusters by Deep Learning. ACS Applied Materials & Interfaces, 2021, 13, 53468-53474.	4.0	8
43	Single-Atom High-Temperature Catalysis on a Rh₁O₅ Cluster for Production of Syngas from Methane. Journal of the American Chemical Society, 2021, 143, 16566-16579.	6.6	22
44	Benchmark CO2 separation achieved by highly fluorinated nanoporous molecular sieve membranes from nonporous precursor via in situ cross-linking. Journal of Membrane Science, 2021, 638, 119698.	4.1	6
45	Proton dynamics in water confined at the interface of the grapheneâ€“MXene heterostructure. Journal of Chemical Physics, 2021, 155, 234707.	1.2	5
46	Understanding the conversion of ethanol to propene on In2O3 from first principles. Catalysis Today, 2020, 350, 19-24.	2.2	16
47	A new trick for an old support: Stabilizing gold single atoms on LaFeO3 perovskite. Applied Catalysis B: Environmental, 2020, 261, 118178.	10.8	31
48	Interlayer separation in hydrogen titanates enables electrochemical proton intercalation. Journal of Materials Chemistry A, 2020, 8, 412-421.	5.2	28
49	Understanding hydrogen in perovskites from first principles. Computational Materials Science, 2020, 174, 109461.	1.4	14
50	Molecular dynamics simulations of structural and transport properties of molten NaCl-UCl3 using the polarizable-ion model. Journal of Molecular Liquids, 2020, 299, 112184.	2.3	30
51	Proton Redox and Transport in MXene-Confined Water. ACS Applied Materials & Interfaces, 2020, 12, 763-770.	4.0	53
52	Transforming Porous Organic Cages into Porous Ionic Liquids via a Supramolecular Complexation Strategy. Angewandte Chemie, 2020, 132, 2288-2292.	1.6	21
53	Transforming Porous Organic Cages into Porous Ionic Liquids via a Supramolecular Complexation Strategy. Angewandte Chemie - International Edition, 2020, 59, 2268-2272.	7.2	101
54	Ethanol Conversion over La_{0.7}Sr_{0.3}MnO_{3â€“x}(100): Autocatalysis, Adjacent O-Vacancies, Disproportionation, and Dehydrogenation. ACS Catalysis, 2020, 10, 12920-12931.	5.5	6

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55	Electrode materialâ€“ionic liquid coupling for electrochemical energy storage. Nature Reviews Materials, 2020, 5, 787-808.	23.3	210
56	Hydrogen in Nanocatalysis. Journal of Physical Chemistry Letters, 2020, 11, 7049-7057.	2.1	18
57	Descriptors for Hydrogen Evolution on Single Atom Catalysts in Nitrogen-Doped Graphene. Journal of Physical Chemistry C, 2020, 124, 19571-19578.	1.5	75
58	Control of single-ligand chemistry on thiolated Au25 nanoclusters. Nature Communications, 2020, 11, 5498.	5.8	63
59	All-Carboxylate-Protected Superatomic Silver Nanocluster with an Unprecedented Rhombohedral Ag₈ Core. Journal of the American Chemical Society, 2020, 142, 16905-16909.	6.6	72
60	Stable Surface Terminations of a Perovskite Oxyhydride from First-Principles. Journal of Physical Chemistry C, 2020, 124, 18557-18563.	1.5	5
61	Sinter-Resistant Nanoparticle Catalysts Achieved by 2D Boron Nitride-Based Strong Metalâ€“Support Interactions: A New Twist on an Old Story. ACS Central Science, 2020, 6, 1617-1627.	5.3	42
62	Structure and Dynamics of Aqueous Electrolytes Confined in 2D-TiO2/Ti3C2T2 MXene Heterostructures. ACS Applied Materials & Interfaces, 2020, 12, 58378-58389.	4.0	25
63	First-principles study of heterostructures of MXene and nitrogen-doped graphene as anode materials for Li-ion batteries. Surfaces and Interfaces, 2020, 21, 100788.	1.5	9
64	Prediction by Convolutional Neural Networks of CO₂/N₂ Selectivity in Porous Carbons from N₂ Adsorption Isotherm at 77â€‰K. Angewandte Chemie, 2020, 132, 19813-19816.	1.6	7
65	Harnessing strong metalâ€“support interactions via a reverse route. Nature Communications, 2020, 11, 3042.	5.8	84
66	Prediction by Convolutional Neural Networks of CO₂/N₂ Selectivity in Porous Carbons from N₂ Adsorption Isotherm at 77â€‰K. Angewandte Chemie - International Edition, 2020, 59, 19645-19648.	7.2	26
67	Interactions between Ultrastable Na₄Ag₄₄(SR)₃₀ Nanoclusters and Coordinating Solvents: Uncovering the Atomic-Scale Mechanism. ACS Nano, 2020, 14, 8433-8441.	7.3	14
68	Nature of Terminating Hydroxyl Groups and Intercalating Water in Ti₃C₂T_x MXenes: A Study by ¹H Solid-State NMR and DFT Calculations. Journal of Physical Chemistry C, 2020, 124, 13649-13655.	1.5	35
69	Highly efficient electrocatalytic hydrogen evolution promoted by Oâ€“Moâ€“C interfaces of ultrafine Î²-Mo₂C nanostructures. Chemical Science, 2020, 11, 3523-3530.	3.7	54
70	Transformation Strategy for Highly Crystalline Covalent Triazine Frameworks: From Staggered AB to Eclipsed AA Stacking. Journal of the American Chemical Society, 2020, 142, 6856-6860.	6.6	136
71	Ion-gated carbon molecular sieve gas separation membranes. Journal of Membrane Science, 2020, 604, 118013.	4.1	15
72	Pseudocapacitance: From Fundamental Understanding to High Power Energy Storage Materials. Chemical Reviews, 2020, 120, 6738-6782.	23.0	1,020

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73	Mechanochemical synthesis of pillar[5]quinone derived multi-microporous organic polymers for radioactive organic iodide capture and storage. Nature Communications, 2020, 11, 1086.	5.8	87
74	The interplay between surface facet and reconstruction on isopropanol conversion over SrTiO3 nanocrystals. Journal of Catalysis, 2020, 384, 49-60.	3.1	19
75	Perovskite-supported Pt single atoms for methane activation. Journal of Materials Chemistry A, 2020, 8, 4362-4368.	5.2	31
76	Surpassing Robeson Upper Limit for CO2/N2 Separation with Fluorinated Carbon Molecular Sieve Membranes. CheM, 2020, 6, 631-645.	5.8	73
77	Highly Polar but Amorphous Polymers with Robust Membrane CO2/N2 Separation Performance. Joule, 2019, 3, 1881-1894.	11.7	60
78	Topotactic Synthesis of Phosphabenzeneâ€Functionalized Porous Organic Polymers: Efficient Ligands in CO 2 Conversion. Angewandte Chemie, 2019, 131, 13901-13905.	1.6	3
79	Methane Chemisorption on Oxideâ€Supported Pt Single Atom. ChemPhysChem, 2019, 20, 2217-2220.	1.0	19
80	Topotactic Synthesis of Phosphabenzeneâ€Functionalized Porous Organic Polymers: Efficient Ligands in CO₂Conversion. Angewandte Chemie - International Edition, 2019, 58, 13763-13767.	7.2	32
81	Entropic selectivity in air separation via a bilayer nanoporous graphene membrane. Physical Chemistry Chemical Physics, 2019, 21, 16310-16315.	1.3	3
82	Influence of fluorination on CO₂adsorption in materials derived from fluorinated covalent triazine framework precursors. Journal of Materials Chemistry A, 2019, 7, 17277-17282.	5.2	47
83	Insights into CO₂/N₂ Selectivity in Porous Carbons from Deep Learning. , 2019, 1, 558-563.		34
84	Real Time Monitoring of the Dynamic Intracluster Diffusion of Single Gold Atoms into Silver Nanoclusters. Journal of the American Chemical Society, 2019, 141, 18977-18983.	6.6	73
85	Confined Interlayer Water Promotes Structural Stability for High-Rate Electrochemical Proton Intercalation in Tungsten Oxide Hydrates. ACS Energy Letters, 2019, 4, 2805-2812.	8.8	88
86	Porous liquid zeolites: hydrogen bonding-stabilized H-ZSM-5 in branched ionic liquids. Nanoscale, 2019, 11, 1515-1519.	2.8	82
87	Computational screening of M/Cu core/shell nanoparticles and their applications for the electro-chemical reduction of CO₂ and CO. Nanoscale, 2019, 11, 11351-11359.	2.8	14
88	Effect of Hydrogen-Induced Metallization on Chemisorption. Journal of Physical Chemistry C, 2019, 123, 15171-15175.	1.5	3
89	Computational Discovery and Design of MXenes for Energy Applications: Status, Successes, and Opportunities. ACS Applied Materials & Interfaces, 2019, 11, 24885-24905.	4.0	105
90	Phosphoreneâ€Supported Transitionâ€Metal Dimer for Effective N₂ Electroreduction. ChemPhysChem, 2019, 20, 3141-3146.	1.0	24

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91	Elucidation of the Reaction Mechanism for High-Temperature Water Gas Shift over an Industrial-Type Copperâ€“Chromiumâ€“Iron Oxide Catalyst. Journal of the American Chemical Society, 2019, 141, 7990-7999.	6.6	60
92	Efficient Absorption of SO₂ by Deep Eutectic Solvents Formed by Biobased Aprotic Organic Compound Succinonitrile and 1-Ethyl-3-methylimidazolium Chloride. ACS Sustainable Chemistry and Engineering, 2019, 7, 9086-9091.	3.2	67
93	Interfacial and electronic properties of heterostructures of MXene and graphene. Physical Review B, 2019, 99, .	1.1	53
94	First-Principles Molecular Dynamics Simulations of UCl_nâ€“NaCl (n = 3, 4) Molten Salts. ACS Applied Energy Materials, 2019, 2, 2122-2128.	2.5	39
95	Density-Functional Tight-Binding for Platinum Clusters and Bulk: Electronic vs Repulsive Parameters. MRS Advances, 2019, 4, 1821-1832.	0.5	3
96	Continuously Tunable Pore Size for Gas Separation via a Bilayer Nanoporous Graphene Membrane. ACS Applied Nano Materials, 2019, 2, 379-384.	2.4	34
97	Deep eutectic solvents formed by quaternary ammonium salts and aprotic organic compound succinonitrile. Journal of Molecular Liquids, 2019, 274, 414-417.	2.3	23
98	Confined Ionic Liquid in an Ionic Porous Aromatic Framework for Gas Separation. ACS Applied Polymer Materials, 2019, 1, 95-102.	2.0	20
99	Structure and Interaction of Ionic Liquid Monolayer on Graphite from First-Principles. Journal of Physical Chemistry C, 2019, 123, 618-624.	1.5	8
100	Computational Screening of MXene Electrodes for Pseudocapacitive Energy Storage. Journal of Physical Chemistry C, 2019, 123, 315-321.	1.5	69
101	Three-orders-of-magnitude variation of carrier lifetimes with crystal phase of gold nanoclusters. Science, 2019, 364, 279-282.	6.0	149
102	Understanding the MXene Pseudocapacitance. Journal of Physical Chemistry Letters, 2018, 9, 1223-1228.	2.1	231
103	Fluorescence of Hydroxyphenyl-Substituted â€œClickâ€•Triazoles. Journal of Physical Chemistry A, 2018, 122, 2956-2973.	1.1	21
104	Selective CO Production by Photoelectrochemical Methane Oxidation on TiO₂. ACS Central Science, 2018, 4, 631-637.	5.3	56
105	Carbon Dioxide Separation: Highly Permeable Oligo(ethylene oxide)-co -poly(dimethylsiloxane) Membranes for Carbon Dioxide Separation (Adv. Sustainable Syst. 4/2018). Advanced Sustainable Systems, 2018, 2, 1870030.	2.7	1
106	Universal molecular-confined synthesis of interconnected porous metal oxides-N-C frameworks for electrocatalytic water splitting. Nano Energy, 2018, 48, 600-606.	8.2	61
107	Displacement of carbonates in Ca₂UO₂(CO₃)₃by amidoxime-based ligands from free-energy simulations. Dalton Transactions, 2018, 47, 1604-1613.	1.6	6
108	Interface Engineering of Earth-Abundant Transition Metals Using Boron Nitride for Selective Electroreduction of CO₂. ACS Applied Materials & Interfaces, 2018, 10, 6694-6700.	4.0	52

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109	Dopant-Dependent Electronic Structures Observed for M₂Au₃₆(SC₆H₁₃)₂₄ Clusters (M = Pt, Pd). Journal of Physical Chemistry Letters, 2018, 9, 982-989.	2.1	55
110	Highly Permeable Oligo(ethylene oxide)â€co â€poly(dimethylsiloxane) Membranes for Carbon Dioxide Separation. Advanced Sustainable Systems, 2018, 2, 1700113.	2.7	6
111	Thiolate-Protected Trimetallic Au_{â^¼20}Ag_{â^¼4}Pd and Au_{â^¼20}Ag_{â^¼4}Pt Alloy Clusters with Controlled Chemical Composition and Metal Positions. Journal of Physical Chemistry Letters, 2018, 9, 2590-2594.	2.1	55
112	SO₂absorption in EmimClâ€“TEG deep eutectic solvents. Physical Chemistry Chemical Physics, 2018, 20, 15168-15173.	1.3	76
113	Single rhodium atoms anchored in micropores for efficient transformation of methane under mild conditions. Nature Communications, 2018, 9, 1231.	5.8	213
114	Understanding Methanol Coupling on SrTiO3 from First Principles. Journal of Physical Chemistry C, 2018, 122, 7210-7216.	1.5	2
115	Stronger-than-Pt hydrogen adsorption in a Au₂₂ nanocluster for the hydrogen evolution reaction. Journal of Materials Chemistry A, 2018, 6, 7532-7537.	5.2	63
116	Trends of Alkane Activation on Doped Cobalt (II,â€…III) Oxide from First Principles. ChemCatChem, 2018, 10, 244-249.	1.8	25
117	Insights into Interfaces, Stability, Electronic Properties, and Catalytic Activities of Atomically Precise Metal Nanoclusters from First Principles. Accounts of Chemical Research, 2018, 51, 2793-2802.	7.6	231
118	Understanding the Binding of a Bifunctional Amidoximateâ€“Carboxylate Ligand with Uranyl in Seawater. Journal of Physical Chemistry B, 2018, 122, 12060-12066.	1.2	8
119	Effects of Metal-Doping on Hydrogen Evolution Reaction Catalyzed by MAu₂₄ and M₂Au₃₆ Nanoclusters (M = Pt, Pd). ACS Applied Materials & Interfaces, 2018, 10, 44645-44653.	4.0	81
120	Rationally designed metal nanocluster for electrocatalytic hydrogen production from water. Journal of Materials Chemistry A, 2018, 6, 19495-19501.	5.2	37
121	Understanding the Impact of Surface Reconstruction of Perovskite Catalysts on CH₄ Activation and Combustion. ACS Catalysis, 2018, 8, 10306-10315.	5.5	50
122	Golden single-atomic-site platinum electrocatalysts. Nature Materials, 2018, 17, 1033-1039.	13.3	266
123	Origins and Implications of Interfacial Capacitance Enhancements in C₆₀-Modified Graphene Supercapacitors. ACS Applied Materials & Interfaces, 2018, 10, 36860-36865.	4.0	23
124	New Bonding Model of Radical Adsorbate on Lattice Oxygen of Perovskites. Journal of Physical Chemistry Letters, 2018, 9, 6321-6325.	2.1	37
125	Revealing isoelectronic size conversion dynamics of metal nanoclusters by a noncrystallization approach. Nature Communications, 2018, 9, 1979.	5.8	88
126	Promotion of catalytic selectivity on transition metal oxide through restructuring surface lattice. Applied Catalysis B: Environmental, 2018, 237, 957-969.	10.8	20

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127	Effect of pore density on gas permeation through nanoporous graphene membranes. Nanoscale, 2018, 10, 14660-14666.	2.8	31
128	First-Principles Insight into Electrocatalytic Reduction of CO₂ to CH₄ on a Copper Nanoparticle. Journal of Physical Chemistry C, 2018, 122, 11392-11398.	1.5	56
129	Low-temperature activation of methane on doped single atoms: descriptor and prediction. Physical Chemistry Chemical Physics, 2018, 20, 22909-22914.	1.3	62
130	Supported bicyclic amidine ionic liquids as a potential CO2/N2 separation medium. Journal of Membrane Science, 2018, 565, 203-212.	4.1	24
131	First Principles Insight into H₂ Activation and Hydride Species on TiO₂ Surfaces. Journal of Physical Chemistry C, 2018, 122, 20323-20328.	1.5	44
132	Hetero-biicosahedral [Au₂₄Pd(PPh₃)₁₀(SC₂H₄Ph)₅Cl₂]<sup>+< nanocluster: selective synthesis and optical and electrochemical properties. Nanoscale, 2018, 10, 18969-18979.	2.8	51
133	Synthesis of Water-Soluble [Au₂₅(SR)₁₈]^{â^'} Using a Stoichiometric Amount of NaBH₄. Journal of the American Chemical Society, 2018, 140, 11370-11377.	6.6	90
134	Exploring perovskites for methane activation from first principles. Catalysis Science and Technology, 2018, 8, 702-709.	2.1	35
135	Exploring Structural Diversity and Fluxionality of Pt_n (n = 10â€“13) Clusters from First-Principles. Journal of Physical Chemistry C, 2017, 121, 10796-10802.	1.5	42
136	Computational insight into the capacitive performance of graphene edge planes. Carbon, 2017, 116, 278-285.	5.4	36
137	Hydrogen functionalisation of transition metal dichalcogenide monolayers from first principles. Molecular Simulation, 2017, 43, 379-383.	0.9	6
138	Impact of tuning CO2-philicity in polydimethylsiloxane-based membranes for carbon dioxide separation. Journal of Membrane Science, 2017, 530, 213-219.	4.1	31
139	Ion-Gated Gas Separation through Porous Graphene. Nano Letters, 2017, 17, 1802-1807.	4.5	109
140	A molecule-like PtAu24(SC6H13)18 nanocluster as an electrocatalyst for hydrogen production. Nature Communications, 2017, 8, 14723.	5.8	274
141	Computational Insights into Materials and Interfaces for Capacitive Energy Storage. Advanced Science, 2017, 4, 1700059.	5.6	176
142	Metallic Hydrogen in Atomically Precise Gold Nanoclusters. Chemistry of Materials, 2017, 29, 4840-4847.	3.2	70
143	General Structureâ€“Reactivity Relationship for Oxygen on Transition-Metal Oxides. Journal of Physical Chemistry Letters, 2017, 8, 2206-2211.	2.1	62
144	Highly Efficient Carbon Monoxide Capture by Carbanionâ€Functionalized Ionic Liquids through Câ€¦Site Interactions. Angewandte Chemie, 2017, 129, 6947-6951.	1.6	26

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145	RÃ¼cktitelbild: Highly Efficient Carbon Monoxide Capture by Carbanionâ€Functionalized Ionic Liquids through Câ€¦Site Interactions (Angew. Chem. 24/2017). Angewandte Chemie, 2017, 129, 7108-7108.	1.6	0
146	Highly Efficient Carbon Monoxide Capture by Carbanionâ€Functionalized Ionic Liquids through Câ€¦Site Interactions. Angewandte Chemie - International Edition, 2017, 56, 6843-6847.	7.2	83
147	Pdâ€Metalated Conjugated Nanoporous Polycarbazoles for Additiveâ€Free Cyanation of Aryl Halides: Boosting Catalytic Efficiency through Spatial Modulation. ChemSusChem, 2017, 10, 2320-2320.	3.6	0
148	Controlling Reaction Selectivity through the Surface Termination of Perovskite Catalysts. Angewandte Chemie, 2017, 129, 9952-9956.	1.6	19
149	Controlling Reaction Selectivity through the Surface Termination of Perovskite Catalysts. Angewandte Chemie - International Edition, 2017, 56, 9820-9824.	7.2	47
150	Lattice-Hydride Mechanism in Electrocatalytic CO₂ Reduction by Structurally Precise Copper-Hydride Nanoclusters. Journal of the American Chemical Society, 2017, 139, 9728-9736.	6.6	261
151	Alkynyl-protected silver nanoclusters featuring an anticuboctahedral kernel. Nanoscale, 2017, 9, 11405-11409.	2.8	73
152	Acidâ€“Base Reactivity of Perovskite Catalysts Probed via Conversion of 2-Propanol over Titanates and Zirconates. ACS Catalysis, 2017, 7, 4423-4434.	5.5	81
153	Capacitive Energy Extraction by Few-Layer Graphene Electrodes. Journal of Physical Chemistry C, 2017, 121, 14010-14018.	1.5	21
154	Pdâ€Metalated Conjugated Nanoporous Polycarbazoles for Additiveâ€Free Cyanation of Aryl Halides: Boosting Catalytic Efficiency through Spatial Modulation. ChemSusChem, 2017, 10, 2348-2351.	3.6	12
155	Design of Calix-Based Cages for CO₂ Capture. Industrial & Engineering Chemistry Research, 2017, 56, 4502-4507.	1.8	7
156	Solvation of the vanadate ion in seawater conditions from molecular dynamics simulations. Inorganica Chimica Acta, 2017, 458, 39-44.	1.2	10
157	Solvent Polarity Governs Ion Interactions and Transport in a Solvated Room-Temperature Ionic Liquid. Journal of Physical Chemistry Letters, 2017, 8, 167-171.	2.1	45
158	Understanding seed-mediated growth of gold nanoclusters at molecular level. Nature Communications, 2017, 8, 927.	5.8	228
159	Optimal Size of a Cylindrical Pore for Post-Combustion CO₂ Capture. Journal of Physical Chemistry C, 2017, 121, 22025-22030.	1.5	9
160	Identify the Removable Substructure in Carbon Activation. Chemistry of Materials, 2017, 29, 7288-7295.	3.2	51
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