Roger Rousseau

List of Publications by Year
in descending order

185	9,057	31902 53	51492 86
papers	citations	h-index	g-index

190	190	190	9336
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Dynamic formation of single-atom catalytic active sites on ceria-supported gold nanoparticles. Nature Communications, 2015, 6, 6511.	5.8	370
2	The Role of Reducible Oxideâ€“Metal Cluster Charge Transfer in Catalytic Processes: New Insights on the Catalytic Mechanism of CO Oxidation on Au/TiO₂ from ab Initio Molecular Dynamics. Journal of the American Chemical Society, 2013, 135, 10673-10683.	6.6	308
3	Thermally-driven processes on rutile TiO2(110)-(1Ã—1): A direct view at the atomic scale. Progress in Surface Science, 2010, 85, 161-205.	3.8	282
4	Water-Lean Solvents for Post-Combustion CO₂Capture: Fundamentals, Uncertainties, Opportunities, and Outlook. Chemical Reviews, 2017, 117, 9594-9624.	23.0	249
5	Distribution of Ti³⁺ Surface Sites in Reduced TiO₂. Journal of Physical Chemistry C, 2011, 115, 7562-7572.	1.5	235
6	First-Principles Study of Phenol Hydrogenation on Pt and Ni Catalysts in Aqueous Phase. Journal of the American Chemical Society, 2014, 136, 10287-10298.	6.6	226
7	Defining the Role of Excess Electrons in the Surface Chemistry of TiO₂. Journal of Physical Chemistry C, 2010, 114, 5891-5897.	1.5	202
8	Localized Electronic States from Surface Hydroxyls and Polarons in TiO₂(110). Journal of Physical Chemistry C, 2009, 113, 14583-14586.	1.5	196
9	Electrocatalytic Hydrogenation of Biomass-Derived Organics: A Review. Chemical Reviews, 2020, 120, 11370-11419.	23.0	185
10	Ethanol synthesis from syngas over Rh-based/SiO2 catalysts: A combined experimental and theoretical modeling study. Journal of Catalysis, 2010, 271, 325-342.	3.1	174
11	Pulling Monatomic Gold Wires with Single Molecules: AnAb InitioSimulation. Physical Review Letters, 2002, 89, 186402.	2.9	169
12	CO Oxidation on Au/TiO₂: Condition-Dependent Active Sites and Mechanistic Pathways. Journal of the American Chemical Society, 2016, 138, 10467-10476.	6.6	159
13	Interaction of short-chain alkane thiols and thiolates with small gold clusters: Adsorption structures and energetics. Journal of Chemical Physics, 2001, 115, 4776-4786.	1.2	136
14	Atomistic Simulation of Water Percolation and Proton Hopping in Nafion Fuel Cell Membrane. Journal of Physical Chemistry B, 2010, 114, 13681-13690.	1.2	125
15	Effects of La₂O₃ on the Mixed Higher Alcohols Synthesis from Syngas over Co Catalysts: A Combined Theoretical and Experimental Study. Journal of Physical Chemistry C, 2011, 115, 17440-17451.	1.5	119
16	Genesis and Stability of Hydronium Ions in Zeolite Channels. Journal of the American Chemical Society, 2019, 141, 3444-3455.	6.6	119
17	Inducing Desorption of Organic Molecules with a Scanning Tunneling Microscope: Theory and Experiments. Physical Review Letters, 2000, 85, 5372-5375.	2.9	112
18	(100) facets of Î³-Al2O3: The Active Surfaces for Alcohol Dehydration Reactions. Catalysis Letters, 2011, 141, 649-655.	1.4	105

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19	Highly active and stable MgAl2O4-supported Rh and Ir catalysts for methane steam reforming: A combined experimental and theoretical study. Journal of Catalysis, 2014, 316, 11-23.	3.1	104
20	Dehydration, dehydrogenation, and condensation of alcohols on supported oxide catalysts based on cyclic (WO₃)₃ and (MoO₃)₃ clusters. Chemical Society Reviews, 2014, 43, 7664-7680.	18.7	99
21	Polarization- and Azimuth-Resolved Infrared Spectroscopy of Water on TiO₂(110): Anisotropy and the Hydrogen-Bonding Network. Journal of Physical Chemistry Letters, 2012, 3, 778-784.	2.1	91
22	Assigning Protonation Patterns in Water Networks in Bacteriorhodopsin Based on Computed IR Spectra. Angewandte Chemie - International Edition, 2004, 43, 4804-4807.	7.2	90
23	Probing equilibrium of molecular and deprotonated water on TiO ₂ (110). Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 1801-1805.	3.3	90
24	Confinement effects and acid strength in zeolites. Nature Communications, 2021, 12, 2630.	5.8	90
25	Theoretical insights into the surface physics and chemistry of redox-active oxides. Nature Reviews Materials, 2020, 5, 460-475.	23.3	89
26	DFT+U Study on the Localized Electronic States and Their Potential Role During H₂O Dissociation and CO Oxidation Processes on CeO₂(111) Surface. Journal of Physical Chemistry C, 2013, 117, 23082-23089.	1.5	85
27	Evaluation of the aromaticity of borepin: synthesis and properties of 1-substituted borepins. Organometallics, 1993, 12, 3225-3231.	1.1	81
28	Dinitrogen Reduction by a Chromium(0) Complex Supported by a 16-Membered Phosphorus Macrocycle. Journal of the American Chemical Society, 2013, 135, 11493-11496.	6.6	81
29	Understanding the Role of Metal and Molecular Structure on the Electrocatalytic Hydrogenation of Oxygenated Organic Compounds. ACS Catalysis, 2019, 9, 9964-9972.	5.5	81
30	Detaching Thiolates from Copper and Gold Clusters:Â Which Bonds to Break?. Journal of the American Chemical Society, 2004, 126, 12103-12111.	6.6	79
31	Carboxyl intermediate formation via an in situ-generated metastable active site during water-gas shift catalysis. Nature Catalysis, 2019, 2, 916-924.	16.1	79
32	Anharmonicity and Confinement in Zeolites: Structure, Spectroscopy, and Adsorption Free Energy of Ethanol in H-ZSM-5. Journal of Physical Chemistry C, 2016, 120, 7172-7182.	1.5	77
33	Catalytic Dehydration of 2-Propanol on (WO₃)₃ Clusters on TiO₂(110). Journal of the American Chemical Society, 2008, 130, 5059-5061.	6.6	76
34	Comprehensive Thermodynamics of Nickel Hydride Bis(Diphosphine) Complexes: A Predictive Model through Computations. Organometallics, 2011, 30, 6108-6118.	1.1	76
35	A Combined Experimental and Theoretical Study on the Activity and Selectivity of the Electrocatalytic Hydrogenation of Aldehydes. ACS Catalysis, 2018, 8, 7645-7658.	5.5	76
36	Towards â€œMechanochemistryâ€• Mechanically Induced Isomerizations of Thiolateâ€“Gold Clusters. Angewandte Chemie - International Edition, 2003, 42, 2251-2253.	7.2	72

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37	Exploring the Electronic Structure of Elemental Lithium: From Small Molecules to Nanoclusters, Bulk Metal, and Surfaces. Chemistry - A European Journal, 2000, 6, 2982-2993.	1.7	71
38	Temperature-Dependent Conformational Transitions and Hydrogen-Bond Dynamics of the Elastin-Like Octapeptide GVG(VPGVG): A Molecular-Dynamics Study. Biophysical Journal, 2004, 86, 1393-1407.	0.2	68
39	Computing Free Energy Landscapes: Application to Ni-based Electrocatalysts with Pendant Amines for H₂ Production and Oxidation. ACS Catalysis, 2014, 4, 229-242.	5.5	68
40	The [(DT-TTF)2M(mnt)2] Family of Radical Ion Salts: From a Spin Ladder to Delocalised Conduction Electrons That Interact with Localised Magnetic Moments. Chemistry - A European Journal, 1999, 5, 2025-2039.	1.7	67
41	Quantum and Thermal Fluctuation Effects on the Photoabsorption Spectra of Clusters. Physical Review Letters, 2004, 92, 183401.	2.9	67
42	Defining Active Catalyst Structure and Reaction Pathways from ab Initio Molecular Dynamics and Operando XAFS: Dehydrogenation of Dimethylaminoborane by Rhodium Clusters. Journal of the American Chemical Society, 2009, 131, 10516-10524.	6.6	67
43	Toward Molecular Catalysts by Computer. Accounts of Chemical Research, 2015, 48, 248-255.	7.6	65
44	Folding and Unfolding of an Elastinlike Oligopeptide: â€œInverse Temperature Transition,â€•Reentrance, and Hydrogen-Bond Dynamics. Physical Review Letters, 2004, 92, 148101.	2.9	63
45	Understanding Heterolytic H₂ Cleavage and Water-Assisted Hydrogen Spillover on Fe₃O₄(001)-Supported Single Palladium Atoms. ACS Catalysis, 2019, 9, 7876-7887.	5.5	63
46	Effect of Collective Dynamics and Anharmonicity on Entropy in Heterogenous Catalysis: Building the Case for Advanced Molecular Simulations. ACS Catalysis, 2020, 10, 9236-9260.	5.5	63
47	Ethanol Conversion on Cyclic (MO3)3 (M = Mo, W) Clusters. Journal of Physical Chemistry C, 2014, 118, 4869-4877.	1.5	62
48	The Nature of Hydrogen Adsorption on Platinum in the Aqueous Phase. Angewandte Chemie - International Edition, 2019, 58, 3527-3532.	7.2	62
49	Structure and Dynamics of CO₂ on Rutile TiO₂(110)-1Ã—1. Journal of Physical Chemistry C, 2012, 116, 26322-26334.	1.5	60
50	Synthesis, Structure, and Bonding in Zirconocene Primary Phosphido (PHR-), Phosphinidene (PR2-), and Phosphide (P3-) Derivatives. Organometallics, 1994, 13, 1918-1926.	1.1	58
51	Polycarbon Ligand Chemistry:Â Electronic Interactions between a Mononuclear Ruthenium Fragment and a Cobaltâ^'Carbon Cluster Core. Organometallics, 1999, 18, 3885-3897.	1.1	56
52	Impact of pH on Aqueous-Phase Phenol Hydrogenation Catalyzed by Carbon-Supported Pt and Rh. ACS Catalysis, 2019, 9, 1120-1128.	5.5	55
53	An Organic Spin-Ladder Molecular Material. Angewandte Chemie International Edition in English, 1997, 36, 2324-2326.	4.4	54
54	The interaction of gold clusters with methanol molecules: Ab initio molecular dynamics of Aun+CH3OH and AunCH3OH. Journal of Chemical Physics, 2000, 112, 761-769.	1.2	54

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55	Environment of Metalâ€“Oâ€“Fe Bonds Enabling High Activity in CO₂ Reduction on Single Metal Atoms and on Supported Nanoparticles. Journal of the American Chemical Society, 2021, 143, 5540-5549.	6.6	54
56	Electronic Structure of Ruthenium(II) Polyynyl Complexes. Organometallics, 2001, 20, 4502-4509.	1.1	53
57	Electrochemically Tunable Protonâ€Coupled Electron Transfer in Pdâ€Catalyzed Benzaldehyde Hydrogenation. Angewandte Chemie - International Edition, 2020, 59, 1501-1505.	7.2	53
58	Structure, dynamics and vibrational spectrum of supercritical CO2/H2O mixtures from ab initio molecular dynamics as a function of water cluster formation. Physical Chemistry Chemical Physics, 2010, 12, 8759.	1.3	51
59	Ab initioSimulation of Phase Transitions and Dissociation ofH2Sat High Pressure. Physical Review Letters, 2000, 85, 1254-1257.	2.9	50
60	Low-Temperature Oxidation of Methanol to Formaldehyde on a Model Single-Atom Catalyst: Pd Atoms on Fe₃O₄(001). ACS Catalysis, 2019, 9, 10977-10982.	5.5	50
61	Carbon-supported Pt during aqueous phenol hydrogenation with and without applied electrical potential: X-ray absorption and theoretical studies of structure and adsorbates. Journal of Catalysis, 2018, 368, 8-19.	3.1	49
62	Mixed Threefold and Fourfold Carbon Coordination in Compressed<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>CO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2008, 100, 163002.	2.9	48
63	Secondary Bonding in Organopnicogen Compounds. Comparison of the Structures of Octamethyl-1,1'-distibaferrocene and Octamethyl-1,1'-diarsaferrocene. Organometallics, 1994, 13, 4067-4071.	1.1	47
64	Dimerization Induced Deprotonation of Water on RuO₂(110). Journal of Physical Chemistry Letters, 2014, 5, 3445-3450.	2.1	47
65	Structural Rearrangement of Auâ€“Pd Nanoparticles under Reaction Conditions: An ab Initio Molecular Dynamics Study. ACS Nano, 2017, 11, 1649-1658.	7.3	47
66	NWPEsSe: An Adaptive-Learning Global Optimization Algorithm for Nanosized Cluster Systems. Journal of Chemical Theory and Computation, 2020, 16, 3947-3958.	2.3	47
67	Steam reforming of hydrocarbons from biomass-derived syngas over MgAl2O4-supported transition metals and bimetallic IrNi catalysts. Applied Catalysis B: Environmental, 2016, 184, 142-152.	10.8	46
68	Norm-Conserving Pseudopotentials and Basis Sets To Explore Lanthanide Chemistry in Complex Environments. Journal of Chemical Theory and Computation, 2019, 15, 5987-5997.	2.3	46
69	Modeling protonated water networks in bacteriorhodopsin. Physical Chemistry Chemical Physics, 2004, 6, 1848-1859.	1.3	45
70	Theoretical Study of Syngas Hydrogenation to Methanol on the Polar Zn-Terminated ZnO(0001) Surface. Journal of Physical Chemistry C, 2012, 116, 15952-15961.	1.5	45
71	Toward control of surface reactions with a scanning tunneling microscope. Structure and dynamics of benzene desorption from a silicon surface. Journal of Chemical Physics, 2000, 113, 4412-4423.	1.2	44
72	Homogeneous Ni Catalysts for H2Oxidation and Production: An Assessment of Theoretical Methods, from Density Functional Theory to Post Hartreeâ^'Fock Correlated Wave-Function Theory. Journal of Physical Chemistry A, 2010, 114, 12716-12724.	1.1	44

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73	Structural Evidence of the Aromaticity of Borepins: A Comparison of 1-Chloroborepin and Tricarbonyl(1-chloroborepin)molybdenum. Angewandte Chemie International Edition in English, 1993, 32, 1065-1066.	4.4	41
74	Anticorrelation between Surface and Subsurface Point Defects and the Impact on the Redox Chemistry of TiO₂(110). ChemPhysChem, 2015, 16, 313-321.	1.0	41
75	Imaging Hindered Rotations of Alkoxy Species on TiO2(110). Journal of the American Chemical Society, 2009, 131, 17926-17932.	6.6	40
76	Growth of Ordered Ultrathin Tungsten Oxide Films on Pt(111). Journal of Physical Chemistry C, 2011, 115, 5773-5783.	1.5	40
77	Hydrogen Bonding Enhances the Electrochemical Hydrogenation of Benzaldehyde in the Aqueous Phase. Angewandte Chemie - International Edition, 2021, 60, 290-296.	7.2	40
78	Phase Stability and Broken-Symmetry Transition of Elemental Lithium up to 140 GPa. ChemPhysChem, 2005, 6, 1703-1706.	1.0	39
79	Comparative Investigation of Benzene Steam Reforming over Spinel Supported Rh and Ir Catalysts. ACS Catalysis, 2013, 3, 1133-1143.	5.5	39
80	Fluctuations and Bonding in Lithium Clusters. Physical Review Letters, 1998, 80, 2574-2577.	2.9	38
81	Ab Initio-Based Kinetic Modeling for the Design of Molecular Catalysts: The Case of H₂ Production Electrocatalysts. ACS Catalysis, 2015, 5, 5436-5452.	5.5	38
82	Oxidation, Reduction, and Condensation of Alcohols over (MO3)3 (M = Mo, W) Nanoclusters. Journal of Physical Chemistry C, 2014, 118, 22620-22634.	1.5	37
83	Directed Hydrogen Bond Placement: Low Viscosity Amine Solvents for CO₂ Capture. ACS Sustainable Chemistry and Engineering, 2019, 7, 7535-7542.	3.2	34
84	Single-Step Conversion of Ethanol to n-Butene over Ag-ZrO₂/SiO₂ Catalysts. ACS Catalysis, 2020, 10, 10602-10613.	5.5	34
85	Progress and challenges in self-healing cementitious materials. Journal of Materials Science, 2021, 56, 201-230.	1.7	34
86	Surface Density Dependent Catalytic Activity of Single Palladium Atoms Supported on Ceria**. Angewandte Chemie - International Edition, 2021, 60, 22769-22775.	7.2	34
87	Static Structure and Dynamical Correlations in High PressureH2S. Physical Review Letters, 1999, 83, 2218-2221.	2.9	33
88	A new stable organic metal based on the BEDO-TTF donor and the doubly charged nitroprusside anion, (BEDO-TTF)4[Fe(CN)5NO]. Journal of Materials Chemistry, 2000, 10, 2017-2023.	6.7	33
89	Deprotonated Water Dimers: The Building Blocks of Segmented Water Chains on Rutile RuO₂(110). Journal of Physical Chemistry C, 2015, 119, 23552-23558.	1.5	33
90	Dynamic Acid/Base Equilibrium in Single Component Switchable Ionic Liquids and Consequences on Viscosity. Journal of Physical Chemistry Letters, 2016, 7, 1646-1652.	2.1	33

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91	Coordination Sphere of Lanthanide Aqua Ions Resolved with Ab Initio Molecular Dynamics and X-ray Absorption Spectroscopy. Inorganic Chemistry, 2021, 60, 3117-3130.	1.9	33
92	Protonation Studies of a Mono-Dinitrogen Complex of Chromium Supported by a 12-Membered Phosphorus Macrocycle Containing Pendant Amines. Inorganic Chemistry, 2015, 54, 4827-4839.	1.9	32
93	Reconciling Work Functions and Adsorption Enthalpies for Implicit Solvent Models: A Pt (111)/Water Interface Case Study. Journal of Chemical Theory and Computation, 2020, 16, 2703-2715.	2.3	32
94	The role of quantum and thermal fluctuations upon properties of lithium clusters. Journal of Chemical Physics, 1999, 111, 5091-5101.	1.2	31
95	Vacancy-Assisted Diffusion of Alkoxy Species on Rutile<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mo stretchy="false">(</mml:mo><mml:mn>110</mml:mn><mml:mo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 567 Td (stretchy="fals	2.9	31
96	An In-Depth Correlation of the Perturbation of the Organicâ€“Inorganic Interface Topology, Electronic Structure, and Transport Properties within an Extended Series of 21 Metallic Pseudopolymorphs, â€³-(BEDT-TTF)4â‹…(guest)nâ‹…[Re6Q6Cl8], (Q=S, Se). Chemistry - A European Journal, 2002, 8, 3884-3900.	1.7	30
97	The Origin of Regioselectivity in 2â€Butanol Dehydration on Solid Acid Catalysts. ChemCatChem, 2011, 3, 1557-1561.	1.8	30
98	Origin of the Metal-to-Insulator Transition in H0.33MoO3. Inorganic Chemistry, 1997, 36, 4627-4632.	1.9	29
99	Ab initio molecular dynamics with enhanced sampling in heterogeneous catalysis. Catalysis Science and Technology, 2022, 12, 12-37.	2.1	29
100	Inverse Temperature Transition of a Biomimetic Elastin Model:Â Reactive Flux Analysis of Folding/Unfolding and Its Coupling to Solvent Dielectric Relaxationâ€. Journal of Physical Chemistry B, 2006, 110, 3576-3587.	1.2	28
101	Structure sensitivity of hydrogenolytic cleavage of endocyclic and exocyclic Câ€“C bonds in methylcyclohexane over supported iridium particles. Journal of Catalysis, 2013, 297, 70-78.	3.1	28
102	Protonation of Ferrous Dinitrogen Complexes Containing a Diphosphine Ligand with a Pendent Amine. Inorganic Chemistry, 2013, 52, 4026-4039.	1.9	28
103	Preparation, Characterization, and Catalytic Properties of Tungsten Trioxide Cyclic Trimers on FeO(111)/Pt(111). Journal of Physical Chemistry C, 2012, 116, 908-916.	1.5	27
104	Lewis acidic titanium species: the synthesis, structure, bonding and molecular modelling considerations of the complexes Ti(NR2)3Cl (Râ€,=â€,Me, Et). Canadian Journal of Chemistry, 1991, 69, 357-362.	0.6	26
105	Structure, dynamics and stability of water/scCO2/mineral interfaces from ab initio molecular dynamics simulations. Scientific Reports, 2015, 5, 14857.	1.6	26
106	Reinventing Design Principles for Developing Lowâ€Viscosity Carbon Dioxideâ€Binding Organic Liquids for Flue Gas Clean Up. ChemSusChem, 2017, 10, 636-642.	3.6	26
107	Molecular Level Investigation of CH₄ and CO₂ Adsorption in Hydrated Calciumâ€“Montmorillonite. Journal of Physical Chemistry C, 2018, 122, 1125-1134.	1.5	26
108	Bonding and conformational aspects of thiolato-bridged early-late heterobimetallics. Organometallics, 1991, 10, 3399-3403.	1.1	24

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109	Binding of Formic Acid on Anatase TiO₂(101). Journal of Physical Chemistry C, 2020, 124, 20228-20239.	1.5	24
110	Atomic Origins of the Self-Healing Function in Cementâ€“Polymer Composites. ACS Applied Materials & Interfaces, 2018, 10, 3011-3019.	4.0	23
111	Molecular Level Understanding of the Free Energy Landscape in Early Stages of Metalâ€“Organic Framework Nucleation. Journal of the American Chemical Society, 2019, 141, 6073-6081.	6.6	23
112	Ab initio molecular dynamics assessment of thermodynamic and transport properties in (K,Li)Cl and (K,) Tj ETQq0 0 0 rgBT /Overlock 10	2.3	23
113	The M(dddt)2 family of conducting complexes: [Ni(dddt)2]3(AuBr2)2, the first quasi-two-dimensional metal stable down to at least 1.3 K. Journal of Materials Chemistry, 1995, 5, 1633.	6.7	22
114	Dimerization of CO2 at High Pressure and Temperature. ChemPhysChem, 2005, 6, 1752-1756.	1.0	22
115	Insights into the physical and chemical properties of a cement-polymer composite developed for geothermal wellbore applications. Cement and Concrete Composites, 2019, 97, 279-287.	4.6	22
116	Influence of Ag metal dispersion on the thermal conversion of ethanol to butadiene over Ag-ZrO2/SiO2 catalysts. Journal of Catalysis, 2020, 386, 30-38.	3.1	22
117	Optimization of the main-group and late-transition-metal elemental structures: Gallium, boron, zinc, cadmium, and manganese. Physical Review B, 1992, 46, 12121-12131.	1.1	21
118	Activity of Cuâ€“Alâ€“Oxo Extra-Framework Clusters for Selective Methane Oxidation on Cu-Exchanged Zeolites. Jacs Au, 2021, 1, 1412-1421.	3.6	21
119	Site-Specific Imaging of Elemental Steps in Dehydration of Diols on TiO₂(110). ACS Nano, 2013, 7, 10414-10423.	7.3	20
120	Structureâ€“property reduced order model for viscosity prediction in single-component CO₂-binding organic liquids. Green Chemistry, 2016, 18, 6004-6011.	4.6	20
121	Shedding light on black titania. Nature Materials, 2018, 17, 856-857.	13.3	19
122	Mesoscopic Structure Facilitates Rapid CO₂ Transport and Reactivity in CO₂ Capture Solvents. Journal of Physical Chemistry Letters, 2018, 9, 5765-5771.	2.1	19
123	Norm-Conserving Pseudopotentials and Basis Sets to Explore Actinide Chemistry in Complex Environments. Journal of Chemical Theory and Computation, 2021, 17, 3360-3371.	2.3	19
124	Actinide Molten Salts: A Machine-Learning Potential Molecular Dynamics Study. ACS Applied Materials & Interfaces, 2021, 13, 53398-53408.	4.0	19
125	Understanding Metalâ€“Organic Framework Nucleation from a Solution with Evolving Graphs. Journal of the American Chemical Society, 2022, 144, 11099-11109.	6.6	19
126	Alcohol Dehydration on Monooxo Wâ•O and Dioxo Oâ•Wâ•O Species. Journal of Physical Chemistry Letters, 2012, 3, 2168-2172.	2.1	18

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127	Are Water-lean Solvent Systems Viable for Post-Combustion CO2 Capture?. Energy Procedia, 2017, 114, 756-763.	1.8	18
128	Electrochemically Tunable Protonâ€Coupled Electron Transfer in Pdâ€Catalyzed Benzaldehyde Hydrogenation. Angewandte Chemie, 2020, 132, 1517-1521.	1.6	18
129	Diffusion and Surface Segregation of Interstitial Ti Defects Induced by Electronic Metalâ€“Support Interactions on a Au/TiO₂ Nanocatalyst. ACS Catalysis, 2022, 12, 4455-4464.	5.5	17
130	A Combined Infrared Photodissociation and Theoretical Study of the Interaction of Ethanol with Small Gold Clusters. Journal of Physical Chemistry A, 2001, 105, 11197-11203.	1.1	16
131	Characterization of the Fermi surface of (BEDO-TTF)5[CsHg(SCN)4]2 by magnetoresistance measurements and tight-binding band structure calculations. Journal of Materials Chemistry, 2002, 12, 483-488.	6.7	16
132	OH Group Dynamics of 1,3-Propanediol on TiO2(110). Journal of Physical Chemistry Letters, 2012, 3, 3257-3263.	2.1	16
133	Impact of Nonadiabatic Charge Transfer on the Rate of Redox Chemistry of Carbon Oxides on Rutile TiO₂(110) Surface. ACS Catalysis, 2015, 5, 1764-1771.	5.5	16
134	Molecularâ€Level Overhaul of Î³â€Aminopropyl Aminosilicone/Triethylene Glycol Postâ€Combustion CO₂â€Capture Solvents. ChemSusChem, 2020, 13, 3429-3438.	3.6	16
135	Electronic Structure of Layered Oxides Containing M2O7(M = V, Nb) Double Octahedral Slabs. Inorganic Chemistry, 1996, 35, 1179-1184.	1.9	15
136	Structure and Phase Stability of Binary Zintl-Phase Compounds: Lithiumâ€“Group 13 Intermetallics and Metal-Doped Group 14 Clathrate Compounds. Chemistry - A European Journal, 2002, 8, 2787.	1.7	15
137	Evaluating Transformational Solvent Systems for Post-combustion CO2 Separations. Energy Procedia, 2014, 63, 8144-8152.	1.8	15
138	Phase-Change Aminopyridines as Carbon Dioxide Capture Solvents. Industrial & Engineering Chemistry Research, 2017, 56, 7534-7540.	1.8	14
139	Formation of Supported Graphene Oxide: Evidence for Enolate Species. Journal of the American Chemical Society, 2018, 140, 5102-5109.	6.6	14
140	The Role of Ir in Ternary Rh-Based Catalysts for Syngas Conversion to C2 + Oxygenates. Topics in Catalysis, 2012, 55, 595-600.	1.3	13
141	Electro-reduction of organics on metal cathodes: A multiscale-modeling study of benzaldehyde on Au (111). Catalysis Today, 2020, 350, 39-46.	2.2	13
142	An evaluation of the rotational barrier about the Bî—¸N bond of 1-aminoborepins. Journal of Organometallic Chemistry, 1994, 468, 21-23.	0.8	12
143	Heterogeneous catalysis in complex, condensed reaction media. Catalysis Today, 2017, 289, 231-236.	2.2	12
144	Structure and Stability of the Ionic Liquid Clusters [EMIM]_n[BF₄]_{n+1}^{â€“} (n = 1â€“9): Implications for Electrochemical Separations. Journal of Physical Chemistry Letters, 2020, 11, 6844-6851.	2.1	12

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145	First-principle investigation on catalytic hydrogenation of benzaldehyde over Pt-group metals. Catalysis Today, 2022, 388-389, 208-215.	2.2	12
146	Selective acetylene hydrogenation over single metal atoms supported on Fe3O4(001): A first-principle study. Journal of Chemical Physics, 2020, 152, 154703.	1.2	12
147	Hydrogen Bonding Enhances the Electrochemical Hydrogenation of Benzaldehyde in the Aqueous Phase. Angewandte Chemie, 2021, 133, 294-300.	1.6	12
148	A Combined Spectroelectrochemical and Computational Study of the Chemically Reversible 2-Electron Reduction of [Ru4(Î¼-RC2R)2(CO)11] Clusters. Organometallics, 2005, 24, 1284-1292.	1.1	11
149	Dynamics, Stability, and Adsorption States of Water on Oxidized RuO₂(110). Journal of Physical Chemistry C, 2017, 121, 18505-18515.	1.5	11
150	How Collective Phenomena Impact CO₂ Reactivity and Speciation in Different Media. Journal of Physical Chemistry A, 2020, 124, 3963-3975.	1.1	11
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