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	First-principle investigation on catalytic hydrogenation of benzaldehyde over Pt-group metals. Catalysis Today, 2022, 388-389, 208-215.	2.2	12
2	Ab initio molecular dynamics with enhanced sampling in heterogeneous catalysis. Catalysis Science and Technology, 2022, 12, 12-37.	2.1	29
3	Impact of functional groups on the electrocatalytic hydrogenation of aromatic carbonyls to alcohols. Catalysis Today, 2022, 397-399, 63-68.	2.2	5
4	Understanding Adsorption of Organics on Pt(111) in the Aqueous Phase: Insights from DFT Based Implicit Solvent and Statistical Thermodynamics Models. Journal of Chemical Theory and Computation, 2022, 18, 1849-1861.	2.3	7
5	The interfacial compatibility between a potential CO2 separation membrane and capture solvents. Carbon Capture Science & Technology, 2022, 2, 100037.	4.9	9
6	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
7	Advanced Theory and Simulation to Guide the Development of CO₂ Capture Solvents. ACS Omega, 2022, 7, 12453-12466.	1.6	2
8	Tuning the Charge and Hydrophobicity of Graphene Oxide Membranes by Functionalization with Ionic Liquids at Epoxide Sites. ACS Applied Materials & Interfaces, 2022, 14, 19031-19042.	4.0	6
9	Understanding Metalâ€“Organic Framework Nucleation from a Solution with Evolving Graphs. Journal of the American Chemical Society, 2022, 144, 11099-11109.	6.6	19
10	Hydrogen Bonding Enhances the Electrochemical Hydrogenation of Benzaldehyde in the Aqueous Phase. Angewandte Chemie, 2021, 133, 294-300.	1.6	12
11	Hydrogen Bonding Enhances the Electrochemical Hydrogenation of Benzaldehyde in the Aqueous Phase. Angewandte Chemie - International Edition, 2021, 60, 290-296.	7.2	40
12	Atomic scale understanding of organic anion separations using ion-exchange resins. Journal of Membrane Science, 2021, 624, 118890.	4.1	5
13	Progress and challenges in self-healing cementitious materials. Journal of Materials Science, 2021, 56, 201-230.	1.7	34
14	Creating self-assembled arrays of mono-oxo (MoO ₃) ₁ species on TiO ₂ (101) via deposition and decomposition of (MoO ₃) _n oligomers. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	10
15	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
16	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
17	Graphene Oxide as a Pb(II) Separation Medium: Has Part of the Story Been Overlooked?. Jacs Au, 2021, 1, 766-776.	3.6	9
18	Conversion of Formic Acid on Single- and Nano-Crystalline Anatase TiO₂(101). Journal of Physical Chemistry C, 2021, 125, 7686-7700.	1.5	10

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19	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
20	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
21	Confinement effects and acid strength in zeolites. Nature Communications, 2021, 12, 2630.	5.8	90
22	Binding and stability of MgO monomers on anatase TiO2(101). Journal of Chemical Physics, 2021, 154, 204703.	1.2	3
23	Surface Density Dependent Catalytic Activity of Single Palladium Atoms Supported on Ceria**. Angewandte Chemie - International Edition, 2021, 60, 22769-22775.	7.2	34
24	Surface Density Dependent Catalytic Activity of Single Palladium Atoms Supported on Ceria**. Angewandte Chemie, 2021, 133, 22951.	1.6	0
25	The role of sub-surface hydrogen on CO2 reduction and dynamics on Ni(110): An ab initio molecular dynamics study. Journal of Chemical Physics, 2021, 155, 044702.	1.2	2
26	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
27	Actinide Molten Salts: A Machine-Learning Potential Molecular Dynamics Study. ACS Applied Materials & Interfaces, 2021, 13, 53398-53408.	4.0	19
28	AMPHIPHILIC WATERâ€LEAN CARBON CAPTURE SOLVENT WETTING BEHAVIOR VIA DECOMPOSITION BY STAINLESSâ€STEEL INTERFACES. ChemSusChem, 2021, 14, 5283-5292.	3.6	1
29	Computational and Experimental Study for the Denitrification of Biomass-Derived Hydrothermal Liquefaction Oil. ACS Sustainable Chemistry and Engineering, 2021, 9, 13406-13413.	3.2	1
30	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
31	Electrochemically Tunable Protonâ€Coupled Electron Transfer in Pdâ€Catalyzed Benzaldehyde Hydrogenation. Angewandte Chemie - International Edition, 2020, 59, 1501-1505.	7.2	53
32	Electrochemically Tunable Protonâ€Coupled Electron Transfer in Pdâ€Catalyzed Benzaldehyde Hydrogenation. Angewandte Chemie, 2020, 132, 1517-1521.	1.6	18
33	Polymer-cement composites with adhesion and re-adhesion (healing) to casing capability for geothermal wellbore applications. Cement and Concrete Composites, 2020, 107, 103490.	4.6	9
34	Impact of Cr and Co on 99Tc retention in magnetite: A combined study of ab initio molecular dynamics and experiments. Journal of Hazardous Materials, 2020, 387, 121721.	6.5	3
35	Synthesizing Clean Transportation Fuels from CO₂ Will at Least Quintuple the Demand for Non-carbogenic Electricity in the United States. Energy & Fuels, 2020, 34, 15433-15442.	2.5	9
36	Single-Step Conversion of Ethanol to n-Butene over Ag-ZrO₂/SiO₂ Catalysts. ACS Catalysis, 2020, 10, 10602-10613.	5.5	34

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37	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
38	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
39	On the Role of Enthalpic and Entropic Contributions to the Conformational Free Energy Landscape of MILâ€101(Cr) Secondary Building Units. Advanced Theory and Simulations, 2020, 3, 2000092.	1.3	7
40	Electrocatalytic Hydrogenation of Biomass-Derived Organics: A Review. Chemical Reviews, 2020, 120, 11370-11419.	23.0	185
41	Binding of Formic Acid on Anatase TiO₂(101). Journal of Physical Chemistry C, 2020, 124, 20228-20239.	1.5	24
42	Subtle changes in hydrogen bond orientation result in glassification of carbon capture solvents. Physical Chemistry Chemical Physics, 2020, 22, 19009-19021.	1.3	3
43	Single-Atom Catalysis: An Analogy between Heterogeneous and Homogeneous Catalysts. ACS Symposium Series, 2020, , 1-15.	0.5	1
44	Molecularâ€Level Overhaul of Î³â€Aminopropyl Aminosilicone/Triethylene Glycol Postâ€Combustion CO₂â€Capture Solvents. ChemSusChem, 2020, 13, 3429-3438.	3.6	16
45	NWPEsSe: An Adaptive-Learning Global Optimization Algorithm for Nanosized Cluster Systems. Journal of Chemical Theory and Computation, 2020, 16, 3947-3958.	2.3	47
46	Theoretical insights into the surface physics and chemistry of redox-active oxides. Nature Reviews Materials, 2020, 5, 460-475.	23.3	89
47	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
48	How Collective Phenomena Impact CO₂ Reactivity and Speciation in Different Media. Journal of Physical Chemistry A, 2020, 124, 3963-3975.	1.1	11
49	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
50	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
51	Mechanistic Understanding of Catalytic Conversion of Ethanol to 1-Butene over 2D-Pillared MFI Zeolite. Journal of Physical Chemistry C, 2020, 124, 28437-28447.	1.5	9
52	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
53	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
54	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

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55	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
56	Genesis and Stability of Hydronium Ions in Zeolite Channels. Journal of the American Chemical Society, 2019, 141, 3444-3455.	6.6	119
57	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
58	Directed Hydrogen Bond Placement: Low Viscosity Amine Solvents for CO₂ Capture. ACS Sustainable Chemistry and Engineering, 2019, 7, 7535-7542.	3.2	34
59	Molecular Simulation of the Catalytic Regeneration of ⁿBuLi through a Hydrometalation Route. Inorganic Chemistry, 2019, 58, 3033-3040.	1.9	2
60	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
61	The Nature of Hydrogen Adsorption on Platinum in the Aqueous Phase. Angewandte Chemie, 2019, 131, 3565-3570.	1.6	2
62	Impact of pH on Aqueous-Phase Phenol Hydrogenation Catalyzed by Carbon-Supported Pt and Rh. ACS Catalysis, 2019, 9, 1120-1128.	5.5	55
63	The Nature of Hydrogen Adsorption on Platinum in the Aqueous Phase. Angewandte Chemie - International Edition, 2019, 58, 3527-3532.	7.2	62
64	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
65	Formation of Supported Graphene Oxide: Evidence for Enolate Species. Journal of the American Chemical Society, 2018, 140, 5102-5109.	6.6	14
66	Atomic Origins of the Self-Healing Function in Cementâ€“Polymer Composites. ACS Applied Materials & Interfaces, 2018, 10, 3011-3019.	4.0	23
67	Molecular Level Investigation of CH₄ and CO₂ Adsorption in Hydrated Calciumâ€“Montmorillonite. Journal of Physical Chemistry C, 2018, 122, 1125-1134.	1.5	26
68	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
69	Shedding light on black titania. Nature Materials, 2018, 17, 856-857.	13.3	19
70	Mesoscopic Structure Facilitates Rapid CO₂ Transport and Reactivity in CO₂ Capture Solvents. Journal of Physical Chemistry Letters, 2018, 9, 5765-5771.	2.1	19
71	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
72	Structural Rearrangement of Auâ€“Pd Nanoparticles under Reaction Conditions: An ab Initio Molecular Dynamics Study. ACS Nano, 2017, 11, 1649-1658.	7.3	47

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73	Trends in Homolytic Bond Dissociation Energies of Five- and Six-Coordinate Hydrides of Group 9 Transition Metals: Co, Rh, Ir. Journal of Physical Chemistry A, 2017, 121, 1993-2000.	1.1	2
74	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
75	Water-Lean Solvents for Post-Combustion CO₂Capture: Fundamentals, Uncertainties, Opportunities, and Outlook. Chemical Reviews, 2017, 117, 9594-9624.	23.0	249
76	Phase-Change Aminopyridines as Carbon Dioxide Capture Solvents. Industrial & Engineering Chemistry Research, 2017, 56, 7534-7540.	1.8	14
77	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
78	Integrated Solvent Design for CO2 Capture and Viscosity Tuning. Energy Procedia, 2017, 114, 726-734.	1.8	10
79	Are Water-lean Solvent Systems Viable for Post-Combustion CO2 Capture?. Energy Procedia, 2017, 114, 756-763.	1.8	18
80	Dynamics, Stability, and Adsorption States of Water on Oxidized RuO₂(110). Journal of Physical Chemistry C, 2017, 121, 18505-18515.	1.5	11
81	Heterogeneous catalysis in complex, condensed reaction media. Catalysis Today, 2017, 289, 231-236.	2.2	12
82	Light Makes a Surface Banana-Bond Split: Photodesorption of Molecular Hydrogen from RuO2(110). Journal of the American Chemical Society, 2016, 138, 8714-8717.	6.6	9
83	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
84	Structureâ€"property reduced order model for viscosity prediction in single-component CO₂-binding organic liquids. Green Chemistry, 2016, 18, 6004-6011.	4.6	20
85	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
86	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
87	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
88	Structure, dynamics and stability of water/scCO2/mineral interfaces from ab initio molecular dynamics simulations. Scientific Reports, 2015, 5, 14857.	1.6	26
89	Toward Molecular Catalysts by Computer. Accounts of Chemical Research, 2015, 48, 248-255.	7.6	65
90	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

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91	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
92	Dynamic formation of single-atom catalytic active sites on ceria-supported gold nanoparticles. Nature Communications, 2015, 6, 6511.	5.8	370
93	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
94	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
95	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
96	Ethanol Conversion on Cyclic (MO3)3 (M = Mo, W) Clusters. Journal of Physical Chemistry C, 2014, 118, 4869-4877.	1.5	62
97	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
98	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
99	Dimerization Induced Deprotonation of Water on RuO₂(110). Journal of Physical Chemistry Letters, 2014, 5, 3445-3450.	2.1	47
100	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
101	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
102	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
103	Evaluating Transformational Solvent Systems for Post-combustion CO2 Separations. Energy Procedia, 2014, 63, 8144-8152.	1.8	15
104	Evaluation of the Role of Water in the H₂ Bond Formation by Ni(II)-Based Electrocatalysts. Journal of Chemical Theory and Computation, 2013, 9, 3505-3514.	2.3	7
105	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
106	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
107	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
108	Protonation of Ferrous Dinitrogen Complexes Containing a Diphosphine Ligand with a Pendent Amine. Inorganic Chemistry, 2013, 52, 4026-4039.	1.9	28

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109	Comparative Investigation of Benzene Steam Reforming over Spinel Supported Rh and Ir Catalysts. ACS Catalysis, 2013, 3, 1133-1143.	5.5	39
110	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
111	Site-Specific Imaging of Elemental Steps in Dehydration of Diols on TiO₂(110). ACS Nano, 2013, 7, 10414-10423.	7.3	20
112	Structure and Dynamics of CO₂ on Rutile TiO₂(110)-1Ã—1. Journal of Physical Chemistry C, 2012, 116, 26322-26334.	1.5	60
113	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
114	Alcohol Dehydration on Monooxo Wâ•O and Dioxo Oâ•Wâ•O Species. Journal of Physical Chemistry Letters, 2012, 3, 2168-2172.	2.1	18
115	OH Group Dynamics of 1,3-Propanediol on TiO2(110). Journal of Physical Chemistry Letters, 2012, 3, 3257-3263.	2.1	16
116	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
117	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
118	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
119	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
120	Growth of Ordered Ultrathin Tungsten Oxide Films on Pt(111). Journal of Physical Chemistry C, 2011, 115, 5773-5783.	1.5	40
121	Distribution of Ti³⁺ Surface Sites in Reduced TiO₂. Journal of Physical Chemistry C, 2011, 115, 7562-7572.	1.5	235
122	The Origin of Regioselectivity in 2â€Butanol Dehydration on Solid Acid Catalysts. ChemCatChem, 2011, 3, 1557-1561.	1.8	30
123	Comprehensive Thermodynamics of Nickel Hydride Bis(Diphosphine) Complexes: A Predictive Model through Computations. Organometallics, 2011, 30, 6108-6118.	1.1	76
124	(100) facets of Î³-Al2O3: The Active Surfaces for Alcohol Dehydration Reactions. Catalysis Letters, 2011, 141, 649-655.	1.4	105
125	Defining the Role of Excess Electrons in the Surface Chemistry of TiO₂. Journal of Physical Chemistry C, 2010, 114, 5891-5897.	1.5	202
126	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

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127	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
128	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
129	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
130	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
131	Imaging Hindered Rotations of Alkoxy Species on TiO2(110). Journal of the American Chemical Society, 2009, 131, 17926-17932.	6.6	40
132	Localized Electronic States from Surface Hydroxyls and Polarons in TiO₂(110). Journal of Physical Chemistry C, 2009, 113, 14583-14586.	1.5	196
133	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
134	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
135	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 50 407 Td (stretchy="fa	2.9	31
136	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
137	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
138	An Effective Pseudopotential for Modeling Gold Surface Slabs for Ab Initio Simulations. ChemPhysChem, 2005, 6, 1756-1760.	1.0	6
139	Dimerization of CO2 at High Pressure and Temperature. ChemPhysChem, 2005, 6, 1752-1756.	1.0	22
140	Phase Stability and Broken-Symmetry Transition of Elemental Lithium up to 140 GPa. ChemPhysChem, 2005, 6, 1703-1706.	1.0	39
141	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
142	Quantum and Thermal Fluctuation Effects on the Photoabsorption Spectra of Clusters. Physical Review Letters, 2004, 92, 183401.	2.9	67
143	Assigning Protonation Patterns in Water Networks in Bacteriorhodopsin Based on Computed IR Spectra. Angewandte Chemie - International Edition, 2004, 43, 4804-4807.	7.2	90
144	Modeling protonated water networks in bacteriorhodopsin. Physical Chemistry Chemical Physics, 2004, 6, 1848-1859.	1.3	45

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145	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
146	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
147	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
148	Towards â€œMechanochemistryâ€: Mechanically Induced Isomerizations of Thiolateâ€“Gold Clusters. Angewandte Chemie - International Edition, 2003, 42, 2251-2253.	7.2	72
149	Computer Modelling of the Structures, Stabilities and Thermoelectric Efficiency of Materials with Clathrate Structures. Key Engineering Materials, 2002, 227, 163-170.	0.4	1
150	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
151	Pulling Monatomic Gold Wires with Single Molecules: AnAb InitioSimulation. Physical Review Letters, 2002, 89, 186402.	2.9	169
152	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
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