List of Publications by Year in descending order

188 papers	11,338 citations	23500 58 h-index	32761 100 g-index
191 all docs	191 docs citations	191 times ranked	12987 citing authors

#	Article	IF	Citations
1	Redox Defect Thermochemistry of FeAl₂O₄ Hercynite in Water Splitting from First-Principles Methods. Chemistry of Materials, 2022, 34, 519-528.	3.2	11
2	Predicting Oxygen Off-Stoichiometry and Hydrogen Incorporation in Complex Perovskite Oxides. Chemistry of Materials, 2022, 34, 510-518.	3.2	7
3	A Computational Framework to Accelerate the Discovery of Perovskites for Solar Thermochemical Hydrogen Production: Identification of Gd Perovskite Oxide Redox Mediators. Advanced Functional Materials, 2022, 32, .	7.8	7
4	Predictive energetic tuning of C-Nucleophiles for the electrochemical capture of carbon dioxide. IScience, 2022, 25, 103997.	1.9	4
5	Ab initio screening of refractory nitrides and carbides for high temperature hydrogen permeation barriers. Journal of Nuclear Materials, 2022, 563, 153611.	1.3	3
6	Bond-Valence Parameterization for the Accurate Description of DFT Energetics. Journal of Chemical Theory and Computation, 2022, 18, 3257-3267.	2.3	3
7	How the Bioinspired Fe₂Mo₆S₈ Chevrel Breaks Electrocatalytic Nitrogen Reduction Scaling Relations. Journal of the American Chemical Society, 2022, 144, 12800-12806.	6.6	29
8	Determining Michael acceptor reactivity from kinetic, mechanistic, and computational analysis for the base-catalyzed thiol-Michael reaction. Polymer Chemistry, 2021, 12, 3619-3628.	1.9	9
9	Reduction of N₂ to Ammonia by Phosphate Molten Salt and Li Electrode: Proof of Concept Using Quantum Mechanics. Journal of Physical Chemistry Letters, 2021, 12, 1696-1701.	2.1	6
10	Kinetics of Hydride Transfer from Catalytic Metal-Free Hydride Donors to CO₂. Journal of Physical Chemistry Letters, 2021, 12, 2306-2311.	2.1	19
11	Mechanistic Studies of Styrene Production from Benzene and Ethylene Using [(Î·²-C₂H₄)₂Rh(Î¼-OAc)]₂ as Catalyst Precursor: Identification of a Bis-Rh^I Mono-Cu^{II} Complex As the Catalyst. ACS Catalysis, 2021, 11, 5688-5702.	5.5	9
12	Machine Learning Guided Synthesis of Multinary Chevrel Phase Chalcogenides. Journal of the American Chemical Society, 2021, 143, 9113-9122.	6.6	22
13	Visible-Light Photoinitiation of (Meth)acrylate Polymerization with Autonomous Post-conversion. Macromolecules, 2021, 54, 7702-7715.	2.2	2
14	Atomic layer deposited boron nitride nanoscale films act as high temperature hydrogen barriers. Applied Surface Science, 2021, 565, 150428.	3.1	9
15	Diazaphospholenes as reducing agents: a thermodynamic and electrochemical DFT study. Physical Chemistry Chemical Physics, 2021, 23, 17794-17802.	1.3	7
16	Electrocatalytic Reduction of CO₂ to CO over Ag(110) and Cu(211) Modeled by Grand-Canonical Density Functional Theory. Journal of Physical Chemistry C, 2021, 125, 23773-23783.	1.5	26
17	Computationally Accelerated Discovery and Experimental Demonstration of Gd0.5La0.5Co0.5Fe0.5O3 for Solar Thermochemical Hydrogen Production. Frontiers in Energy Research, 2021, 9, .	1.2	12
18	Altering Linear Scaling Relationships on Metal Catalysts via Ligandâ€“Adsorbate Hydrogen Bonding. Journal of Physical Chemistry C, 2021, 125, 23791-23802.	1.5	4

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19	Relocation and reinforcement of the adhesive/composite interface with spontaneous amine-peroxide interfacial polymerization. Dental Materials, 2021, 37, 1865-1872.	1.6	0
20	Immobilization of â€œCapping Areneâ€•Cobalt(II) Complexes on Ordered Mesoporous Carbon for Electrocatalytic Water Oxidation. ACS Catalysis, 2021, 11, 15068-15082.	5.5	8
21	Surface Hydrides on Fe₂P Electrocatalyst Reduce CO₂ at Low Overpotential: Steering Selectivity to Ethylene Glycol. Journal of the American Chemical Society, 2021, 143, 21275-21285.	6.6	34
22	Atomic layer deposition of tungsten nitride films as protective barriers to hydrogen. Applied Surface Science, 2020, 507, 145019.	3.1	5
23	Stabilizing Hydrogen Adsorption through Theory-Guided Chalcogen Substitution in Chevrel-Phase Mo₆X₈ (X=S, Se, Te) Electrocatalysts. ACS Applied Materials & Interfaces, 2020, 12, 35995-36003.	4.0	26
24	Computational and Experimental Evaluation of Peroxide Oxidants for Amineâ€“Peroxide Redox Polymerization. Macromolecules, 2020, 53, 9736-9746.	2.2	5
25	A Synergistic Approach to Unraveling the Thermodynamic Stability of Binary and Ternary Chevrel Phase Sulfides. Chemistry of Materials, 2020, 32, 7044-7051.	3.2	10
26	Computationally Predicted High-Throughput Free-Energy Phase Diagrams for the Discovery of Solid-State Hydrogen Storage Reactions. ACS Applied Materials & Interfaces, 2020, 12, 48553-48564.	4.0	6
27	Modified Single Iteration Synchronous-Transit Approach to Bound Diffusion Barriers for Solid-State Reactions. Journal of Chemical Theory and Computation, 2020, 16, 5912-5922.	2.3	3
28	Predicting Spinel Disorder and Its Effect on Oxygen Transport Kinetics in Hercynite. ACS Applied Materials & Interfaces, 2020, 12, 23831-23843.	4.0	11
29	Highâ€Throughput Analysis of Materials for Chemical Looping Processes. Advanced Energy Materials, 2020, 10, 2000685.	10.2	18
30	Oxidation kinetics of hercynite spinels for solar thermochemical fuel production. Chemical Engineering Journal, 2020, 401, 126015.	6.6	17
31	High-Efficiency Radical Photopolymerization Enhanced by Autonomous Dark Cure. Macromolecules, 2020, 53, 5034-5046.	2.2	13
32	Solidâ€state sintering of coreâ€shell ceramic powders fabricated by particle atomic layer deposition. Journal of the American Ceramic Society, 2020, 103, 4101-4109.	1.9	1
33	Highly dispersed Co deposited on Al₂O₃ particles via CoCp₂ + H₂ ALD. Nanotechnology, 2020, 31, 175703.	1.3	4
34	Inorganic Halide Double Perovskites with Optoelectronic Properties Modulated by Sublattice Mixing. Journal of the American Chemical Society, 2020, 142, 5135-5145.	6.6	62
35	Metalloradical intermediates in electrocatalytic reduction of CO₂ to CO: Mn versus Re bis-N-heterocyclic carbene pincers. Dalton Transactions, 2020, 49, 2053-2057.	1.6	18
36	Mn-Based Molecular Catalysts for the Electrocatalytic Disproportionation of CO₂ into CO and CO₃^{2â€“}. ACS Catalysis, 2020, 10, 1961-1968.	5.5	25

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37	Nonuniform Growth of Sub-2 Nanometer Atomic Layer Deposited Alumina Films on Lithium Nickel Manganese Cobalt Oxide Cathode Battery Materials. ACS Applied Nano Materials, 2019, 2, 6989-6997.	2.4	23
38	Enhancing Au/TiO₂ Catalyst Thermostability and Coking Resistance with Alkyl Phosphonic-Acid Self-Assembled Monolayers. ACS Applied Materials & Interfaces, 2019, 11, 41289-41296.	4.0	26
39	The role of decomposition reactions in assessing first-principles predictions of solid stability. Npj Computational Materials, 2019, 5, .	3.5	63
40	Independent Control of Singlet Oxygen and Radical Generation via Irradiation of a Two-Color Photosensitive Molecule. Macromolecules, 2019, 52, 4968-4978.	2.2	21
41	Continuous on-sun solar thermochemical hydrogen production via an isothermal redox cycle. Applied Energy, 2019, 249, 368-376.	5.1	49
42	Rational Design of Efficient Amine Reductant Initiators for Amineâ€“Peroxide Redox Polymerization. Journal of the American Chemical Society, 2019, 141, 6279-6291.	6.6	19
43	High-Throughput Equilibrium Analysis of Active Materials for Solar Thermochemical Ammonia Synthesis. ACS Applied Materials & Interfaces, 2019, 11, 24850-24858.	4.0	21
44	The effect of ultrathin ALD films on the oxidation kinetics of SiC in high-temperature steam. Chemical Engineering Science, 2019, 201, 230-236.	1.9	5
45	Importance of proton-coupled electron transfer in cathodic regeneration of organic hydrides. Chemical Communications, 2019, 55, 5583-5586.	2.2	24
46	New tolerance factor to predict the stability of perovskite oxides and halides. Science Advances, 2019, 5, eaav0693.	4.7	778
47	Catalyst-free, aza-Michael polymerization of hydrazides: polymerizability, kinetics, and mechanistic origin of an Î±-effect. Polymer Chemistry, 2019, 10, 5790-5804.	1.9	9
48	Particle atomic layer deposition of alumina for sintering yttriaâ€stabilized cubic zirconia. Journal of the American Ceramic Society, 2019, 102, 2283-2293.	1.9	8
49	Benzimidazoles as Metal-Free and Recyclable Hydrides for CO₂ Reduction to Formate. Journal of the American Chemical Society, 2019, 141, 272-280.	6.6	67
50	Amine Induced Retardation of the Radical-Mediated Thiolâ€“Ene Reaction via the Formation of Metastable Disulfide Radical Anions. Journal of Organic Chemistry, 2018, 83, 2912-2919.	1.7	32
51	Nanostructured mullite steam oxidation resistant coatings for silicon carbide deposited via atomic layer deposition. Journal of the American Ceramic Society, 2018, 101, 2493-2505.	1.9	11
52	Predicting Hydride Donor Strength via Quantum Chemical Calculations of Hydride Transfer Activation Free Energy. Journal of Physical Chemistry B, 2018, 122, 1278-1288.	1.2	15
53	Thermodynamic and kinetic hydricities of metal-free hydrides. Chemical Society Reviews, 2018, 47, 2809-2836.	18.7	103
54	Renewable Hydride Donors for the Catalytic Reduction of CO₂: A Thermodynamic and Kinetic Study. Journal of Physical Chemistry B, 2018, 122, 10179-10189.	1.2	13

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55	Dynamic and Responsive DNA-like Polymers. Journal of the American Chemical Society, 2018, 140, 13594-13598.	6.6	45
56	Physical descriptor for the Gibbs energy of inorganic crystalline solids and temperature-dependent materials chemistry. Nature Communications, 2018, 9, 4168.	5.8	152
57	Bistable and photoswitchable states of matter. Nature Communications, 2018, 9, 2804.	5.8	111
58	A user's guide to the thiol-thioester exchange in organic media: scope, limitations, and applications in material science. Polymer Chemistry, 2018, 9, 4523-4534.	1.9	78
59	The Unified Electrochemical Band Diagram Framework: Understanding the Driving Forces of Materials Electrochemistry. Advanced Functional Materials, 2018, 28, 1803439.	7.8	8
60	Predicting kinetics of polymorphic transformations from structure mapping and coordination analysis. Physical Review Materials, 2018, 2, .	0.9	13
61	Implications of heterostructural alloying for enhanced piezoelectric performance of (Al,Sc)N. Physical Review Materials, 2018, 2, .	0.9	47
62	Adatom surface diffusion of catalytic metals on the anatase TiO₂(101) surface. Physical Chemistry Chemical Physics, 2017, 19, 4541-4552.	1.3	28
63	Dihydropteridine/Pteridine as a 2H⁺/2e^{â€“} Redox Mediator for the Reduction of CO₂ to Methanol: A Computational Study. Journal of Physical Chemistry B, 2017, 121, 4158-4167.	1.2	13
64	Solvent effects on the intramolecular charge transfer character of N,Nâ€diaryl dihydrophenazine catalysts for organocatalyzed atom transfer radical polymerization. Journal of Polymer Science Part A, 2017, 55, 3017-3027.	2.5	56
65	Intramolecular Charge Transfer and Ion Pairing in N,N-Diaryl Dihydrophenazine Photoredox Catalysts for Efficient Organocatalyzed Atom Transfer Radical Polymerization. Journal of the American Chemical Society, 2017, 139, 348-355.	6.6	207
66	Controlling the Surface Reactivity of Titania via Electronic Tuning of Self-Assembled Monolayers. ACS Catalysis, 2017, 7, 8351-8357.	5.5	30
67	A review and perspective of efficient hydrogen generation via solar thermal water splitting. Wiley Interdisciplinary Reviews: Energy and Environment, 2016, 5, 261-287.	1.9	168
68	Organocatalyzed atom transfer radical polymerization driven by visible light. Science, 2016, 352, 1082-1086.	6.0	649
69	Rapid Growth of Crystalline Mn₅O₈ by Self-Limited Multilayer Deposition using Mn(EtCp)₂ and O₃. ACS Applied Materials & Interfaces, 2016, 8, 18560-18569.	4.0	17
70	Organocatalyzed Atom Transfer Radical Polymerization Using N-Aryl Phenoxazines as Photoredox Catalysts. Journal of the American Chemical Society, 2016, 138, 11399-11407.	6.6	300
71	Degradation of Ethylene Carbonate Electrolytes of Lithium Ion Batteries via Ring Opening Activated by LiCoO₂ Cathode Surfaces and Electrolyte Species. ACS Applied Materials & Interfaces, 2016, 8, 26664-26674.	4.0	67
72	Band Diagram and Rate Analysis of Thin Film Spinel LiMn₂O₄ Formed by Electrochemical Conversion of ALDâ€Grown MnO. Advanced Functional Materials, 2016, 26, 7895-7907.	7.8	37

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73	Aluminum Nitride Hydrolysis Enabled by Hydroxyl-Mediated Surface Proton Hopping. ACS Applied Materials & Interfaces, 2016, 8, 18550-18559.	4.0	21
74	First-Principles Analysis of Cation Diffusion in Mixed Metal Ferrite Spinels. Chemistry of Materials, 2016, 28, 214-226.	3.2	80
75	Growth and Characterization of Al₂O₃ Atomic Layer Deposition Films on sp²-Graphitic Carbon Substrates Using NO₂/Trimethylaluminum Pretreatment. ACS Applied Materials & Interfaces, 2015, 7, 12030-12037.	4.0	34
76	Sodium Charge Storage in Thin Films of MnO₂Derived by Electrochemical Oxidation of MnO Atomic Layer Deposition Films. Journal of the Electrochemical Society, 2015, 162, A2753-A2761.	1.3	42
77	Charge Storage in Cation Incorporated Î±-MnO₂. Chemistry of Materials, 2015, 27, 1172-1180.	3.2	122
78	Solvent Control of Surface Plasmon-Mediated Chemical Deposition of Au Nanoparticles from Alkylgold Phosphine Complexes. ACS Applied Materials & Interfaces, 2015, 7, 13384-13394.	4.0	8
79	Intrinsic Material Properties Dictating Oxygen Vacancy Formation Energetics in Metal Oxides. Journal of Physical Chemistry Letters, 2015, 6, 1948-1953.	2.1	103
80	Predicting the solar thermochemical water splitting ability and reaction mechanism of metal oxides: a case study of the hercynite family of water splitting cycles. Energy and Environmental Science, 2015, 8, 3687-3699.	15.6	68
81	Mechanisms of LiCoO₂ Cathode Degradation by Reaction with HF and Protection by Thin Oxide Coatings. ACS Applied Materials & Interfaces, 2015, 7, 24265-24278.	4.0	98
82	Mechanism of hydrofluoric acid formation in ethylene carbonate electrolytes with fluorine salt additives. Journal of Power Sources, 2015, 297, 427-435.	4.0	35
83	Catalytic Reduction of CO₂ by Renewable Organohydrides. Journal of Physical Chemistry Letters, 2015, 6, 5078-5092.	2.1	59
84	Extracting Kinetic Information from Complex Gasâ€“Solid Reaction Data. Industrial & Engineering Chemistry Research, 2015, 54, 4113-4122.	1.8	26
85	Electronic and dielectric properties of Ruddlesdenâ€“Popper type and MagnÃ©li type SrTiO3. Computational Materials Science, 2015, 96, 223-228.	1.4	15
86	Tunable Oxygen Vacancy Formation Energetics in the Complex Perovskite Oxide Sr_xLa_{1â€“x}Mn_yAl_{1â€“y}O<sub>3<sub>. Chemistry of Materials, 2014, 26, 6595-6602.	8.2	90
87	Reduction of CO₂ to Methanol Catalyzed by a Biomimetic Organo-Hydride Produced from Pyridine. Journal of the American Chemical Society, 2014, 136, 16081-16095.	6.6	131
88	Increasing the Photocatalytic Activity of Anatase TiO₂ through B, C, and N Doping. Journal of Physical Chemistry C, 2014, 118, 27415-27427.	1.5	55
89	Visible-Light Organic Photocatalysis for Latent Radical-Initiated Polymerization via 2e^{â€“}/1H⁺ Transfers: Initiation with Parallels to Photosynthesis. Journal of the American Chemical Society, 2014, 136, 7418-7427.	6.6	78
90	Oxide enthalpy of formation and band gap energy as accurate descriptors of oxygen vacancy formation energetics. Energy and Environmental Science, 2014, 7, 1996.	15.6	109

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92	Roles of the Lewis Acid and Base in the Chemical Reduction of CO₂ Catalyzed by Frustrated Lewis Pairs. Inorganic Chemistry, 2013, 52, 10062-10066.	1.9	58
93	Efficient Generation of H ₂ by Splitting Water with an Isothermal Redox Cycle. Science, 2013, 341, 540-542.	6.0	296
94	Mechanistic Basis for High Stereoselectivity and Broad Substrate Scope in the (salen)Co(III)-Catalyzed Hydrolytic Kinetic Resolution. Journal of the American Chemical Society, 2013, 135, 15595-15608.	6.6	115
95	A Correlated Electron View of Singlet Fission. Accounts of Chemical Research, 2013, 46, 1339-1347.	7.6	150
96	The Effect of N and B Doping on Graphene and the Adsorption and Migration Behavior of Pt Atoms. Journal of Physical Chemistry C, 2013, 117, 10523-10535.	1.5	71
97	Mechanism of Homogeneous Reduction of CO₂ by Pyridine: Proton Relay in Aqueous Solvent and Aromatic Stabilization. Journal of the American Chemical Society, 2013, 135, 142-154.	6.6	151
98	Growth of Pt Particles on the Anatase TiO₂ (101) Surface. Journal of Physical Chemistry C, 2012, 116, 12114-12123.	1.5	63
99	Effect of Surface Deposited Pt on the Photoactivity of TiO₂. Journal of Physical Chemistry C, 2012, 116, 10138-10149.	1.5	92
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101	Atomic Layer Deposition of Tantalum Nitride Using A Novel Precursor. Journal of Physical Chemistry C, 2011, 115, 11507-11513.	1.5	25
102	Reactions of Amino Acids on the Si(100)-2Ã—1 Surface. Journal of Physical Chemistry C, 2011, 115, 7477-7486.	1.5	13
103	Effects of Water and Formic Acid Adsorption on the Electronic Structure of Anatase TiO₂(101). Journal of Physical Chemistry C, 2011, 115, 2738-2749.	1.5	41
104	Dynamic Mechanisms for Ammonia Borane Thermolysis in Solvent: Deviation from Gas-Phase Minimum-Energy Pathways. Journal of Physical Chemistry Letters, 2011, 2, 276-281.	2.1	27
105	Effect of interface structure on the Ru on HfO2 work function. Journal of Materials Science, 2010, 45, 4924-4928.	1.7	2
106	Singlet fission in pentacene through multi-exciton quantum states. Nature Chemistry, 2010, 2, 648-652.	6.6	356
107	Reaction Mechanism, Bonding, and Thermal Stability of 1-Alkanethiols Self-Assembled on Halogenated Ge Surfaces. Langmuir, 2010, 26, 8419-8429.	1.6	22
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109	Excited states of methylene from quantum Monte Carlo. Journal of Chemical Physics, 2009, 131, 124103.	1.2	70
110	The Role of Free Nâ€Heterocyclic Carbene (NHC) in the Catalytic Dehydrogenation of Ammoniaâ€“Borane in the Nickel NHC System. Angewandte Chemie - International Edition, 2009, 48, 2201-2205.	7.2	115
111	Oligomerization and Autocatalysis of NH2BH2 with Ammoniaâˆ’Borane. Inorganic Chemistry, 2009, 48, 1069-1081.	1.9	108
112	Catalytic Dehydrogenation of Ammonia Borane at Ni Monocarbene and Dicarbene Catalysts. Inorganic Chemistry, 2009, 48, 5418-5433.	1.9	72
113	Formation of Alkanethiolate Self-Assembled Monolayers at Halide-Terminated Ge Surfaces. Langmuir, 2009, 25, 2013-2025.	1.6	38
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116	Atomic Layer Deposition of Hafnium Oxide from Hafnium Chloride and Water. Journal of the American Chemical Society, 2008, 130, 11996-12006.	6.6	45
117	Comparison of DFT Methods for Molecular Orbital Eigenvalue Calculations. Journal of Physical Chemistry A, 2007, 111, 1554-1561.	1.1	693
118	A Detailed Theoretical Study of the Mechanism and Energetics of Methane to Methanol Conversion by Cisplatin and Catalytica. Organometallics, 2007, 26, 793-809.	1.1	49
119	The role of ammonia in atomic layer deposition of tungsten nitride. Applied Physics Letters, 2007, 90, 173120.	1.5	17
120	Attachment of Alanine and Arginine to the Ge(100)-2Ã—1 Surface. Journal of Physical Chemistry C, 2007, 111, 3692-3699.	1.5	18
121	Carbonâˆ’Oxygen Coupling in the Reaction of Formaldehyde on Ge(100)-2Ã—1. Journal of Physical Chemistry C, 2007, 111, 1739-1746.	1.5	12
122	First-Principles Investigation of the Structure, Energetics, and Electronic Properties of Ru/HfO2Interfaces. Journal of Physical Chemistry C, 2007, 111, 9203-9210.	1.5	11
123	Carbon Dioxide Reduction by Pincer Rhodium Î·2-Dihydrogen Complexes:Â Hydrogen-Binding Modes and Mechanistic Studies by Density Functional Theory Calculations. Organometallics, 2007, 26, 508-513.	1.1	62
124	Catalyzed Dehydrogenation of Ammoniaâ€“Borane by Iridium Dihydrogen Pincer Complex Differs from Ethane Dehydrogenation. Angewandte Chemie - International Edition, 2007, 46, 8153-8156.	7.2	194
125	First-Principles Investigation of Hydroxylated Monoclinic HfO2 Surfaces. Chemistry of Materials, 2006, 18, 3397-3403.	3.2	30
126	First-principles calculations of structural and electronic properties of monoclinic hafnia surfaces. Physical Review B, 2006, 73, .	1.1	71

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127	Density Functional Theory Calculations of Tiâˆ’TEMPO Complexes:Â Influence of Ancillary Ligation on the Strength of the Tiâˆ’O Bond. Organometallics, 2006, 25, 3317-3323.	1.1	20
128	Non-growth ligand exchange reactions in atomic layer deposition of HfO2. Chemical Physics Letters, 2006, 421, 215-220.	1.2	23
129	A chemical mechanism for nitrogen incorporation into HfO2 ALD films using ammonia and alkylamide as precursors. Surface Science, 2005, 591, L280-L285.	0.8	11
130	Atomic layer deposition of hafnium nitrides using ammonia and alkylamide precursors. Chemical Physics Letters, 2005, 407, 272-275.	1.2	11
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135	Initial Nitridation of the Ge(100)-2 Ã— 1 Surface by Ammonia. Langmuir, 2005, 21, 5230-5232.	1.6	18
136	Density Functional Theory Study of the Geometry, Energetics, and Reconstruction Process of Si(111) Surfaces. Langmuir, 2005, 21, 12404-12414.	1.6	21
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139	Indirect adsorbateâ€“adsorbate interactions mediated through the surface electronic structure of the Si(100) surface. Journal of Chemical Physics, 2004, 120, 1555-1559.	1.2	33
140	A quantum chemical study of ZrO2 atomic layer deposition growth reactions on the SiO2 surface. Surface Science, 2004, 550, 199-212.	0.8	45
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146	Quantum Chemistry Based Statistical Mechanical Model of Hydrogen Desorption from Si(100)-2 Ã— 1, Ge(100)-2 Ã— 1, and SiGe Alloy Surfaces. Journal of Physical Chemistry B, 2004, 108, 18243-18253.	1.2	9
147	Initial Oxidation and Hydroxylation of the Ge(100)-2Ã—1 Surface by Water and Hydrogen Peroxide. Langmuir, 2004, 20, 7604-7609.	1.6	16
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150	A shock tube study of the reaction NH2 + CH4 ? NH3 + CH3 and comparison with transition state theory. International Journal of Chemical Kinetics, 2003, 35, 304-309.	1.0	23
151	Temperature and pressure dependence of the reaction of OH and CO: Master equation modeling on a high-level potential energy surface. International Journal of Chemical Kinetics, 2003, 35, 464-474.	1.0	49
152	Kinetic lattice Monte Carlo simulations of processes on the silicon (100) surface. Physica E: Low-Dimensional Systems and Nanostructures, 2003, 19, 183-187.	1.3	3
153	Reactions of Nitriles at Semiconductor Surfaces. Journal of Physical Chemistry B, 2003, 107, 12256-12267.	1.2	35
154	Quantum Chemical Study of Zirconium Oxide Deposition on the Si(100)â^'(2Ã—1) Surface. Journal of Physical Chemistry B, 2003, 107, 9319-9324.	1.2	31
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