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	New tolerance factor to predict the stability of perovskite oxides and halides. Science Advances, 2019, 5, eaav0693.	4.7	778
2	Comparison of DFT Methods for Molecular Orbital Eigenvalue Calculations. Journal of Physical Chemistry A, 2007, 111, 1554-1561.	1.1	693
3	Organocatalyzed atom transfer radical polymerization driven by visible light. Science, 2016, 352, 1082-1086.	6.0	649
4	Singlet fission in pentacene through multi-exciton quantum states. Nature Chemistry, 2010, 2, 648-652.	6.6	356
5	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
6	Efficient Generation of H ₂ by Splitting Water with an Isothermal Redox Cycle. Science, 2013, 341, 540-542.	6.0	296
7	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
8	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
9	Quantum chemical study of the mechanism of aluminum oxide atomic layer deposition. Applied Physics Letters, 2002, 80, 3304-3306.	1.5	178
10	Prediction of transition state barriers and enthalpies of reaction by a new hybrid density-functional approximation. Journal of Chemical Physics, 2001, 115, 11040-11051.	1.2	177
11	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
12	Predicting ionic conductivity of solid oxide fuel cell electrolyte from first principles. Journal of Applied Physics, 2005, 98, 103513.	1.1	162
13	Proton Transfer Reactions on Semiconductor Surfaces. Journal of the American Chemical Society, 2002, 124, 4027-4038.	6.6	152
14	Physical descriptor for the Gibbs energy of inorganic crystalline solids and temperature-dependent materials chemistry. Nature Communications, 2018, 9, 4168.	5.8	152
15	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
16	A Correlated Electron View of Singlet Fission. Accounts of Chemical Research, 2013, 46, 1339-1347.	7.6	150
17	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
18	Reactions of methylamines at the Si(100)-2Ã—1 surface. Journal of Chemical Physics, 2001, 114, 10170-10180.	1.2	130

#	Article	IF	Citations
19	Charge Storage in Cation Incorporated Î±-MnO₂. Chemistry of Materials, 2015, 27, 1172-1180.	3.2	122
20	Adsorption of organic matter at mineral/water interfaces: I. ATR-FTIR spectroscopic and quantum chemical study of oxalate adsorbed at boehmite/water and corundum/water interfaces. Geochimica Et Cosmochimica Acta, 2004, 68, 4505-4518.	1.6	120
21	Ab Initio Study of Adsorption and Decomposition of NH3on Si(100)-(2Ã—1). Journal of Physical Chemistry B, 2000, 104, 2527-2533.	1.2	118
22	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
23	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
24	Bistable and photoswitchable states of matter. Nature Communications, 2018, 9, 2804.	5.8	111
25	A density functional theory study of the nonlocal effects of NH3 adsorption and dissociation on Si(100)-(2Ã—1). Surface Science, 2000, 469, 9-20.	0.8	110
26	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
27	Oligomerization and Autocatalysis of NH2BH2 with Ammoniaâ^'Borane. Inorganic Chemistry, 2009, 48, 1069-1081.	1.9	108
28	Intrinsic Material Properties Dictating Oxygen Vacancy Formation Energetics in Metal Oxides. Journal of Physical Chemistry Letters, 2015, 6, 1948-1953.	2.1	103
29	Thermodynamic and kinetic hydricities of metal-free hydrides. Chemical Society Reviews, 2018, 47, 2809-2836.	18.7	103
30	The mechanism of HF/H[sub 2]O chemical etching of SiO[sub 2]. Journal of Chemical Physics, 2002, 116, 275.	1.2	99
31	Atomic layer deposition of hafnium oxide: A detailed reaction mechanism from first principles. Journal of Chemical Physics, 2002, 117, 1931-1934.	1.2	99
32	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
33	Effect of Surface Deposited Pt on the Photoactivity of TiO₂. Journal of Physical Chemistry C, 2012, 116, 10138-10149.	1.5	92
34	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.	3.2	90
35	Competition and Selectivity of Organic Reactions on Semiconductor Surfaces:Â Reaction of Unsaturated Ketones on Si(100)-2Ã—1 and Ge(100)-2Ã—1. Journal of the American Chemical Society, 2002, 124, 8990-9004.	6.6	87
36	Reactions of Cyclic Aliphatic and Aromatic Amines on Ge(100)-2Ã—1 and Si(100)-2Ã—1. Journal of Physical Chemistry B, 2003, 107, 4982-4996.	1.2	84

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37	A DFT Study of the Al2O3Atomic Layer Deposition on SAMs:Â Effect of SAM Termination. Chemistry of Materials, 2004, 16, 646-653.	3.2	83
38	First-Principles Analysis of Cation Diffusion in Mixed Metal Ferrite Spinels. Chemistry of Materials, 2016, 28, 214-226.	3.2	80
39	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
40	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
41	First-principles calculation of intrinsic defect formation volumes in silicon. Physical Review B, 2005, 72, .	1.1	76
42	A Theoretical Study of the Structure and Thermochemistry of 1,3-Butadiene on the Ge/Si(100)-2 Ã— 1 Surface. Journal of Physical Chemistry A, 2000, 104, 2457-2462.	1.1	74
43	Catalytic Dehydrogenation of Ammonia Borane at Ni Monocarbene and Dicarbene Catalysts. Inorganic Chemistry, 2009, 48, 5418-5433.	1.9	72
44	First-principles calculations of structural and electronic properties of monoclinic hafnia surfaces. Physical Review B, 2006, 73, .	1.1	71
45	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
46	Excited states of methylene from quantum Monte Carlo. Journal of Chemical Physics, 2009, 131, 124103.	1.2	70
47	Simultaneous Two-Hydrogen Transfer as a Mechanism for Efficient CO₂ Reduction. Inorganic Chemistry, 2010, 49, 8724-8728.	1.9	70
48	Example of a Thermodynamically Controlled Reaction on a Semiconductor Surface:Â Acetone on Ge(100)-2 Ã— 1. Journal of Physical Chemistry B, 2001, 105, 12559-12565.	1.2	69
49	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
50	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
51	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
52	Topological Disorder and Reactivity of Borosilicate Glasses:Â Quantum Chemical Calculations and17O and11B NMR Study. Journal of Physical Chemistry B, 2001, 105, 12583-12595.	1.2	64
53	A Quantum Chemical Study of the Atomic Layer Deposition of Al2O3 Using AlCl3 and H2O as Precursors. Journal of Physical Chemistry B, 2004, 108, 5718-5725.	1.2	64
54	Growth of Pt Particles on the Anatase TiO₂ (101) Surface. Journal of Physical Chemistry C, 2012, 116, 12114-12123.	1.5	63

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55	The role of decomposition reactions in assessing first-principles predictions of solid stability. Npj Computational Materials, 2019, 5, .	3.5	63
56	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
57	Inorganic Halide Double Perovskites with Optoelectronic Properties Modulated by Sublattice Mixing. Journal of the American Chemical Society, 2020, 142, 5135-5145.	6.6	62
58	Catalytic Reduction of CO₂ by Renewable Organohydrides. Journal of Physical Chemistry Letters, 2015, 6, 5078-5092.	2.1	59
59	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
60	A quantum chemical study of the self-directed growth mechanism of styrene and propylene molecular nanowires on the silicon (100) 2Ã—1 surface. Journal of Chemical Physics, 2002, 116, 9907-9913.	1.2	56
61	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
62	Mechanism of atomic layer deposition of SiO2 on the silicon (100)-2Ã—1 surface using SiCl4 and H2O as precursors. Journal of Applied Physics, 2002, 91, 3408-3414.	1.1	55
63	In-Situ Infrared Spectroscopy and Density Functional Theory Modeling of Hafnium Alkylamine Adsorption on Siâ^'OH and Siâ^'H Surfaces. Chemistry of Materials, 2005, 17, 5305-5314.	3.2	55
64	Adsorption of Organic Matter at Mineral/Water Interfaces: 7. ATR-FTIR and Quantum Chemical Study of Lactate Interactions with Hematite Nanoparticles. Langmuir, 2008, 24, 6683-6692.	1.6	55
65	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
66	Quantum chemical study of the elementary reactions in zirconium oxide atomic layer deposition. Applied Physics Letters, 2002, 81, 304-306.	1.5	54
67	Bulk and Surface Tunneling Hydrogen Defects in Alumina. Physical Review Letters, 2013, 111, 065901.	2.9	51
68	Cycloaddition of Cyclopentadiene and Dicyclopentadiene on Si(100)-2Ã—1:Â Comparison of Monomer and Dimer Adsorption. Journal of Physical Chemistry B, 1999, 103, 6803-6808.	1.2	50
69	Ab initiostudy of the initial growth mechanism of silicon nitride onSi(100)â^'(2Ã—1)usingNH3. Physical Review B, 2001, 64, .	1.1	49
70	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
71	Homolysis of Weak Tiâ^'O Bonds:Â Experimental and Theoretical Studies of Titanium Oxygen Bonds Derived from Stable Nitroxyl Radicals. Journal of the American Chemical Society, 2005, 127, 3807-3816.	6.6	49
72	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

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73	Continuous on-sun solar thermochemical hydrogen production via an isothermal redox cycle. Applied Energy, 2019, 249, 368-376.	5.1	49
74	Implications of heterostructural alloying for enhanced piezoelectric performance of (Al,Sc)N. Physical Review Materials, 2018, 2, .	0.9	47
75	Use of quantum methods for a consistent approach to combustion modelling: Hydrocarbon bond dissociation energies. Faraday Discussions, 2001, 119, 173-189.	1.6	45
76	A quantum chemical study of ZrO2 atomic layer deposition growth reactions on the SiO2 surface. Surface Science, 2004, 550, 199-212.	0.8	45
77	Atomic Layer Deposition of Hafnium Oxide from Hafnium Chloride and Water. Journal of the American Chemical Society, 2008, 130, 11996-12006.	6.6	45
78	Dynamic and Responsive DNA-like Polymers. Journal of the American Chemical Society, 2018, 140, 13594-13598.	6.6	45
79	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
80	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
81	Competition and Selectivity in the Reaction of Nitriles on Ge(100)â”2Ã—1. Journal of the American Chemical Society, 2003, 125, 4928-4936.	6.6	40
82	Atomistic mechanism of the initial oxidation of the clean Si(100)-(2Ã—1) surface by O2 and SiO2 decomposition. Journal of Chemical Physics, 2002, 116, 5774-5780.	1.2	39
83	Formation of Alkanethiolate Self-Assembled Monolayers at Halide-Terminated Ge Surfaces. Langmuir, 2009, 25, 2013-2025.	1.6	38
84	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
85	Reactions of Nitriles at Semiconductor Surfaces. Journal of Physical Chemistry B, 2003, 107, 12256-12267.	1.2	35
86	Mechanism of hydrofluoric acid formation in ethylene carbonate electrolytes with fluorine salt additives. Journal of Power Sources, 2015, 297, 427-435.	4.0	35
87	Surface reaction mechanisms for atomic layer deposition of silicon nitride. Surface Science, 2004, 557, 159-170.	0.8	34
88	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
89	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
90	Effect of a Methyl-Protecting Group on the Adsorption of Pyrrolidine on Si(100)-2 Ã— 1. Journal of Physical Chemistry B, 2001, 105, 3295-3299.	1.2	33

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91	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
92	Molecular Layer Deposition of Conductive Hybrid Organic-Inorganic Thin Films Using Diethylzinc and Hydroquinone. ECS Transactions, 2011, 33, 191-195.	0.3	33
93	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
94	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
95	Use of Quantum Methods with Transition State Theory:Â Application to H-Atom Metathesis Reactionsâ€. Journal of Physical Chemistry A, 2001, 105, 1669-1675.	1.1	30
96	Theoretical study of the chemical vapor deposition of (100) silicon from silane. Physical Review B, 2001, 64, .	1.1	30
97	First-Principles Investigation of Hydroxylated Monoclinic HfO2 Surfaces. Chemistry of Materials, 2006, 18, 3397-3403.	3.2	30
98	Controlling the Surface Reactivity of Titania via Electronic Tuning of Self-Assembled Monolayers. ACS Catalysis, 2017, 7, 8351-8357.	5.5	30
99	How the Bioinspired Fe₂Mo₆S₈ Chevrel Breaks Electrocatalytic Nitrogen Reduction Scaling Relations. Journal of the American Chemical Society, 2022, 144, 12800-12806.	6.6	29
100	Atomic Layer Deposition of HfO2 Using Alkoxides as Precursors. Journal of Physical Chemistry B, 2004, 108, 15150-15164.	1.2	28
101	Adatom surface diffusion of catalytic metals on the anatase TiO₂(101) surface. Physical Chemistry Chemical Physics, 2017, 19, 4541-4552.	1.3	28
102	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
103	Extracting Kinetic Information from Complex Gasâ€“Solid Reaction Data. Industrial & Engineering Chemistry Research, 2015, 54, 4113-4122.	1.8	26
104	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
105	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
106	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
107	DFT Study of the Adsorption of Chlorosilanes on the Si(100)-2 Ã— 1 Surface. Journal of Physical Chemistry B, 2001, 105, 12068-12075.	1.2	25
108	Atomic Layer Deposition of Tantalum Nitride Using A Novel Precursor. Journal of Physical Chemistry C, 2011, 115, 11507-11513.	1.5	25

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109	Mn-Based Molecular Catalysts for the Electrocatalytic Disproportionation of CO₂ into CO and CO₃^{2â€“}. ACS Catalysis, 2020, 10, 1961-1968.	5.5	25
110	Importance of proton-coupled electron transfer in cathodic regeneration of organic hydrides. Chemical Communications, 2019, 55, 5583-5586.	2.2	24
111	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
112	Non-growth ligand exchange reactions in atomic layer deposition of HfO2. Chemical Physics Letters, 2006, 421, 215-220.	1.2	23
113	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
114	Reaction Mechanism, Bonding, and Thermal Stability of 1-Alkanethiols Self-Assembled on Halogenated Ge Surfaces. Langmuir, 2010, 26, 8419-8429.	1.6	22
115	Machine Learning Guided Synthesis of Multinary Chevrel Phase Chalcogenides. Journal of the American Chemical Society, 2021, 143, 9113-9122.	6.6	22
116	A theoretical study of the chemical vapor deposition of (100) diamond: An explanation for the slow growth of the (100) surface. Journal of Chemical Physics, 2000, 113, 7582-7587.	1.2	21
117	Density Functional Theory Study of the Geometry, Energetics, and Reconstruction Process of Si(111) Surfaces. Langmuir, 2005, 21, 12404-12414.	1.6	21
118	Aluminum Nitride Hydrolysis Enabled by Hydroxyl-Mediated Surface Proton Hopping. ACS Applied Materials & Interfaces, 2016, 8, 18550-18559.	4.0	21
119	Independent Control of Singlet Oxygen and Radical Generation via Irradiation of a Two-Color Photosensitive Molecule. Macromolecules, 2019, 52, 4968-4978.	2.2	21
120	High-Throughput Equilibrium Analysis of Active Materials for Solar Thermochemical Ammonia Synthesis. ACS Applied Materials & Interfaces, 2019, 11, 24850-24858.	4.0	21
121	Density Functional Theory Calculations of Tiâ^'TEMPO Complexes:Â Influence of Ancillary Ligation on the Strength of the Tiâ^'O Bond. Organometallics, 2006, 25, 3317-3323.	1.1	20
122	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
123	Kinetics of Hydride Transfer from Catalytic Metal-Free Hydride Donors to CO₂. Journal of Physical Chemistry Letters, 2021, 12, 2306-2311.	2.1	19
124	Initial Nitridation of the Ge(100)-2 Ã— 1 Surface by Ammonia. Langmuir, 2005, 21, 5230-5232.	1.6	18
125	Attachment of Alanine and Arginine to the Ge(100)-2Ã—1 Surface. Journal of Physical Chemistry C, 2007, 111, 3692-3699.	1.5	18
126	Highâ€Throughput Analysis of Materials for Chemical Looping Processes. Advanced Energy Materials, 2020, 10, 2000685.	10.2	18

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127	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
128	The role of ammonia in atomic layer deposition of tungsten nitride. Applied Physics Letters, 2007, 90, 173120.	1.5	17
129	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
130	Oxidation kinetics of hercynite spinels for solar thermochemical fuel production. Chemical Engineering Journal, 2020, 401, 126015.	6.6	17
131	Initial Oxidation and Hydroxylation of the Ge(100)-2Ã—1 Surface by Water and Hydrogen Peroxide. Langmuir, 2004, 20, 7604-7609.	1.6	16
132	Density Functional Theory Study of Atomic Nitrogen on the Si(100)â˜’(2 Ã— 1) Surface. Journal of Physical Chemistry B, 2002, 106, 2643-2648.	1.2	15
133	Atomic layer deposition of high-Îº dielectrics on nitrided silicon surfaces. Applied Physics Letters, 2005, 86, 192110.	1.5	15
134	Electronic and dielectric properties of Ruddlesdenâ€“Popper type and MagnÃ©li type SrTiO3. Computational Materials Science, 2015, 96, 223-228.	1.4	15
135	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
136	Hessian biased force field for polysilane polymers. The Journal of Physical Chemistry, 1995, 99, 13321-13333.	2.9	13
137	Theoretical study of the Cl-passivated Si(111) surface. Surface Science, 1999, 430, 116-125.	0.8	13
138	Reactions of Amino Acids on the Si(100)-2Ã—1 Surface. Journal of Physical Chemistry C, 2011, 115, 7477-7486.	1.5	13
139	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
140	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
141	High-Efficiency Radical Photopolymerization Enhanced by Autonomous Dark Cure. Macromolecules, 2020, 53, 5034-5046.	2.2	13
142	Predicting kinetics of polymorphic transformations from structure mapping and coordination analysis. Physical Review Materials, 2018, 2, .	0.9	13
143	Calculating Cumulene/Poly-yne Isomerization Energies. Journal of Physical Chemistry A, 2004, 108, 4030-4035.	1.1	12
144	Carbonâ˜’Oxygen Coupling in the Reaction of Formaldehyde on Ge(100)-2Ã—1. Journal of Physical Chemistry C, 2007, 111, 1739-1746.	1.5	12

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145	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
146	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
147	Atomic layer deposition of hafnium nitrides using ammonia and alkylamide precursors. Chemical Physics Letters, 2005, 407, 272-275.	1.2	11
148	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
149	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
150	Predicting Spinel Disorder and Its Effect on Oxygen Transport Kinetics in Hercynite. ACS Applied Materials & Interfaces, 2020, 12, 23831-23843.	4.0	11
151	Redox Defect Thermochemistry of FeAl₂O₄ Hercynite in Water Splitting from First-Principles Methods. Chemistry of Materials, 2022, 34, 519-528.	3.2	11
152	The surface-radical-surface-olefin recombination step for CVD growth of diamond. Calculation of the rate constant from first principles. Chemical Physics Letters, 1995, 247, 359-365.	1.2	10
153	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
154	A Density Functional Theory Study on the Effect of Ge Alloying on Hydrogen Desorption from SiGe Alloy Surfaces. Journal of Physical Chemistry B, 2004, 108, 6336-6350.	1.2	9
155	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
156	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
157	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
158	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
159	Atomic layer deposited boron nitride nanoscale films act as high temperature hydrogen barriers. Applied Surface Science, 2021, 565, 150428.	3.1	9
160	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
161	The Unified Electrochemical Band Diagram Framework: Understanding the Driving Forces of Materials Electrochemistry. Advanced Functional Materials, 2018, 28, 1803439.	7.8	8
162	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

#	Article	IF	Citations
163	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
164	First-principles calculation of free Si(100) surface impurity enrichment. Applied Physics Letters, 2005, 87, 232101.	1.5	7
165	Diazaphospholenes as reducing agents: a thermodynamic and electrochemical DFT study. Physical Chemistry Chemical Physics, 2021, 23, 17794-17802.	1.3	7
166	Predicting Oxygen Off-Stoichiometry and Hydrogen Incorporation in Complex Perovskite Oxides. Chemistry of Materials, 2022, 34, 510-518.	3.2	7
167	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
168	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
169	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
170	Modeling Copper Diffusion in Silicon Oxide, Nitride, and Carbide. Materials Research Society Symposia Proceedings, 2002, 716, 841.	0.1	5
171	Quantum dot properties in the multiband envelope-function approximation using boundary conditions based upon first-principles quantum calculations. Physical Review B, 2008, 77, .	1.1	5
172	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
173	Atomic layer deposition of tungsten nitride films as protective barriers to hydrogen. Applied Surface Science, 2020, 507, 145019.	3.1	5
174	Computational and Experimental Evaluation of Peroxide Oxidants for Amineâ€“Peroxide Redox Polymerization. Macromolecules, 2020, 53, 9736-9746.	2.2	5
175	Highly dispersed Co deposited on Al₂O₃ particles via CoCp₂ + H₂ ALD. Nanotechnology, 2020, 31, 175703.	1.3	4
176	Altering Linear Scaling Relationships on Metal Catalysts via Ligandâ€“Adsorbate Hydrogen Bonding. Journal of Physical Chemistry C, 2021, 125, 23791-23802.	1.5	4
177	Hydrolysis protection and sintering of aluminum nitride powders with yttria nanofilms. Journal of the American Ceramic Society, 0, , .	1.9	4
178	Predictive energetic tuning of C-Nucleophiles for the electrochemical capture of carbon dioxide. IScience, 2022, 25, 103997.	1.9	4
179	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
180	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

#	Article	IF	Citations
181	Ab initio screening of refractory nitrides and carbides for high temperature hydrogen permeation barriers. Journal of Nuclear Materials, 2022, 563, 153611.	1.3	3
182	Bond-Valence Parameterization for the Accurate Description of DFT Energetics. Journal of Chemical Theory and Computation, 2022, 18, 3257-3267.	2.3	3
183	Effect of interface structure on the Ru on HfO2 work function. Journal of Materials Science, 2010, 45, 4924-4928.	1.7	2
184	Visible-Light Photoinitiation of (Meth)acrylate Polymerization with Autonomous Post-conversion. Macromolecules, 2021, 54, 7702-7715.	2.2	2
185	The effect of an electric field on the chemical vapour deposition of (100) diamond. Nanotechnology, 2001, 12, 258-264.	1.3	1
186	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
187	Relocation and reinforcement of the adhesive/composite interface with spontaneous amine-peroxide interfacial polymerization. Dental Materials, 2021, 37, 1865-1872.	1.6	0
188	X-ray absorption spectroscopy insights on the structure anisotropy and charge transfer in Chevrel Phase chalcogenides. Physical Chemistry Chemical Physics, 0, , .	1.3	0