

Charles B Musgrave Iii

List of Publications by Year in descending order

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186
papers

10,892
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26630

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12289
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#	ARTICLE	IF	CITATIONS
1	Redox Defect Thermochemistry of FeAl_2O_4 Hercynite in Water Splitting from First-Principles Methods. <i>Chemistry of Materials</i> , 2022, 34, 519-528.	6.7	11
2	Predicting Oxygen Off-Stoichiometry and Hydrogen Incorporation in Complex Perovskite Oxides. <i>Chemistry of Materials</i> , 2022, 34, 510-518.	6.7	7
3	Experimental and Theoretical Comparison of Potential-dependent Methylation on Chemically Exfoliated WS_2 and MoS_2 . <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 9744-9753.	8.0	2
4	A Computational Framework to Accelerate the Discovery of Perovskites for Solar Thermochemical Hydrogen Production: Identification of Gd Perovskite Oxide Redox Mediators. <i>Advanced Functional Materials</i> , 2022, 32, .	14.9	7
5	Predictive energetic tuning of C-Nucleophiles for the electrochemical capture of carbon dioxide. <i>IScience</i> , 2022, 25, 103997.	4.1	4
6	Ab initio screening of refractory nitrides and carbides for high temperature hydrogen permeation barriers. <i>Journal of Nuclear Materials</i> , 2022, 563, 153611.	2.7	3
7	Bond-Valence Parameterization for the Accurate Description of DFT Energetics. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3257-3267.	5.3	3
8	Manganese Catalyzed Partial Oxidation of Light Alkanes. <i>ACS Catalysis</i> , 2022, 12, 5356-5370.	11.2	9
9	How the Bioinspired $\text{Fe}_2\text{Mo}_6\text{S}_8$ Chevrel Breaks Electrocatalytic Nitrogen Reduction Scaling Relations. <i>Journal of the American Chemical Society</i> , 2022, 144, 12800-12806.	13.7	29
10	Determining Michael acceptor reactivity from kinetic, mechanistic, and computational analysis for the base-catalyzed thiol-Michael reaction. <i>Polymer Chemistry</i> , 2021, 12, 3619-3628.	3.9	9
11	Reduction of N_2 to Ammonia by Phosphate Molten Salt and Li Electrode: Proof of Concept Using Quantum Mechanics. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 1696-1701.	4.6	6
12	Kinetics of Hydride Transfer from Catalytic Metal-Free Hydride Donors to CO_2 . <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2306-2311.	4.6	19
13	Mechanistic Studies of Styrene Production from Benzene and Ethylene Using $[(\text{I}^{\text{II}}\text{-C}_2\text{H}_4)_2\text{Rh}(\text{I}^{\text{I}}\text{-OAc})_2]$ as Catalyst Precursor: Identification of a Bis-Rh Mono-Cu Complex As the Catalyst. <i>ACS Catalysis</i> , 2021, 11, 5688-5702.	11.2	9
14	Functionalization of RhIII^{Me} Bonds: Use of σ -Capping Arene Ligands to Facilitate Me^{X} Reductive Elimination. <i>Organometallics</i> , 2021, 40, 1889-1906.	2.3	3
15	Electrocatalytic Water Oxidation by a Trinuclear Copper(II) Complex. <i>ACS Catalysis</i> , 2021, 11, 7223-7240.	11.2	35
16	Machine Learning Guided Synthesis of Multinary Chevrel Phase Chalcogenides. <i>Journal of the American Chemical Society</i> , 2021, 143, 9113-9122.	13.7	22
17	Role of Ferryl Ion Intermediates in Fast Fenton Chemistry on Aqueous Microdroplets. <i>Environmental Science & Technology</i> , 2021, 55, 14370-14377.	10.0	21
18	Noncovalent Immobilization of Pentamethylcyclopentadienyl Iridium Complexes on Ordered Mesoporous Carbon for Electrocatalytic Water Oxidation. <i>Small Science</i> , 2021, 1, 2100037.	9.9	7

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19	Rhodium and Iridium Complexes Bearing π -Capping Arene-Ligands: Synthesis and Characterization. <i>Organometallics</i> , 2021, 40, 2808-2825.	2.3	4
20	Visible-Light Photoinitiation of (Meth)acrylate Polymerization with Autonomous Post-conversion. <i>Macromolecules</i> , 2021, 54, 7702-7715.	4.8	2
21	Atomic layer deposited boron nitride nanoscale films act as high temperature hydrogen barriers. <i>Applied Surface Science</i> , 2021, 565, 150428.	6.1	9
22	Diazaphospholenes as reducing agents: a thermodynamic and electrochemical DFT study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 17794-17802.	2.8	7
23	Electrocatalytic Reduction of CO_2 to CO over Ag(110) and Cu(211) Modeled by Grand-Canonical Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2021, 125, 23773-23783.	3.1	26
24	Computationally Accelerated Discovery and Experimental Demonstration of $\text{Gd}_{0.5}\text{La}_{0.5}\text{Co}_{0.5}\text{Fe}_{0.5}\text{O}_3$ for Solar Thermochemical Hydrogen Production. <i>Frontiers in Energy Research</i> , 2021, 9, .	2.3	12
25	Altering Linear Scaling Relationships on Metal Catalysts via Ligand-Adsorbate Hydrogen Bonding. <i>Journal of Physical Chemistry C</i> , 2021, 125, 23791-23802.	3.1	4
26	Relocation and reinforcement of the adhesive/composite interface with spontaneous amine-peroxide interfacial polymerization. <i>Dental Materials</i> , 2021, 37, 1865-1872.	3.5	0
27	Immobilization of π -Capping Arene-Cobalt(II) Complexes on Ordered Mesoporous Carbon for Electrocatalytic Water Oxidation. <i>ACS Catalysis</i> , 2021, 11, 15068-15082.	11.2	8
28	Surface Hydrides on Fe_2P Electrocatalyst Reduce CO_2 at Low Overpotential: Steering Selectivity to Ethylene Glycol. <i>Journal of the American Chemical Society</i> , 2021, 143, 21275-21285.	13.7	34
29	Atomic layer deposition of tungsten nitride films as protective barriers to hydrogen. <i>Applied Surface Science</i> , 2020, 507, 145019.	6.1	5
30	Templated Growth of Metastable Polymorphs on Amorphous Substrates with Seed Layers. <i>Physical Review Applied</i> , 2020, 13, .	3.8	7
31	Stabilizing Hydrogen Adsorption through Theory-Guided Chalcogen Substitution in Chevrel-Phase Mo_6X_8 (X=S, Se, Te) Electrocatalysts. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 35995-36003.	8.0	26
32	Computational and Experimental Evaluation of Peroxide Oxidants for Amine-Peroxide Redox Polymerization. <i>Macromolecules</i> , 2020, 53, 9736-9746.	4.8	5
33	A Synergistic Approach to Unraveling the Thermodynamic Stability of Binary and Ternary Chevrel Phase Sulfides. <i>Chemistry of Materials</i> , 2020, 32, 7044-7051.	6.7	10
34	Computationally Predicted High-Throughput Free-Energy Phase Diagrams for the Discovery of Solid-State Hydrogen Storage Reactions. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 48553-48564.	8.0	6
35	Modified Single Iteration Synchronous-Transit Approach to Bound Diffusion Barriers for Solid-State Reactions. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5912-5922.	5.3	3
36	Predicting Spinel Disorder and Its Effect on Oxygen Transport Kinetics in Hercynite. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 23831-23843.	8.0	11

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37	High-Throughput Analysis of Materials for Chemical Looping Processes. <i>Advanced Energy Materials</i> , 2020, 10, 2000685.	19.5	18
38	Oxidation kinetics of hercynite spinels for solar thermochemical fuel production. <i>Chemical Engineering Journal</i> , 2020, 401, 126015.	12.7	17
39	High-Efficiency Radical Photopolymerization Enhanced by Autonomous Dark Cure. <i>Macromolecules</i> , 2020, 53, 5034-5046.	4.8	13
40	Solid-state sintering of core-shell ceramic powders fabricated by particle atomic layer deposition. <i>Journal of the American Ceramic Society</i> , 2020, 103, 4101-4109.	3.8	1
41	Highly dispersed Co deposited on Al ₂ O ₃ particles via CoCp ₂ + H ₂ ALD. <i>Nanotechnology</i> , 2020, 31, 175703.	2.6	4
42	Inorganic Halide Double Perovskites with Optoelectronic Properties Modulated by Sublattice Mixing. <i>Journal of the American Chemical Society</i> , 2020, 142, 5135-5145.	13.7	62
43	Metalloradical intermediates in electrocatalytic reduction of CO ₂ to CO: Mn <i>versus</i> Re bis-N-heterocyclic carbene pincers. <i>Dalton Transactions</i> , 2020, 49, 2053-2057.	3.3	18
44	Mn-Based Molecular Catalysts for the Electrocatalytic Disproportionation of CO ₂ into CO and CO ₃ ²⁻ . <i>ACS Catalysis</i> , 2020, 10, 1961-1968.	11.2	25
45	Wurtzite materials in alloys of rock salt compounds. <i>Journal of Materials Research</i> , 2020, 35, 972-980.	2.6	2
46	Nonuniform Growth of Sub-2 Nanometer Atomic Layer Deposited Alumina Films on Lithium Nickel Manganese Cobalt Oxide Cathode Battery Materials. <i>ACS Applied Nano Materials</i> , 2019, 2, 6989-6997.	5.0	23
47	Enhancing Au/TiO ₂ Catalyst Thermostability and Coking Resistance with Alkyl Phosphonic-Acid Self-Assembled Monolayers. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 41289-41296.	8.0	26
48	The role of decomposition reactions in assessing first-principles predictions of solid stability. <i>Npj Computational Materials</i> , 2019, 5, .	8.7	63
49	Independent Control of Singlet Oxygen and Radical Generation via Irradiation of a Two-Color Photosensitive Molecule. <i>Macromolecules</i> , 2019, 52, 4968-4978.	4.8	21
50	Continuous on-sun solar thermochemical hydrogen production via an isothermal redox cycle. <i>Applied Energy</i> , 2019, 249, 368-376.	10.1	49
51	Rational Design of Efficient Amine Reductant Initiators for Amine Peroxide Redox Polymerization. <i>Journal of the American Chemical Society</i> , 2019, 141, 6279-6291.	13.7	19
52	High-Throughput Equilibrium Analysis of Active Materials for Solar Thermochemical Ammonia Synthesis. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 24850-24858.	8.0	21
53	The effect of ultrathin ALD films on the oxidation kinetics of SiC in high-temperature steam. <i>Chemical Engineering Science</i> , 2019, 201, 230-236.	3.8	5
54	Importance of proton-coupled electron transfer in cathodic regeneration of organic hydrides. <i>Chemical Communications</i> , 2019, 55, 5583-5586.	4.1	24

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55	New tolerance factor to predict the stability of perovskite oxides and halides. <i>Science Advances</i> , 2019, 5, eaav0693.	10.3	778
56	Catalyst-free, aza-Michael polymerization of hydrazides: polymerizability, kinetics, and mechanistic origin of an I±-effect. <i>Polymer Chemistry</i> , 2019, 10, 5790-5804.	3.9	9
57	Particle atomic layer deposition of alumina for sintering yttria-stabilized cubic zirconia. <i>Journal of the American Ceramic Society</i> , 2019, 102, 2283-2293.	3.8	8
58	Benzimidazoles as Metal-Free and Recyclable Hydrides for CO ₂ Reduction to Formate. <i>Journal of the American Chemical Society</i> , 2019, 141, 272-280.	13.7	67
59	Amine Induced Retardation of the Radical-Mediated Thiol-ene Reaction via the Formation of Metastable Disulfide Radical Anions. <i>Journal of Organic Chemistry</i> , 2018, 83, 2912-2919.	3.2	32
60	Nanostructured mullite steam oxidation resistant coatings for silicon carbide deposited via atomic layer deposition. <i>Journal of the American Ceramic Society</i> , 2018, 101, 2493-2505.	3.8	11
61	Predicting Hydride Donor Strength via Quantum Chemical Calculations of Hydride Transfer Activation Free Energy. <i>Journal of Physical Chemistry B</i> , 2018, 122, 1278-1288.	2.6	15
62	Thermodynamic and kinetic hydricities of metal-free hydrides. <i>Chemical Society Reviews</i> , 2018, 47, 2809-2836.	38.1	103
63	Renewable Hydride Donors for the Catalytic Reduction of CO ₂ : A Thermodynamic and Kinetic Study. <i>Journal of Physical Chemistry B</i> , 2018, 122, 10179-10189.	2.6	13
64	Dynamic and Responsive DNA-like Polymers. <i>Journal of the American Chemical Society</i> , 2018, 140, 13594-13598.	13.7	45
65	Physical descriptor for the Gibbs energy of inorganic crystalline solids and temperature-dependent materials chemistry. <i>Nature Communications</i> , 2018, 9, 4168.	12.8	152
66	Bistable and photoswitchable states of matter. <i>Nature Communications</i> , 2018, 9, 2804.	12.8	111
67	A user's guide to the thiol-thioester exchange in organic media: scope, limitations, and applications in material science. <i>Polymer Chemistry</i> , 2018, 9, 4523-4534.	3.9	78
68	The Unified Electrochemical Band Diagram Framework: Understanding the Driving Forces of Materials Electrochemistry. <i>Advanced Functional Materials</i> , 2018, 28, 1803439.	14.9	8
69	Implications of heterostructural alloying for enhanced piezoelectric performance of (Al,Sc)N. <i>Physical Review Materials</i> , 2018, 2, .	2.4	47
70	Adatom surface diffusion of catalytic metals on the anatase TiO ₂ (101) surface. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 4541-4552.	2.8	28
71	Dihydropteridine/Pteridine as a 2H ⁺ /2e ⁻ Redox Mediator for the Reduction of CO ₂ to Methanol: A Computational Study. <i>Journal of Physical Chemistry B</i> , 2017, 121, 4158-4167.	2.6	13
72	Solvent effects on the intramolecular charge transfer character of <i>N,N</i> -diaryl dihydrophenazine catalysts for organocatalyzed atom transfer radical polymerization. <i>Journal of Polymer Science Part A</i> , 2017, 55, 3017-3027.	2.3	56

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73	Intramolecular Charge Transfer and Ion Pairing in <i>N,N</i> -Diaryl Dihydrophenazine Photoredox Catalysts for Efficient Organocatalyzed Atom Transfer Radical Polymerization. <i>Journal of the American Chemical Society</i> , 2017, 139, 348-355.	13.7	207
74	Controlling the Surface Reactivity of Titania via Electronic Tuning of Self-Assembled Monolayers. <i>ACS Catalysis</i> , 2017, 7, 8351-8357.	11.2	30
75	A review and perspective of efficient hydrogen generation via solar thermal water splitting. <i>Wiley Interdisciplinary Reviews: Energy and Environment</i> , 2016, 5, 261-287.	4.1	168
76	Organocatalyzed atom transfer radical polymerization driven by visible light. <i>Science</i> , 2016, 352, 1082-1086.	12.6	649
77	Rapid Growth of Crystalline Mn ₅ O ₈ by Self-Limited Multilayer Deposition using Mn(EtCp) ₂ and O ₃ . <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 18560-18569.	8.0	17
78	Organocatalyzed Atom Transfer Radical Polymerization Using <i>N</i> -Aryl Phenoxazines as Photoredox Catalysts. <i>Journal of the American Chemical Society</i> , 2016, 138, 11399-11407.	13.7	300
79	Degradation of Ethylene Carbonate Electrolytes of Lithium Ion Batteries via Ring Opening Activated by LiCoO ₂ Cathode Surfaces and Electrolyte Species. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 26664-26674.	8.0	67
80	Band Diagram and Rate Analysis of Thin Film Spinel LiMn ₂ O ₄ Formed by Electrochemical Conversion of ALD-Grown MnO. <i>Advanced Functional Materials</i> , 2016, 26, 7895-7907.	14.9	37
81	Aluminum Nitride Hydrolysis Enabled by Hydroxyl-Mediated Surface Proton Hopping. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 18550-18559.	8.0	21
82	First-Principles Analysis of Cation Diffusion in Mixed Metal Ferrite Spinel. <i>Chemistry of Materials</i> , 2016, 28, 214-226.	6.7	80
83	Growth and Characterization of Al ₂ O ₃ Atomic Layer Deposition Films on sp ² -Graphitic Carbon Substrates Using NO ₂ /Trimethylaluminum Pretreatment. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 12030-12037.	8.0	34
84	Sodium Charge Storage in Thin Films of MnO ₂ Derived by Electrochemical Oxidation of MnO Atomic Layer Deposition Films. <i>Journal of the Electrochemical Society</i> , 2015, 162, A2753-A2761.	2.9	42
85	Charge Storage in Cation Incorporated δ -MnO ₂ . <i>Chemistry of Materials</i> , 2015, 27, 1172-1180.	6.7	122
86	Solvent Control of Surface Plasmon-Mediated Chemical Deposition of Au Nanoparticles from Alkylgold Phosphine Complexes. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 13384-13394.	8.0	8
87	Intrinsic Material Properties Dictating Oxygen Vacancy Formation Energetics in Metal Oxides. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 1948-1953.	4.6	103
88	Predicting the solar thermochemical water splitting ability and reaction mechanism of metal oxides: a case study of the hercynite family of water splitting cycles. <i>Energy and Environmental Science</i> , 2015, 8, 3687-3699.	30.8	68
89	Mechanisms of LiCoO ₂ Cathode Degradation by Reaction with HF and Protection by Thin Oxide Coatings. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 24265-24278.	8.0	98
90	Mechanism of hydrofluoric acid formation in ethylene carbonate electrolytes with fluorine salt additives. <i>Journal of Power Sources</i> , 2015, 297, 427-435.	7.8	35

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91	Catalytic Reduction of CO ₂ by Renewable Organohydrides. Journal of Physical Chemistry Letters, 2015, 6, 5078-5092.	4.6	59
92	Extracting Kinetic Information from Complex Gas-Solid Reaction Data. Industrial & Engineering Chemistry Research, 2015, 54, 4113-4122.	3.7	26
93	Tunable Oxygen Vacancy Formation Energetics in the Complex Perovskite Oxide Sr _{1-x} La _x Mn _y Al _{1-y} O ₃ . Chemistry of Materials, 2014, 26, 6595-6602.		90
94	Reduction of CO ₂ to Methanol Catalyzed by a Biomimetic Organo-Hydride Produced from Pyridine. Journal of the American Chemical Society, 2014, 136, 16081-16095.	13.7	131
95	Increasing the Photocatalytic Activity of Anatase TiO ₂ through B, C, and N Doping. Journal of Physical Chemistry C, 2014, 118, 27415-27427.	3.1	55
96	Visible-Light Organic Photocatalysis for Latent Radical-Initiated Polymerization via 2e ⁻ /1H ⁺ Transfers: Initiation with Parallels to Photosynthesis. Journal of the American Chemical Society, 2014, 136, 7418-7427.	13.7	78
97	Oxide enthalpy of formation and band gap energy as accurate descriptors of oxygen vacancy formation energetics. Energy and Environmental Science, 2014, 7, 1996.	30.8	109
98	Bulk and Surface Tunneling Hydrogen Defects in Alumina. Physical Review Letters, 2013, 111, 065901.	7.8	51
99	Roles of the Lewis Acid and Base in the Chemical Reduction of CO ₂ Catalyzed by Frustrated Lewis Pairs. Inorganic Chemistry, 2013, 52, 10062-10066.	4.0	58
100	Efficient Generation of H ₂ by Splitting Water with an Isothermal Redox Cycle. Science, 2013, 341, 540-542.	12.6	296
101	A Correlated Electron View of Singlet Fission. Accounts of Chemical Research, 2013, 46, 1339-1347.	15.6	150
102	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.	3.1	71
103	Mechanism of Homogeneous Reduction of CO ₂ by Pyridine: Proton Relay in Aqueous Solvent and Aromatic Stabilization. Journal of the American Chemical Society, 2013, 135, 142-154.	13.7	151
104	Growth of Pt Particles on the Anatase TiO ₂ (101) Surface. Journal of Physical Chemistry C, 2012, 116, 12114-12123.	3.1	63
105	Effect of Surface Deposited Pt on the Photoactivity of TiO ₂ . Journal of Physical Chemistry C, 2012, 116, 10138-10149.	3.1	92
106	Atomic Layer Deposition of Tantalum Nitride Using A Novel Precursor. Journal of Physical Chemistry C, 2011, 115, 11507-11513.	3.1	25
107	Reactions of Amino Acids on the Si(100)-2 \times 1 Surface. Journal of Physical Chemistry C, 2011, 115, 7477-7486.	3.1	13
108	Dynamic Mechanisms for Ammonia Borane Thermolysis in Solvent: Deviation from Gas-Phase Minimum-Energy Pathways. Journal of Physical Chemistry Letters, 2011, 2, 276-281.	4.6	27

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109	Effect of interface structure on the Ru on HfO ₂ work function. <i>Journal of Materials Science</i> , 2010, 45, 4924-4928.	3.7	2
110	Singlet fission in pentacene through multi-exciton quantum states. <i>Nature Chemistry</i> , 2010, 2, 648-652.	13.6	356
111	Reaction Mechanism, Bonding, and Thermal Stability of 1-Alkanethiols Self-Assembled on Halogenated Ge Surfaces. <i>Langmuir</i> , 2010, 26, 8419-8429.	3.5	22
112	Simultaneous Two-Hydrogen Transfer as a Mechanism for Efficient CO ₂ Reduction. <i>Inorganic Chemistry</i> , 2010, 49, 8724-8728.	4.0	70
113	Excited states of methylene from quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2009, 131, 124103.	3.0	70
114	The Role of Free N-Heterocyclic Carbene (NHC) in the Catalytic Dehydrogenation of Ammonia-Borane in the Nickel NHC System. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 2201-2205.	13.8	115
115	Oligomerization and Autocatalysis of NH ₂ BH ₂ with Ammonia-Borane. <i>Inorganic Chemistry</i> , 2009, 48, 1069-1081.	4.0	108
116	Catalytic Dehydrogenation of Ammonia Borane at Ni Monocarbene and Dicarbene Catalysts. <i>Inorganic Chemistry</i> , 2009, 48, 5418-5433.	4.0	72
117	Formation of Alkanethiolate Self-Assembled Monolayers at Halide-Terminated Ge Surfaces. <i>Langmuir</i> , 2009, 25, 2013-2025.	3.5	38
118	Atomic Layer Deposition of Hafnium Oxide from Hafnium Chloride and Water. <i>Journal of the American Chemical Society</i> , 2008, 130, 11996-12006.	13.7	45
119	Comparison of DFT Methods for Molecular Orbital Eigenvalue Calculations. <i>Journal of Physical Chemistry A</i> , 2007, 111, 1554-1561.	2.5	693
120	A Detailed Theoretical Study of the Mechanism and Energetics of Methane to Methanol Conversion by Cisplatin and Catalyca. <i>Organometallics</i> , 2007, 26, 793-809.	2.3	49
121	The role of ammonia in atomic layer deposition of tungsten nitride. <i>Applied Physics Letters</i> , 2007, 90, 173120.	3.3	17
122	Attachment of Alanine and Arginine to the Ge(100)-2 \times 1 Surface. <i>Journal of Physical Chemistry C</i> , 2007, 111, 3692-3699.	3.1	18
123	Carbon-Oxygen Coupling in the Reaction of Formaldehyde on Ge(100)-2 \times 1. <i>Journal of Physical Chemistry C</i> , 2007, 111, 1739-1746.	3.1	12
124	First-Principles Investigation of the Structure, Energetics, and Electronic Properties of Ru/HfO ₂ Interfaces. <i>Journal of Physical Chemistry C</i> , 2007, 111, 9203-9210.	3.1	11
125	Carbon Dioxide Reduction by Pincer Rhodium η -2-Dihydrogen Complexes: Hydrogen-Binding Modes and Mechanistic Studies by Density Functional Theory Calculations. <i>Organometallics</i> , 2007, 26, 508-513.	2.3	62
126	Catalyzed Dehydrogenation of Ammonia-Borane by Iridium Dihydrogen Pincer Complex Differs from Ethane Dehydrogenation. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 8153-8156.	13.8	194

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127	First-Principles Investigation of Hydroxylated Monoclinic HfO ₂ Surfaces. <i>Chemistry of Materials</i> , 2006, 18, 3397-3403.	6.7	30
128	First-principles calculations of structural and electronic properties of monoclinic hafnia surfaces. <i>Physical Review B</i> , 2006, 73, .	3.2	71
129	Density Functional Theory Calculations of Ti ^{IV} -TEMPO Complexes: Influence of Ancillary Ligation on the Strength of the Ti ^{IV} -O Bond. <i>Organometallics</i> , 2006, 25, 3317-3323.	2.3	20
130	Non-growth ligand exchange reactions in atomic layer deposition of HfO ₂ . <i>Chemical Physics Letters</i> , 2006, 421, 215-220.	2.6	23
131	A chemical mechanism for nitrogen incorporation into HfO ₂ ALD films using ammonia and alkylamide as precursors. <i>Surface Science</i> , 2005, 591, L280-L285.	1.9	11
132	Atomic layer deposition of hafnium nitrides using ammonia and alkylamide precursors. <i>Chemical Physics Letters</i> , 2005, 407, 272-275.	2.6	11
133	First-principles calculation of free Si(100) surface impurity enrichment. <i>Applied Physics Letters</i> , 2005, 87, 232101.	3.3	7
134	Atomic layer deposition of high- ϵ_r dielectrics on nitrided silicon surfaces. <i>Applied Physics Letters</i> , 2005, 86, 192110.	3.3	15
135	First-principles calculation of intrinsic defect formation volumes in silicon. <i>Physical Review B</i> , 2005, 72, .	3.2	76
136	Initial Nitridation of the Ge(100)-2 \times 1 Surface by Ammonia. <i>Langmuir</i> , 2005, 21, 5230-5232.	3.5	18
137	In-Situ Infrared Spectroscopy and Density Functional Theory Modeling of Hafnium Alkylamine Adsorption on Si ^{IV} -OH and Si ^{IV} -H Surfaces. <i>Chemistry of Materials</i> , 2005, 17, 5305-5314.	6.7	55
138	Predicting ionic conductivity of solid oxide fuel cell electrolyte from first principles. <i>Journal of Applied Physics</i> , 2005, 98, 103513.	2.5	162
139	Indirect adsorbate-adsorbate interactions mediated through the surface electronic structure of the Si(100) surface. <i>Journal of Chemical Physics</i> , 2004, 120, 1555-1559.	3.0	33
140	A quantum chemical study of ZrO ₂ atomic layer deposition growth reactions on the SiO ₂ surface. <i>Surface Science</i> , 2004, 550, 199-212.	1.9	45
141	Surface reaction mechanisms for atomic layer deposition of silicon nitride. <i>Surface Science</i> , 2004, 557, 159-170.	1.9	34
142	Atomic Layer Deposition of HfO ₂ Using Alkoxides as Precursors. <i>Journal of Physical Chemistry B</i> , 2004, 108, 15150-15164.	2.6	28
143	A Density Functional Theory Study on the Effect of Ge Alloying on Hydrogen Desorption from SiGe Alloy Surfaces. <i>Journal of Physical Chemistry B</i> , 2004, 108, 6336-6350.	2.6	9
144	Calculating Cumulene/Poly-yne Isomerization Energies. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4030-4035.	2.5	12

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