Mark Allendorf

List of Publications by Year
in descending order

185 papers	28,194 citations	17776 65 h-index	5873 166 g-index
203 all docs	203 docs citations	203 times ranked	25731 citing authors

#	Article	IF	Citations
1	Understanding Hydrogenation Chemistry at MgB₂Reactive Edges fromAb InitioMolecular Dynamics. ACS Applied Materials & Interfaces, 2022, 14, 20430-20442.	4.0	4
2	Reversible dehydrogenation and rehydrogenation of cyclohexane and methylcyclohexane by single-site platinum catalyst. Nature Communications, 2022, 13, 1092.	5.8	41
3	Magnesium- and intermetallic alloys-based hydrides for energy storage: modelling, synthesis and properties. Progress in Energy, 2022, 4, 032007.	4.6	29
4	Tailored porous carbons enabled by persistent micelles with glassy cores. Materials Advances, 2021, 2, 5381-5395.	2.6	10
5	Data-Driven Discovery and Synthesis of High Entropy Alloy Hydrides with Targeted Thermodynamic Stability. Chemistry of Materials, 2021, 33, 4067-4076.	3.2	33
6	What Lies beneath a Metalâ€“Organic Framework Crystal Structure? New Design Principles from Unexpected Behaviors. Journal of the American Chemical Society, 2021, 143, 6705-6723.	6.6	48
7	Reversing the Irreversible: Thermodynamic Stabilization of LiAlH₄ Nanoconfined Within a Nitrogen-Doped Carbon Host. ACS Nano, 2021, 15, 10163-10174.	7.3	24
8	From n- to p-Type Material: Effect of Metal Ion on Charge Transport in Metalâ€“Organic Materials. ACS Applied Materials & Interfaces, 2021, 13, 52055-52062.	4.0	10
9	Defying Thermodynamics: Stabilization of Alane Within Covalent Triazine Frameworks for Reversible Hydrogen Storage. Angewandte Chemie, 2021, 133, 26019-26028.	1.6	2
10	Defying Thermodynamics: Stabilization of Alane Within Covalent Triazine Frameworks for Reversible Hydrogen Storage. Angewandte Chemie - International Edition, 2021, 60, 25815-25824.	7.2	11
11	Stabilized open metal sites in bimetallic metalâ€“organic framework catalysts for hydrogen production from alcohols. Journal of Materials Chemistry A, 2021, 9, 10869-10881.	5.2	20
12	RÃ¼cktitelbild: Defying Thermodynamics: Stabilization of Alane Within Covalent Triazine Frameworks for Reversible Hydrogen Storage (Angew. Chem. 49/2021). Angewandte Chemie, 2021, 133, 26204-26204.	1.6	0
13	Spontaneous dynamical disordering of borophenes in MgB2 and related metal borides. Nature Communications, 2021, 12, 6268.	5.8	14
14	Extracting an Empirical Intermetallic Hydride Design Principle from Limited Data via Interpretable Machine Learning. Journal of Physical Chemistry Letters, 2020, 11, 40-47.	2.1	28
15	Electronic Devices Using Open Framework Materials. Chemical Reviews, 2020, 120, 8581-8640.	23.0	185
16	Nanoconfinement of Molecular Magnesium Borohydride Captured in a Bipyridine-Functionalized Metalâ€“Organic Framework. ACS Nano, 2020, 14, 10294-10304.	7.3	40
17	Design principles for the ultimate gas deliverable capacity material: nonporous to porous deformations without volume change. Molecular Systems Design and Engineering, 2020, 5, 1491-1503.	1.7	5
18	Melting of Magnesium Borohydride under High Hydrogen Pressure: Thermodynamic Stability and Effects of Nanoconfinement. Chemistry of Materials, 2020, 32, 5604-5615.	3.2	18

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19	The Insideâ€Outs of Metal Hydride Dehydrogenation: Imaging the Phase Evolution of the Liâ€Nâ€H Hydrogen Storage System. Advanced Materials Interfaces, 2020, 7, 1901905.	1.9	9
20	Efficient Hydrogen Production from Methanol Using a Single-Site Pt₁/CeO₂ Catalyst. Journal of the American Chemical Society, 2019, 141, 17995-17999.	6.6	114
21	IRMOF-74(n)â€“Mg: a novel catalyst series for hydrogen activation and hydrogenolysis of Câ€“O bonds. Chemical Science, 2019, 10, 9880-9892.	3.7	23
22	Desulfurization of Liquid Hydrocarbon Fuels with Microporous and Mesoporous Materials: Metal-Organic Frameworks, Zeolites, and Mesoporous Silicas. Industrial & Engineering Chemistry Research, 2019, 58, 19322-19352.	1.8	34
23	An International Laboratory Comparison Study of Volumetric and Gravimetric Hydrogen Adsorption Measurements. ChemPhysChem, 2019, 20, 1997-2009.	1.0	26
24	Morphologyâ€Dependent Stability of Complex Metal Hydrides and Their Intermediates Using Firstâ€Principles Calculations. ChemPhysChem, 2019, 20, 1340-1347.	1.0	11
25	Get the light out: nanoscaling MOFs for luminescence sensing and optical applications. Chemical Communications, 2019, 55, 4647-4650.	2.2	38
26	Design Rules for Metalâ€Organic Framework Stability in Highâ€Pressure Hydrogen Environments. ChemPhysChem, 2019, 20, 1305-1310.	1.0	9
27	Inâ€Situ/Operando Xâ€ray Characterization of Metal Hydrides. ChemPhysChem, 2019, 20, 1261-1271.	1.0	12
28	An Analytical Bond Order Potential for Mgâ€“H Systems. ChemPhysChem, 2019, 20, 1404-1411.	1.0	3
29	Identifying the Role of Dynamic Surface Hydroxides in the Dehydrogenation of Ti-Doped NaAlH₄. ACS Applied Materials & Interfaces, 2019, 11, 4930-4941.	4.0	19
30	Effect of Solvent and Substrate on the Surface Binding Mode of Carboxylate-Functionalized Aromatic Molecules. Journal of Physical Chemistry C, 2018, 122, 10846-10856.	1.5	5
31	Anomalous H₂ Desorption Rate of NaAlH₄ Confined in Nitrogen-Doped Nanoporous Carbon Frameworks. Chemistry of Materials, 2018, 30, 2930-2938.	3.2	45
32	Thermally activated delayed fluorescence of a Zr-based metalâ€“organic framework. Chemical Communications, 2018, 54, 631-634.	2.2	30
33	Unraveling the Semiconducting/Metallic Discrepancy in Ni₃(HITP)₂. Journal of Physical Chemistry Letters, 2018, 9, 481-486.	2.1	70
34	Mechanical Properties in Metalâ€“Organic Frameworks: Emerging Opportunities and Challenges for Device Functionality and Technological Applications. Advanced Materials, 2018, 30, e1704124.	11.1	165
35	Nanostructured Metal Hydrides for Hydrogen Storage. Chemical Reviews, 2018, 118, 10775-10839.	23.0	461
36	Surface Morphology and Electrical Properties of Cu₃BTC₂ Thin Films Before and After Reaction with TCNQ. ACS Applied Materials & Interfaces, 2018, 10, 39400-39410.	4.0	30

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37	Efficient conversion of lignin into a water-soluble polymer by a chelator-mediated Fenton reaction: optimization of H₂O₂use and performance as a dispersant. Green Chemistry, 2018, 20, 3024-3037.	4.6	36
38	Hybrid Polymer/Metalâ€“Organic Framework Films for Colorimetric Water Sensing over a Wide Concentration Range. ACS Applied Materials & Interfaces, 2018, 10, 24201-24208.	4.0	46
39	Critical Factors in Computational Characterization of Hydrogen Storage in Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2018, 122, 18957-18967.	1.5	21
40	Metallic Metalâ€“Organic Frameworks Predicted by the Combination of Machine Learning Methods and Ab Initio Calculations. Journal of Physical Chemistry Letters, 2018, 9, 4562-4569.	2.1	84
41	Molecular dynamics studies of fundamental bulk properties of palladium hydrides for hydrogen storage. Journal of Applied Physics, 2018, 123, .	1.1	10
42	An assessment of strategies for the development of solid-state adsorbents for vehicular hydrogen storage. Energy and Environmental Science, 2018, 11, 2784-2812.	15.6	162
43	High electrical conductivity and high porosity in a Guest@MOF material: evidence of TCNQ ordering within Cu₃BTC₂ micropores. Chemical Science, 2018, 9, 7405-7412.	3.7	73
44	Hydrogenation properties of lithium and sodium hydride â€“ closo-borate, [B₁₀H₁₀]^{2â^'} and [B₁₂H₁₂]^{2â^'}, composites. Physical Chemistry Chemical Physics, 2018, 20, 16266-16275.	1.3	18
45	MOF-Sensitized Solar Cells Enabled by a Pillared Porphyrin Framework. Journal of Physical Chemistry C, 2017, 121, 4816-4824.	1.5	83
46	An updated roadmap for the integration of metalâ€“organic frameworks with electronic devices and chemical sensors. Chemical Society Reviews, 2017, 46, 3185-3241.	18.7	987
47	Correction: An updated roadmap for the integration of metalâ€“organic frameworks with electronic devices and chemical sensors. Chemical Society Reviews, 2017, 46, 3853-3853.	18.7	30
48	Understanding Charge Transfer at Mg/MgH ₂ Interfaces for Hydrogen Storage. ECS Transactions, 2017, 77, 81-90.	0.3	6
49	A Microporous and Naturally Nanostructured Thermoelectric Metal-Organic Framework with Ultralow Thermal Conductivity. Joule, 2017, 1, 168-177.	11.7	159
50	Two-dimensional metalâ€“organic frameworks with high thermoelectric efficiency through metal ion selection. Physical Chemistry Chemical Physics, 2017, 19, 19461-19467.	1.3	30
51	Nanophotonic Atomic Force Microscope Transducers Enable Chemical Composition and Thermal Conductivity Measurements at the Nanoscale. Nano Letters, 2017, 17, 5587-5594.	4.5	93
52	Finite-Temperature Behavior of PdHx Elastic Constants Computed by Direct Molecular Dynamics. MRS Advances, 2017, 2, 3341-3346.	0.5	2
53	Thermoelectric Properties of 2D Ni₃(hitp)₂and 3D Cu₃(btc)₂MOFs: First-Principles Studies. ECS Journal of Solid State Science and Technology, 2017, 6, N236-N242.	0.9	7
54	Transforming MOFs for Energy Applications Using the Guest@MOF Concept. Inorganic Chemistry, 2016, 55, 7233-7249.	1.9	65

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55	Linkers with Optical Functionality. , 2016, , 463-489.		1
56	Longâ€Lived Roomâ€Temperature Phosphorescence of Coronene in Zeolitic Imidazolate Framework ZIFâ€8. Advanced Optical Materials, 2016, 4, 1015-1021.	3.6	209
57	Guest molecules as a design element for metalâ€“organic frameworks. MRS Bulletin, 2016, 41, 865-869.	1.7	26
58	Virtual Special Issue on Catalysis at the U.S. Department of Energyâ€™s National Laboratories. ACS Catalysis, 2016, 6, 3227-3235.	5.5	2
59	Thin Film Growth of nbo MOFs and their Integration with Electroacoustic Devices. Advanced Functional Materials, 2016, 26, 1699-1707.	7.8	53
60	Proposed Modification of the Graphene Analogue Ni₃(HITP)₂ To Yield a Semiconducting Material. Journal of Physical Chemistry C, 2016, 120, 15001-15008.	1.5	67
61	From conventional to conformal. Nature Materials, 2016, 15, 255-257.	13.3	2
62	Molecular Dynamics Simulations of Hydrogen Diffusion in Aluminum. Journal of Physical Chemistry C, 2016, 120, 7500-7509.	1.5	36
63	Versatile Synthesis and Fluorescent Labeling of ZIF-90 Nanoparticles for Biomedical Applications. ACS Applied Materials & Interfaces, 2016, 8, 7623-7630.	4.0	60
64	MOF-Based Catalysts for Selective Hydrogenolysis of Carbonâ€“Oxygen Ether Bonds. ACS Catalysis, 2016, 6, 55-59.	5.5	82
65	Molecular simulation of size-selective gas adsorption in idealised carbon nanotubes. Molecular Simulation, 2015, 41, 1388-1395.	0.9	5
66	Thin Film Thermoelectric Metalâ€“Organic Framework with High Seebeck Coefficient and Low Thermal Conductivity. Advanced Materials, 2015, 27, 3453-3459.	11.1	227
67	Guest-Induced Emergent Properties in Metalâ€“Organic Frameworks. Journal of Physical Chemistry Letters, 2015, 6, 1182-1195.	2.1	150
68	DFT-based force field development for noble gas adsorption in metal organic frameworks. Journal of Materials Chemistry A, 2015, 3, 23539-23548.	5.2	33
69	Crystal engineering, structureâ€“function relationships, and the future of metalâ€“organic frameworks. CrystEngComm, 2015, 17, 229-246.	1.3	237
70	Considerations in the Design of Materials for Solarâ€Driven Fuel Production Using Metalâ€Oxide Thermochemical Cycles. Advanced Energy Materials, 2014, 4, 1300469.	10.2	138
71	Energy and charge transfer by donorâ€“acceptor pairs confined in a metalâ€“organic framework: a spectroscopic and computational investigation. Journal of Materials Chemistry A, 2014, 2, 3389-3398.	5.2	100
72	Novel metalâ€“organic framework linkers for light harvesting applications. Chemical Science, 2014, 5, 2081-2090.	3.7	152

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73	Noble Gas Adsorption in Metalâ€“Organic Frameworks Containing Open Metal Sites. Journal of Physical Chemistry C, 2014, 118, 11685-11698.	1.5	165
74	Homo- and heterometallic luminescent 2-D stilbene metalâ€“organic frameworks. Dalton Transactions, 2014, 43, 2925-2935.	1.6	28
75	Tunable Electrical Conductivity in Metal-Organic Framework Thin-Film Devices. Science, 2014, 343, 66-69.	6.0	1,061
76	Efficiency maximization in solar-thermochemical fuel production: challenging the concept of isothermal water splitting. Physical Chemistry Chemical Physics, 2014, 16, 8418-8427.	1.3	112
77	MOF-based electronic and opto-electronic devices. Chemical Society Reviews, 2014, 43, 5994-6010.	18.7	1,145
78	Controlled Nucleation and Growth of Pillared Paddlewheel Framework Nanostacks onto Chemically Modified Surfaces. ACS Applied Materials & Interfaces, 2014, 6, 1509-1514.	4.0	20
79	Molecular dynamics simulation of framework flexibility effects on noble gas diffusion in HKUST-1 and ZIF-8. Microporous and Mesoporous Materials, 2014, 194, 190-199.	2.2	75
80	Probing the unusual anion mobility of LiBH4 confined in highly ordered nanoporous carbon frameworks via solid state NMR and quasielastic neutron scattering. Journal of Materials Chemistry A, 2013, 1, 9935.	5.2	42
81	Screening metalâ€“organic frameworks for selective noble gas adsorption in air: effect of pore size and framework topology. Physical Chemistry Chemical Physics, 2013, 15, 9093.	1.3	92
82	Nanoconfined light metal hydrides for reversible hydrogen storage. MRS Bulletin, 2013, 38, 488-494.	1.7	105
83	Surface mediated assembly of small, metastable gold nanoclusters. Nanoscale, 2013, 5, 6558.	2.8	10
84	Kinetics and mechanism of solar-thermochemical H2 production by oxidation of a cobalt ferriteâ€“zirconia composite. Energy and Environmental Science, 2013, 6, 963.	15.6	123
85	HKUSTâ€1 coated piezoresistive microcantilever array for volatile organic compound sensing. Micro and Nano Letters, 2013, 8, 766-769.	0.6	32
86	Characterization of Piezoresistive Microcantilever Sensors with Metal Organic Frameworks for the Detection of Volatile Organic Compounds. ECS Transactions, 2013, 50, 469-476.	0.3	17
87	Predicting Lowâ€Pressure O₂ Adsorption in Nanoporous Framework Materials for Sensing Applications. ChemPhysChem, 2013, 14, 3740-3750.	1.0	11
88	Nano-Ordering of Donor-Acceptor Interactions Using Metal-Organic Frameworks as Scaffolds. ECS Transactions, 2013, 58, 21-28.	0.3	0
89	Design of Materials for Solar-Driven Fuel Production by Metal-Oxide Thermochemical Cycles. Electrochemical Society Interface, 2013, 22, 63-68.	0.3	26
90	Thermodynamics and kinetics of NaAlH4 nanocluster decomposition. Physical Chemistry Chemical Physics, 2012, 14, 8160.	1.3	41

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91	Spectral- and Pulse-Shape Discrimination in Triplet-Harvesting Plastic Scintillators. IEEE Transactions on Nuclear Science, 2012, 59, 3312-3319.	1.2	41
92	Grand Canonical Monte Carlo Simulation of Low-Pressure Methane Adsorption in Nanoporous Framework Materials for Sensing Applications. Journal of Physical Chemistry C, 2012, 116, 3492-3502.	1.5	30
93	Reversible Hydrogen Storage by NaAlH₄ Confined within a Titanium-Functionalized MOF-74(Mg) Nanoreactor. ACS Nano, 2012, 6, 9807-9817.	7.3	146
94	Connecting structure with function in metalâ€“organic frameworks to design novel photo- and radioluminescent materials. Journal of Materials Chemistry, 2012, 22, 10235.	6.7	105
95	Identification of Metalâ€“Organic Framework Materials for Adsorption Separation of Rare Gases: Applicability of Ideal Adsorbed Solution Theory (IAST) and Effects of Inaccessible Framework Regions. Journal of Physical Chemistry C, 2012, 116, 13183-13195.	1.5	102
96	Effects of Polarizability on the Adsorption of Noble Gases at Low Pressures in Monohalogenated Isoreticular Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2012, 116, 19765-19772.	1.5	99
97	Ultrasensitive Humidity Detection Using Metalâ€“Organic Framework-Coated Microsensors. Analytical Chemistry, 2012, 84, 7043-7051.	3.2	111
98	Tuning metal hydride thermodynamics via size and composition: Liâ€“H, Mgâ€“H, Alâ€“H, and Mgâ€“Alâ€“H nanoclusters for hydrogen storage. Physical Chemistry Chemical Physics, 2012, 14, 6611.	1.3	23
99	Metalâ€“Organic Framework Materials as Chemical Sensors. Chemical Reviews, 2012, 112, 1105-1125.	23.0	6,221
100	Charge-transfer guest interactions in luminescent MOFs: implications for solid-state temperature and environmental sensing. Dalton Transactions, 2012, 41, 8869.	1.6	78
101	Kinetics and mechanism of metalâ€“organic framework thin film growth: systematic investigation of HKUST-1 deposition on QCM electrodes. Chemical Science, 2012, 3, 1531.	3.7	169
102	MOF @ MEMS: Design optimization for high sensitivity chemical detection. Sensors and Actuators B: Chemical, 2012, 168, 256-262.	4.0	50
103	Ordered metal nanostructureself-assembly using metalâ€“organic frameworks as templates. Chemical Science, 2011, 2, 411-416.	3.7	64
104	Thermochemistry of Alane Complexes for Hydrogen Storage: A Theoretical and Experimental Investigation. Journal of Physical Chemistry C, 2011, 115, 7778-7786.	1.5	41
105	Hydrogen Production via Chemical Looping Redox Cycles Using Atomic Layer Deposition-Synthesized Iron Oxide and Cobalt Ferrites. Chemistry of Materials, 2011, 23, 2030-2038.	3.2	153
106	Designing metal-organic frameworks for radiation detection. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2011, 652, 295-298.	0.7	28
107	Complete Series of Monohalogenated Isoreticular Metalâ€“Organic Frameworks: Synthesis and the Importance of Activation Method. Crystal Growth and Design, 2011, 11, 4309-4312.	1.4	53
108	Metalâ€Organic Frameworks: A Rapidly Growing Class of Versatile Nanoporous Materials. Advanced Materials, 2011, 23, 249-267.	11.1	1,232

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109	A Roadmap to Implementing Metalâ€“Organic Frameworks in Electronic Devices: Challenges and Critical Directions. Chemistry - A European Journal, 2011, 17, 11372-11388.	1.7	403
110	Electron beam synthesis of metal and semiconductor nanoparticles using metalâ€“organic frameworks as ordered precursors. Nanotechnology, 2011, 22, 375601.	1.3	20
111	MOF Films for Microsensor Coatings. Materials Research Society Symposia Proceedings, 2011, 1366, 1.	0.1	4
112	Conductivity, Doping, and Redox Chemistry of a Microporous Dithiolene-Based Metalâ^'Organic Framework. Chemistry of Materials, 2010, 22, 4120-4122.	3.2	459
113	Investigation of microcantilever array with ordered nanoporous coatings for selective chemical detection. Proceedings of SPIE, 2010, , .	0.8	13
114	Predicting impurity gases and phases during hydrogen evolution from complex metal hydrides using free energy minimization enabled by first-principles calculations. Physical Chemistry Chemical Physics, 2010, 12, 9918.	1.3	20
115	Assessing the Purity of Metalâ^'Organic Frameworks Using Photoluminescence: MOF-5, ZnO Quantum Dots, and Framework Decomposition. Journal of the American Chemical Society, 2010, 132, 15487-15489.	6.6	140
116	Luminescent Metal-Organic Frameworks: A Nanolaboratory for Probing Energy Transfer via Interchromophore Interactions. ECS Transactions, 2010, 28, 137-143.	0.3	5
117	Computational screening of metalâ€“organic frameworks for large-molecule chemical sensing. Physical Chemistry Chemical Physics, 2010, 12, 12621.	1.3	83
118	Characterization of HKUST-1 Crystals and Their Application to MEMS Microcantilever Array Sensors. ECS Transactions, 2010, 33, 229-238.	0.3	16
119	Scintillating Metal Organic Frameworks: A New Class of Radiation Detection Materials. Materials Research Society Symposia Proceedings, 2009, 1164, 1.	0.1	3
120	Scintillating Metalâ€Organic Frameworks: A New Class of Radiation Detection Materials. Advanced Materials, 2009, 21, 95-101.	11.1	157
121	Luminescent metalâ€“organic frameworks. Chemical Society Reviews, 2009, 38, 1330.	18.7	4,545
122	Silver Cluster Formation, Dynamics, and Chemistry in Metalâ^'Organic Frameworks. Nano Letters, 2009, 9, 3413-3418.	4.5	245
123	Adsorption and Separation of Noble Gases by IRMOF-1: Grand Canonical Monte Carlo Simulations. Industrial & Engineering Chemistry Research, 2009, 48, 3425-3431.	1.8	137
124	Metalâ^'Organic Frameworks As Templates for Nanoscale NaAlH₄. Journal of the American Chemical Society, 2009, 131, 13198-13199.	6.6	123
125	Quantum Monte Carlo Simulation of Nanoscale MgH2 Cluster Thermodynamics. Journal of the American Chemical Society, 2009, 131, 13918-13919.	6.6	57
126	The Metal Organic Films for Tailorable Chemical Sensing on Microcantilevers. ECS Transactions, 2009, 19, 267-278.	0.3	6

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127	Metal oxide composites and structures for ultra-high temperature solar thermochemical cycles. Journal of Materials Science, 2008, 43, 4714-4728.	1.7	213
128	Force Field Validation for Molecular Dynamics Simulations of IRMOF-1 and Other Isoreticular Zinc Carboxylate Coordination Polymers. Journal of Physical Chemistry C, 2008, 112, 5795-5802.	1.5	142
129	Stress-Induced Chemical Detection Using Flexible Metalâ^'Organic Frameworks. Journal of the American Chemical Society, 2008, 130, 14404-14405.	6.6	469
130	Two-Step Water Splitting Using Mixed-Metal Ferrites: Thermodynamic Analysis and Characterization of Synthesized Materials. Energy & Fuels, 2008, 22, 4115-4124.	2.5	152
131	Influence of Surface Reactions on Complex Hydride Reversibility. Journal of Physical Chemistry C, 2008, 112, 18270-18279.	1.5	4
132	Solar Thermochemical Water-Splitting Ferrite-Cycle Heat Engines. Journal of Solar Energy Engineering, Transactions of the ASME, 2008, 130, .	1.1	227
133	Mechanical properties of cubic zinc carboxylate IRMOF-1 metal-organic framework crystals. Physical Review B, 2007, 76, .	1.1	124
134	Theoretical and Experimental Investigation of the Thermochemistry of CrO2(OH)2(g). Journal of Physical Chemistry A, 2007, 111, 1971-1980.	1.1	189
135	Influence of Connectivity and Porosity on Ligand-Based Luminescence in Zinc Metalâ^'Organic Frameworks. Journal of the American Chemical Society, 2007, 129, 7136-7144.	6.6	625
136	The Interaction of Water with MOF-5 Simulated by Molecular Dynamics. Journal of the American Chemical Society, 2006, 128, 10678-10679.	6.6	533
137	Thermochemistry of the Chromium Hydroxides Cr(OH)n, n = 2â^'6, and the Oxyhydroxide CrO(OH)4:â€‰ Ab Initio Predictions. Journal of Physical Chemistry A, 2006, 110, 4093-4099.	1.1	11
138	BAC-MP4 Predictions of Thermochemistry for Gas-Phase Antimony Compounds in the Sbâ^'Hâ^'Câ^'Oâ^'Cl System. Journal of Physical Chemistry A, 2006, 110, 5919-5928.	1.1	11
139	BAC-MP4 Predictions of Thermochemistry for Gas-Phase Indium Compounds in the Inâ^'Hâ^'Câ^'Oâ^'Cl System. Journal of Physical Chemistry A, 2006, 110, 281-290.	1.1	8
140	Models for the Chemical Vapor Deposition of Tin Oxide from Monobutyltintrichloride. Journal of the Electrochemical Society, 2006, 153, C309.	1.3	15
141	From the President: Multiple Realities. Electrochemical Society Interface, 2006, 15, 7-7.	0.3	0
142	BAC-MP4 Predictions of Thermochemistry for Gas-Phase Tin Compounds in the Snâ^'Hâ^'Câ^'Cl System. Journal of Physical Chemistry A, 2005, 109, 4939-4949.	1.1	19
143	High-Level ab Initio Thermochemical Data for Halides of Chromium, Manganese, and Iron. Journal of Physical Chemistry A, 2005, 109, 928-933.	1.1	25
144	Gas-Phase Thermochemistry and Mechanism of Organometallic Tin Oxide CVD Precursors. Topics in Organometallic Chemistry, 2005, , 1-48.	0.7	9

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145	Stagnation Flow Reactor Investigation of Tin Oxide CVD from Monobutyltin Trichloride. Journal of the Electrochemical Society, 2004, 151, C527.	1.3	13
146	Theoretical Study of the Adsorption of Acetylene on the (111) Surfaces of Pd, Pt, Ni, and Rh. Journal of Physical Chemistry B, 2003, 107, 217-223.	1.2	107
147	Ab Initio Predictions for Thermochemical Parameters for Tinâ^'Oxygen Compounds. Journal of Physical Chemistry A, 2003, 107, 5122-5127.	1.1	9
148	In Situ Diagnostics and Modeling of Methane Catalytic Partial Oxidation on Pt in a Stagnation-Flow Reactor. Industrial & Engineering Chemistry Research, 2003, 42, 6559-6566.	1.8	22
149	Effects of competitive carbon monoxide adsorption on the hydrogen response of metalâ€"insulatorâ€"semiconductor sensors: the role of metal film morphology. Journal of Applied Physics, 2003, 93, 2267-2274.	1.1	15
150	Thermodynamic Analysis of Alumina Refractory Corrosion by Sodium or Potassium Hydroxide in Glass Melting Furnaces. Journal of the Electrochemical Society, 2002, 149, B551.	1.3	28
151	BAC-G2 Predictions of Thermochemistry for Gas-Phase Aluminum Compounds. Journal of Physical Chemistry A, 2002, 106, 2629-2640.	1.1	41
152	High pressure, high temperature shock tube studies of ethane pyrolysis and oxidation. Physical Chemistry Chemical Physics, 2002, 4, 2001-2010.	1.3	32
153	The Influence of Carbon Precursors on the Gas-Phase Chemistry of Titanium Carbide CVD. Chemical Vapor Deposition, 2002, 8, 63-73.	1.4	4
154	Effects of Methane and Ethane on the Heterogeneous Production of Water from Hydrogen and Oxygen over Platinum in Stagnation Flow. Journal of Catalysis, 2002, 208, 21-29.	3.1	12
155	BAC-MP4 Predictions of Thermochemistry for Gas-Phase Compounds in the Siâ^'Hâ^'Oâ^'Cl System. Journal of Physical Chemistry A, 2002, 106, 6370-6380.	1.1	11
156	Research needs for coatings on glass. Summary of the US Department of Energy roadmapping workshop. Thin Solid Films, 2001, 392, 155-163.	0.8	16
157	Thermodynamic Analysis of Silica Refractory Corrosion in Glass-Melting Furnaces. Journal of the Electrochemical Society, 2001, 148, B59.	1.3	66
158	EUROCVD-12. Chemical Vapor Deposition, 2000, 6, 9-11.	1.4	1
159	Understanding Homogeneous and Heterogeneous Contributions to the Platinum-Catalyzed Partial Oxidation of Ethane in a Short-Contact-Time Reactor. Journal of Catalysis, 2000, 196, 18-39.	3.1	157
160	Bond Additivity Corrections for Quantum Chemistry Methods. Journal of Physical Chemistry A, 2000, 104, 2168-2177.	1.1	37
161	Autocatalytic Behavior of Trimethylindium during Thermal Decomposition. Chemistry of Materials, 2000, 12, 450-460.	3.2	17
162	Gallium compounds, a possible problem for the G2 approaches. Journal of Chemical Physics, 1999, 110, 1879-1881.	1.2	28

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163	Thermodynamics and Kinetics of Gasâ€Phase Reactions in the Tiâ€Clâ€H System. Journal of the Electrochemical Society, 1998, 145, 2167-2178.	1.3	29
164	Flow-Tube Investigation of the High-Temperature Reaction between BCl3 and NH3. Journal of Physical Chemistry A, 1998, 102, 7804-7812.	1.1	27
165	Thermochemistry and Kinetics of Gas-Phase Reactions Relevant to the CVD of Coatings: New Data for Process Models. Materials Research Society Symposia Proceedings, 1998, 555, 121.	0.1	0
166	From Bunsen to VLSI. Electrochemical Society Interface, 1998, 7, 36-39.	0.3	14
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