Thomas Autrey

List of Publications by Year in descending order

116 papers	7,994 citations	57631 44 h-index	48187 88 g-index
125 all docs	125 docs citations	125 times ranked	5899 citing authors

#	Article	IF	Citations
1	Analysis of Intermediates and Products from the Dehydrogenation of Mg(BH₄)₂. Journal of Physical Chemistry A, 2022, 126, 444-452.	1.1	6
2	First-Principles Elucidation of Initial Dehydrogenation Pathways in Mg(BH₄)₂. Journal of Physical Chemistry Letters, 2022, 13, 1908-1913.	2.1	4
3	Thermal stability and structural studies on the mixtures of Mg(BH₄)₂ and glymes. Dalton Transactions, 2022, 51, 7268-7273.	1.6	2
4	Cost and potential of metalâ€“organic frameworks for hydrogen back-up power supply. Nature Energy, 2022, 7, 448-458.	19.8	28
5	Hydrogen storage in complex hydrides: past activities and new trends. Progress in Energy, 2022, 4, 032009.	4.6	23
6	Mg(BH₄)₂-Based Hybrid Metalâ€“Organic Borohydride System Exhibiting Enhanced Chemical Stability in Melt. ACS Applied Energy Materials, 2021, 4, 1704-1713.	2.5	5
7	Thermal Conversion of Unsolvated Mg(B₃H₈)₂ to BH₄^{â€“} in the Presence of MgH₂. ACS Applied Energy Materials, 2021, 4, 3737-3747.	2.5	17
8	Effects of Glymes on the Distribution of Mg(B10H10) and Mg(B12H12) from the Thermolysis of Mg(BH4)2. Inorganics, 2021, 9, 41.	1.2	9
9	A comparison of hydrogen release kinetics from 5- and 6-membered 1,2-BN-cycloalkanes. RSC Advances, 2021, 11, 34132-34136.	1.7	1
10	Challenges and opportunities for using formate to store, transport, and use hydrogen. Journal of Energy Chemistry, 2020, 41, 216-224.	7.1	65
11	Structural and reorientational dynamics of tetrahydroborate (BH₄^{â^’}) and tetrahydrofuran (THF) in a Mg(BH₄)₂Â·3THF adduct: neutron-scattering characterization. Physical Chemistry Chemical Physics, 2020, 22, 368-378.	1.3	6
12	Heterolytic Scission of Hydrogen Within a Crystalline Frustrated Lewis Pair. Inorganic Chemistry, 2020, 59, 15295-15301.	1.9	8
13	Nanoconfinement of Molecular Magnesium Borohydride Captured in a Bipyridine-Functionalized Metalâ€“Organic Framework. ACS Nano, 2020, 14, 10294-10304.	7.3	40
14	Development of an Autothermal Formate-Based Hydrogen Generator: From Optimization of Formate Dehydrogenation Conditions to Thermal Integration with Fuel Cells. ACS Sustainable Chemistry and Engineering, 2020, 8, 9846-9856.	3.2	21
15	Physi-Sorption of H2 on Pure and Boronâ€“Doped Graphene Monolayers: A Dispersionâ€“Corrected DFT Study. Journal of Carbon Research, 2020, 6, 15.	1.4	13
16	Immobilization of highly active bimetallic PdAu nanoparticles onto nanocarbons for dehydrogenation of formic acid. Journal of Materials Chemistry A, 2019, 7, 18835-18839.	5.2	45
17	Solid-state hydrogen rich boronâ€“nitrogen compounds for energy storage. Chemical Society Reviews, 2019, 48, 5350-5380.	18.7	82
18	Hydrogen Energy. ChemPhysChem, 2019, 20, 1157-1157.	1.0	22

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19	Reversible Hydrogen Uptake/Release over a Sodium Phenoxideâ€“Cyclohexanolate Pair. Angewandte Chemie, 2019, 131, 3134-3139.	1.6	6
20	Reversible Hydrogen Uptake/Release over a Sodium Phenoxideâ€“Cyclohexanolate Pair. Angewandte Chemie - International Edition, 2019, 58, 3102-3107.	7.2	23
21	Complexation Chemistry in N,N-Dimethylformamide-Based Molecular Inks for Chalcogenide Semiconductors and Photovoltaic Devices. Journal of the American Chemical Society, 2019, 141, 298-308.	6.6	57
22	A solvent-switched in situ confinement approach for immobilizing highly-active ultrafine palladium nanoparticles: boosting catalytic hydrogen evolution. Journal of Materials Chemistry A, 2018, 6, 5544-5549.	5.2	58
23	Releasing Hydrogen at High Pressures from Liquid Carriers: Aspects for the H₂ Delivery to Fueling Stations. Energy & Fuels, 2018, 32, 10008-10015.	2.5	25
24	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
25	Tandem Nitrogen Functionalization of Porous Carbon: Toward Immobilizing Highly Active Palladium Nanoclusters for Dehydrogenation of Formic Acid. ACS Catalysis, 2017, 7, 2720-2724.	5.5	175
26	Calorimetric Study of the Activation of Hydrogen by Tris(pentafluorophenyl)borane and Trimesitylphosphine. Journal of Physical Chemistry A, 2017, 121, 8785-8790.	1.1	21
27	Hydrogen Storage in Formic Acid: A Comparison of Process Options. Energy & Fuels, 2017, 31, 12603-12611.	2.5	94
28	Lewis Base Complexes of Magnesium Borohydride: Enhanced Kinetics and Product Selectivity upon Hydrogen Release. Inorganics, 2017, 5, 89.	1.2	23
29	Blending materials composed of boron, nitrogen and carbon to transform approaches to liquid hydrogen stores. Dalton Transactions, 2016, 45, 6196-6203.	1.6	7
30	Heterolysis of H2Across a Classical Lewis Pair, 2,6-Lutidineâ‹…BCl3: Synthesis, Characterization, and Mechanism. Chemistry - A European Journal, 2015, 21, 15713-15719.	1.7	6
31	Kinetic and Thermodynamic Study of the Reduction of 1,1â€Ðiphenylethylene by a Thermally Frustrated Diethyl Etherâ€BCF Lewis Pair. Israel Journal of Chemistry, 2015, 55, 196-201.	1.0	9
32	Selective Reversible Hydrogenation of Mg(B₃H₈)₂/MgH₂ to Mg(BH₄)₂: Pathway to Reversible Borane-Based Hydrogen Storage?. Inorganic Chemistry, 2015, 54, 4120-4125.	1.9	53
33	Capacity enhancement of aqueous borohydride fuels for hydrogen storage in liquids. Journal of Alloys and Compounds, 2015, 645, S196-S199.	2.8	16
34	Catalytic reduction of polar substrates without metals: A thermodynamic and kinetic study of heterolytic activation of hydrogen by vacancies in frustrated Lewis pairs. Catalysis Today, 2015, 251, 28-33.	2.2	35
35	Bis-BN Cyclohexane: A Remarkably Kinetically Stable Chemical Hydrogen Storage Material. Journal of the American Chemical Society, 2015, 137, 134-137.	6.6	62
36	Experimental and Theoretical Study of Molecular Response of Amine Bases in Organic Solvents. Journal of Physical Chemistry B, 2014, 118, 4883-4888.	1.2	9

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37	Methods to stabilize and destabilize ammonium borohydride. Dalton Transactions, 2013, 42, 680-687.	1.6	22
38	A thermodynamic and kinetic study of the heterolytic activation of hydrogen by frustrated boraneâ€“amine Lewis pairs. Dalton Transactions, 2013, 42, 615-619.	1.6	43
39	3-Methyl-1,2-BN-cyclopentane: a promising H₂storage material?. Dalton Transactions, 2013, 42, 611-614.	1.6	26
40	Understanding Vibrational Anharmonicity and Phonon Dispersion in Solid Ammonia Borane. Journal of Physical Chemistry C, 2012, 116, 5926-5931.	1.5	10
41	Role of Solvents on the Thermodynamics and Kinetics of Forming Frustrated Lewis Pairs. Journal of Physical Chemistry Letters, 2012, 3, 3312-3319.	2.1	20
42	First-Principles Prediction of Intermediate Products in the Decomposition of Metal Amidoboranes. Journal of Physical Chemistry C, 2012, 116, 26728-26734.	1.5	8
43	Boronâ€“nitrogenâ€“hydrogen (BNH) compounds: recent developments in hydrogen storage, applications in hydrogenation and catalysis, and new syntheses. Energy and Environmental Science, 2012, 5, 9257.	15.6	233
44	Immobilizing Highly Catalytically Active Pt Nanoparticles inside the Pores of Metalâ€“Organic Framework: A Double Solvents Approach. Journal of the American Chemical Society, 2012, 134, 13926-13929.	6.6	834
45	Mechanistic Investigation on the Formation and Dehydrogenation of Calcium Amidoborane Ammoniate. ChemSusChem, 2012, 5, 927-931.	3.6	10
46	Analysis of the Activation and Heterolytic Dissociation of H₂ by Frustrated Lewis Pairs: NH₃/BX₃ (X = H, F, and Cl). Journal of Physical Chemistry A, 2012, 116, 7228-7237.	1.1	51
47	Kinetic and thermodynamic investigation of hydrogen release from ethane 1,2-di-amineborane. Energy and Environmental Science, 2011, 4, 4187.	15.6	70
48	Reversible dehydrogenation of magnesium borohydride to magnesium triborane in the solid state under moderate conditions. Chemical Communications, 2011, 47, 1330-1332.	2.2	149
49	Control of hydrogen release and uptake in amine borane molecular complexes: thermodynamics of ammonia borane, ammonium borohydride, and the diammoniate of diborane. Faraday Discussions, 2011, 151, 157.	1.6	36
50	Characterization and mechanistic studies of the dehydrogenation of NHxBHx materials. Current Opinion in Solid State and Materials Science, 2011, 15, 73-79.	5.6	33
51	The tetragonal-to-orthorhombic phase transformation in ammonia borane and in its deuterium substituted compounds. Journal of Alloys and Compounds, 2011, 509, S709-S713.	2.8	4
52	Hydrogen isotope effects on the structural phase transition of NH3BH3. International Journal of Hydrogen Energy, 2011, 36, 7927-7931.	3.8	2
53	High-capacity hydrogen storage in lithium and sodium amidoboranes. , 2010, , 276-279.		0
54	Decomposition of NH3BH3 at sub-ambient pressures: A combined thermogravimetryâ€“differential thermal analysisâ€“mass spectrometry study. Journal of Power Sources, 2010, 195, 1615-1618.	4.0	29

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55	Highâ€Pressure Hydrogen Interactions with Polyaminoborane and Polyiminoborane. ChemPhysChem, 2010, 11, 93-96.	1.0	19
56	Growth of Crystalline Polyaminoborane through Catalytic Dehydrogenation of Ammonia Borane on FeB Nanoalloy. Chemistry - A European Journal, 2010, 16, 12814-12817.	1.7	40
57	Synthesis, structure and dehydrogenation of magnesium amidoborane monoammoniate. Chemical Communications, 2010, 46, 5752.	2.2	65
58	Characterization of a new phase of ammonia borane. Energy and Environmental Science, 2010, 3, 796.	15.6	48
59	Hydrogen Release Studies of Alkali Metal Amidoboranes. Inorganic Chemistry, 2010, 49, 3905-3910.	1.9	108
60	Thermal Stability of Ammonia Borane: A Case Study for Exothermic Hydrogen Storage Materials. Energy & Fuels, 2010, 24, 2596-2606.	2.5	57
61	Theoretical Investigations on the Formation and Dehydrogenation Reaction Pathways of H(NH₂BH₂)_nH (n = 1â^'4) Oligomers: Importance of Dihydrogen Interactions. Inorganic Chemistry, 2010, 49, 7710-7720.	1.9	38
62	The diammoniate of diborane: crystal structure and hydrogen release. Chemical Communications, 2010, 46, 8564.	2.2	47
63	Decomposition Pathway of Ammonia Borane on the Surface of Nano-BN. Journal of Physical Chemistry C, 2010, 114, 13935-13941.	1.5	39
64	Interaction of ammonia borane with Li2NH and Li3N. Dalton Transactions, 2010, 39, 720-722.	1.6	18
65	Pressure-induced complexation of NH3BH3â€"H2. Journal of Chemical Physics, 2009, 131, 224515.	1.2	40
66	Experimental and computational studies on collective hydrogen dynamics in ammonia borane: Incoherent inelastic neutron scattering. Journal of Chemical Physics, 2009, 130, 024507.	1.2	25
67	Bonding in boranes and their interaction with molecular hydrogen at extreme conditions. Journal of Chemical Physics, 2009, 131, 144508.	1.2	18
68	Hydrogen Dynamics and Characterization of the Tetragonal-to-Orthorhombic Phase Transformation in Ammonia Borane. Journal of Physical Chemistry C, 2009, 113, 5872-5878.	1.5	34
69	Absence of the Structural Phase Transition in Ammonia Borane Dispersed in Mesoporous Silica: Evidence of Novel Thermodynamic Properties. Journal of Physical Chemistry C, 2009, 113, 10319-10321.	1.5	65
70	Hyperpolarized 129Xe NMR Investigation of Ammonia Borane in Mesoporous Silica. Journal of Physical Chemistry C, 2009, 113, 6485-6490.	1.5	37
71	Thermodynamic and Structural Investigations of Ammonium Borohydride, a Solid with a Highest Content of Thermodynamically and Kinetically Accessible Hydrogen. Chemistry of Materials, 2009, 21, 4356-4358.	3.2	55
72	Determination of Structure and Phase Transition of Light Element Nanocomposites in Mesoporous Silica: Case study of NH₃BH₃ in MCM-41. Journal of the American Chemical Society, 2009, 131, 13749-13755.	6.6	93

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73	Neutron Powder Diffraction and Molecular Simulation Study of the Structural Evolution of Ammonia Borane from 15 to 340 K. Journal of Physical Chemistry A, 2009, 113, 5723-5735.	1.1	56
74	Defining Active Catalyst Structure and Reaction Pathways from ab Initio Molecular Dynamics and Operando XAFS: Dehydrogenation of Dimethylaminoborane by Rhodium Clusters. Journal of the American Chemical Society, 2009, 131, 10516-10524.	6.6	67
75	Promotion of Hydrogen Release from Ammonia Borane with Mechanically Activated Hexagonal Boron Nitride. Journal of Physical Chemistry C, 2009, 113, 1098-1103.	1.5	89
76	An investigation of the structural phase transition of ammonia borane. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2009, 521-522, 169-171.	2.6	4
77	The thermal decomposition of ammonia borane: A potential hydrogen storage material. Current Applied Physics, 2008, 8, 498-500.	1.1	98
78	In Situ Multinuclear NMR Spectroscopic Studies of the Thermal Decomposition of Ammonia Borane in Solution. Angewandte Chemie - International Edition, 2008, 47, 7493-7496.	7.2	168
79	Quasielastic neutron scattering of â€“NH3 and â€“BH3 rotational dynamics in orthorhombic ammonia borane. Chemical Physics Letters, 2008, 459, 85-88.	1.2	27
80	High-capacity hydrogen storage in lithium and sodium amidoboranes. Nature Materials, 2008, 7, 138-141.	13.3	583
81	Spectroscopic studies of the phase transition in ammonia borane: Raman spectroscopy of single crystal NH3BH3 as a function of temperature from 88to330K. Journal of Chemical Physics, 2008, 128, 034508.	1.2	90
82	Automated gas burette system for evolved hydrogen measurements. Review of Scientific Instruments, 2008, 79, 084103.	0.6	36
83	The Effects of Chemical Additives on the Induction Phase in Solid-State Thermal Decomposition of Ammonia Borane. Chemistry of Materials, 2008, 20, 5332-5336.	3.2	188
84	Materials for hydrogen storage: structure and dynamics of borane ammonia complex. Dalton Transactions, 2008, , 4514.	1.6	43
85	Synthesis of ammonia borane for hydrogen storage applications. Energy and Environmental Science, 2008, 1, 156.	15.6	233
86	Interaction of lithium hydride and ammonia borane in THF. Chemical Communications, 2008, , 5595.	2.2	70
87	Iridium-Catalyzed Dehydrogenation of Substituted Amine Boranes: Kinetics, Thermodynamics, and Implications for Hydrogen Storage. Inorganic Chemistry, 2008, 47, 8583-8585.	1.9	156
88	In situ solid state 11B MAS-NMR studies of the thermal decomposition of ammonia borane: mechanistic studies of the hydrogen release pathways from a solid state hydrogen storage material. Physical Chemistry Chemical Physics, 2007, 9, 1831.	1.3	356
89	When is a Nanoparticle a Cluster? An Operando EXAFS Study of Amine Borane Dehydrocoupling by Rh₄₋₆ Clusters. Journal of the American Chemical Society, 2007, 129, 11936-11949.	6.6	144
90	Spectroscopic Studies of Dehydrogenation of Ammonia Borane in Carbon Cryogel. Journal of Physical Chemistry B, 2007, 111, 14285-14289.	1.2	79

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91	Coherent Carbon Cryogelâ˜Ammonia Borane Nanocomposites for H2 Storage. Journal of Physical Chemistry B, 2007, 111, 7469-7472.	1.2	177
92	Dynamics of ammonia borane using neutron scattering. Physica B: Condensed Matter, 2006, 385-386, 266-268.	1.3	23
93	Mechanistic Studies of Hydrogen Release from Solid Amine Borane Materials. Materials Research Society Symposia Proceedings, 2006, 927, 1.	0.1	6
94	Nanoscaffold Mediates Hydrogen Release and the Reactivity of Ammonia Borane. Angewandte Chemie - International Edition, 2005, 44, 3578-3582.	7.2	751
95	In Situ XAFS and NMR Study of Rhodium-Catalyzed Dehydrogenation of Dimethylamine Borane. Journal of the American Chemical Society, 2005, 127, 3254-3255.	6.6	207
96	Thermochemistry of Aqueous Hydroxyl Radical from Advances in Photoacoustic Calorimetry and ab Initio Continuum Solvation Theory. Journal of the American Chemical Society, 2004, 126, 3680-3681.	6.6	32
97	Spectroscopic Studies of Tributylstannyl Radical. Rates of Formation, Termination, and Abstraction Determined by Transient Absorption Spectroscopy. Organometallics, 2004, 23, 2080-2086.	1.1	10
98	Absolute Rate Constants for Reactions of Tributylstannyl Radicals with Bromoalkanes, Episulfides, and Î±-Halomethyl-Episulfides, -Cyclopropanes, and -Oxiranes:Â New Rate Expressions for Sulfur and Bromine Atom Abstraction. Journal of Organic Chemistry, 2004, 69, 1020-1027.	1.7	9
99	azideDedicated to Professor Dr Z. R. Grabowski and Professor Dr J. Wirz on the occasions of their 75th and 60th birthdays.Electronic supplementary information (ESI) available: Cartesian coordinates and details of the CASSCF/CASPT2 calculations, details of the excited-state calculations on formylnitrene, the full IR spectra, additional results from the TRIR experiments and two tables with results from CASPT2 calculat. Physical Chemistry Chemical Physics, 2003, 5, 1010-1018.	1.3	94
100	Counting particles by means of optoacoustics: Potential limits in real solutions. Review of Scientific Instruments, 2003, 74, 628-631.	0.6	12
101	Model Compound Studies of the Î²-O-4 Linkage in Lignin:â€‰ Absolute Rate Expressions for Î²-Scission of Phenoxyl Radical from 1-Phenyl-2-phenoxyethanol-1-yl Radical. Journal of Organic Chemistry, 2002, 67, 7937-7945.	1.7	43
102	Comparison of Diffusion Coefficients of Aryl Carbonyls and Aryl Alcohols in Hydroxylic Solvents. Evidence that the Diffusion of Ketyl Radicals in Hydrogen-Bonding Solvents Is Not Anomalous?. Journal of Physical Chemistry A, 2001, 105, 5948-5953.	1.1	29
103	Detection of trace levels of water in oil by photoacoustic spectroscopy. Sensors and Actuators B: Chemical, 2001, 77, 620-624.	4.0	51
104	Tunable ultraviolet visible photoacoustic detection. Analytica Chimica Acta, 2001, 434, 217-222.	2.6	8
105	Measurement of select radical processes in hydrocarbon pyrolysis. Journal of Analytical and Applied Pyrolysis, 2000, 54, 37-64.	2.6	15
106	Listening to Colloidal Silica Samples: Simultaneous Measurement of Absorbed and Scattered Light Using Pulsed-Laser Photoacoustics. Applied Spectroscopy, 2000, 54, 1142-1150.	1.2	13
107	Nanojoules, nanoliters and nanosecond calorimetry. Journal of Photochemistry and Photobiology A: Chemistry, 1999, 125, 13-19.	2.0	8
108	â€œFeSâ€•Assisted Scission of Strong Bonds in Phenoxydiphenylmethanes. Competition between Hydrogen Atom Transfer and Free Radical Rearrangement Pathways. Energy & Fuels, 1999, 13, 927-933.	2.5	5

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109	A new angle into time-resolved photoacoustic spectroscopy: A layered prism cell increases experimental flexibility. Review of Scientific Instruments, 1998, 69, 2246-2258.	0.6	29
110	Mechanistic investigations of iron/sulfur-catalyzed bond scission in aromatic hydrocarbons. A catalytic hydrogen atom transfer step involving a late transition state. Catalysis Today, 1996, 31, 105-111.	2.2	15
111	Role of aromatic structure in pathways of hydrogen transfer and bond cleavage in coal liquefaction: Theoretical studies.. Coal Science and Technology, 1995, 24, 1411-1414.	0.0	1
112	Solvent Cage Recombination of 4-Benzoylphenylthiyl Radicals: Fast Intersystem Crossing of Triplet Sulfur-Centered Radical Pairs. The Journal of Physical Chemistry, 1995, 99, 869-871.	2.9	18
113	Solvent-Induced Scission of Diarylmethanes in Dihydroarene Donor Solvents: An Experimental and Mechanistic Modeling Study of Hydrogen-Transfer Pathways. Energy & Fuels, 1995, 9, 420-428.	2.5	25
114	THE PHOTOCHEMISTRY OF 3-NITROBENZOYL AND 4-NITROBENZOYL AZIDES: POSSIBLE REAGENTS FOR PHOTOAFFINITY LABELING. Photochemistry and Photobiology, 1988, 47, 497-501.	1.3	16
115	Aroylnitrenes with singlet ground states: photochemistry of acetyl-substituted aroyl and aryloxycarbonyl azides. Journal of the American Chemical Society, 1988, 110, 4297-4305.	6.6	59
116	Are aroylnitrenes ground-state singlets? Photochemistry of .beta.-naphthoyl azide. Journal of the American Chemical Society, 1987, 109, 5814-5820.	6.6	44