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	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
2	Nanoscaffold Mediates Hydrogen Release and the Reactivity of Ammonia Borane. Angewandte Chemie - International Edition, 2005, 44, 3578-3582.	7.2	751
3	High-capacity hydrogen storage in lithium and sodium amidoboranes. Nature Materials, 2008, 7, 138-141.	13.3	583
4	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
5	Synthesis of ammonia borane for hydrogen storage applications. Energy and Environmental Science, 2008, 1, 156.	15.6	233
6	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
7	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
8	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
9	Coherent Carbon Cryogelâ^'Ammonia Borane Nanocomposites for H2 Storage. Journal of Physical Chemistry B, 2007, 111, 7469-7472.	1.2	177
10	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
11	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
12	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
13	Iridium-Catalyzed Dehydrogenation of Substituted Amine Boranes: Kinetics, Thermodynamics, and Implications for Hydrogen Storage. Inorganic Chemistry, 2008, 47, 8583-8585.	1.9	156
14	Reversible dehydrogenation of magnesium borohydride to magnesium triborane in the solid state under moderate conditions. Chemical Communications, 2011, 47, 1330-1332.	2.2	149
15	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
16	Hydrogen Release Studies of Alkali Metal Amidoboranes. Inorganic Chemistry, 2010, 49, 3905-3910.	1.9	108
17	The thermal decomposition of ammonia borane: A potential hydrogen storage material. Current Applied Physics, 2008, 8, 498-500.	1.1	98
18	Matrix isolation, time-resolved IR, and computational study of the photochemistry of benzoyl 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

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19	Hydrogen Storage in Formic Acid: A Comparison of Process Options. Energy & Fuels, 2017, 31, 12603-12611.	2.5	94
20	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
21	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
22	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
23	Solid-state hydrogen rich boronâ€“nitrogen compounds for energy storage. Chemical Society Reviews, 2019, 48, 5350-5380.	18.7	82
24	Spectroscopic Studies of Dehydrogenation of Ammonia Borane in Carbon Cryogel. Journal of Physical Chemistry B, 2007, 111, 14285-14289.	1.2	79
25	Interaction of lithium hydride and ammonia borane in THF. Chemical Communications, 2008, , 5595.	2.2	70
26	Kinetic and thermodynamic investigation of hydrogen release from ethane 1,2-di-amineborane. Energy and Environmental Science, 2011, 4, 4187.	15.6	70
27	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
28	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
29	Synthesis, structure and dehydrogenation of magnesium amidoborane monoammoniate. Chemical Communications, 2010, 46, 5752.	2.2	65
30	Challenges and opportunities for using formate to store, transport, and use hydrogen. Journal of Energy Chemistry, 2020, 41, 216-224.	7.1	65
31	Bis-BN Cyclohexane: A Remarkably Kinetically Stable Chemical Hydrogen Storage Material. Journal of the American Chemical Society, 2015, 137, 134-137.	6.6	62
32	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
33	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
34	Thermal Stability of Ammonia Borane: A Case Study for Exothermic Hydrogen Storage Materials. Energy & Fuels, 2010, 24, 2596-2606.	2.5	57
35	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
36	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

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37	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
38	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
39	Detection of trace levels of water in oil by photoacoustic spectroscopy. Sensors and Actuators B: Chemical, 2001, 77, 620-624.	4.0	51
40	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
41	Characterization of a new phase of ammonia borane. Energy and Environmental Science, 2010, 3, 796.	15.6	48
42	The diammoniate of diborane: crystal structure and hydrogen release. Chemical Communications, 2010, 46, 8564.	2.2	47
43	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
44	Are aroylnitrenes ground-state singlets? Photochemistry of .beta.-naphthoyl azide. Journal of the American Chemical Society, 1987, 109, 5814-5820.	6.6	44
45	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
46	Materials for hydrogen storage: structure and dynamics of borane ammonia complex. Dalton Transactions, 2008, , 4514.	1.6	43
47	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
48	Pressure-induced complexation of NH3BH3â€“H2. Journal of Chemical Physics, 2009, 131, 224515.	1.2	40
49	Growth of Crystalline Polyaminoborane through Catalytic Dehydrogenation of Ammonia Borane on FeB Nanoalloy. Chemistry - A European Journal, 2010, 16, 12814-12817.	1.7	40
50	Nanoconfinement of Molecular Magnesium Borohydride Captured in a Bipyridine-Functionalized Metalâ€“Organic Framework. ACS Nano, 2020, 14, 10294-10304.	7.3	40
51	Decomposition Pathway of Ammonia Borane on the Surface of Nano-BN. Journal of Physical Chemistry C, 2010, 114, 13935-13941.	1.5	39
52	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
53	Hyperpolarized 129Xe NMR Investigation of Ammonia Borane in Mesoporous Silica. Journal of Physical Chemistry C, 2009, 113, 6485-6490.	1.5	37
54	Automated gas burette system for evolved hydrogen measurements. Review of Scientific Instruments, 2008, 79, 084103.	0.6	36

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55	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
56	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
57	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
58	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
59	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
60	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
61	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
62	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
63	Cost and potential of metalâ€“organic frameworks for hydrogen back-up power supply. Nature Energy, 2022, 7, 448-458.	19.8	28
64	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
65	3-Methyl-1,2-BN-cyclopentane: a promising H₂storage material?. Dalton Transactions, 2013, 42, 611-614.	1.6	26
66	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
67	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
68	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
69	Dynamics of ammonia borane using neutron scattering. Physica B: Condensed Matter, 2006, 385-386, 266-268.	1.3	23
70	Lewis Base Complexes of Magnesium Borohydride: Enhanced Kinetics and Product Selectivity upon Hydrogen Release. Inorganics, 2017, 5, 89.	1.2	23
71	Reversible Hydrogen Uptake/Release over a Sodium Phenoxideâ€“Cyclohexanolate Pair. Angewandte Chemie - International Edition, 2019, 58, 3102-3107.	7.2	23
72	Hydrogen storage in complex hydrides: past activities and new trends. Progress in Energy, 2022, 4, 032009.	4.6	23

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73	Methods to stabilize and destabilize ammonium borohydride. Dalton Transactions, 2013, 42, 680-687.	1.6	22
74	Hydrogen Energy. ChemPhysChem, 2019, 20, 1157-1157.	1.0	22
75	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
76	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
77	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
78	Highâ€Pressure Hydrogen Interactions with Polyaminoborane and Polyiminoborane. ChemPhysChem, 2010, 11, 93-96.	1.0	19
79	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
80	Bonding in boranes and their interaction with molecular hydrogen at extreme conditions. Journal of Chemical Physics, 2009, 131, 144508.	1.2	18
81	Interaction of ammonia borane with Li2NH and Li3N. Dalton Transactions, 2010, 39, 720-722.	1.6	18
82	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
83	THE PHOTOCHEMISTRY OF 3-NITROBENZOYL AND 4-NITROBENZOYL AZIDES: POSSIBLE REAGENTS FOR PHOTOAFFINITY LABELING. Photochemistry and Photobiology, 1988, 47, 497-501.	1.3	16
84	Capacity enhancement of aqueous borohydride fuels for hydrogen storage in liquids. Journal of Alloys and Compounds, 2015, 645, S196-S199.	2.8	16
85	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
86	Measurement of select radical processes in hydrocarbon pyrolysis. Journal of Analytical and Applied Pyrolysis, 2000, 54, 37-64.	2.6	15
87	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
88	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
89	Counting particles by means of optoacoustics: Potential limits in real solutions. Review of Scientific Instruments, 2003, 74, 628-631.	0.6	12
90	Spectroscopic Studies of Tributylstannyl Radical. Rates of Formation, Termination, and Abstraction Determined by Transient Absorption Spectroscopy. Organometallics, 2004, 23, 2080-2086.	1.1	10

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91	Understanding Vibrational Anharmonicity and Phonon Dispersion in Solid Ammonia Borane. Journal of Physical Chemistry C, 2012, 116, 5926-5931.	1.5	10
92	Mechanistic Investigation on the Formation and Dehydrogenation of Calcium Amidoborane Ammoniate. ChemSusChem, 2012, 5, 927-931.	3.6	10
93	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
94	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
95	Kinetic and Thermodynamic Study of the Reduction of 1,1â€Diphenylethylene by a Thermally Frustrated Diethyl Etherâ€BCF Lewis Pair. Israel Journal of Chemistry, 2015, 55, 196-201.	1.0	9
96	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
97	Nanojoules, nanoliters and nanosecond calorimetry. Journal of Photochemistry and Photobiology A: Chemistry, 1999, 125, 13-19.	2.0	8
98	Tunable ultraviolet visible photoacoustic detection. Analytica Chimica Acta, 2001, 434, 217-222.	2.6	8
99	First-Principles Prediction of Intermediate Products in the Decomposition of Metal Amidoboranes. Journal of Physical Chemistry C, 2012, 116, 26728-26734.	1.5	8
100	Heterolytic Scission of Hydrogen Within a Crystalline Frustrated Lewis Pair. Inorganic Chemistry, 2020, 59, 15295-15301.	1.9	8
101	Blending materials composed of boron, nitrogen and carbon to transform approaches to liquid hydrogen stores. Dalton Transactions, 2016, 45, 6196-6203.	1.6	7
102	Mechanistic Studies of Hydrogen Release from Solid Amine Borane Materials. Materials Research Society Symposia Proceedings, 2006, 927, 1.	0.1	6
103	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
104	Reversible Hydrogen Uptake/Release over a Sodium Phenoxideâ€“Cyclohexanolate Pair. Angewandte Chemie, 2019, 131, 3134-3139.	1.6	6
105	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
106	Analysis of Intermediates and Products from the Dehydrogenation of Mg(BH₄)₂. Journal of Physical Chemistry A, 2022, 126, 444-452.	1.1	6
107	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
108	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

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109	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
110	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
111	First-Principles Elucidation of Initial Dehydrogenation Pathways in Mg(BH₄)₂. Journal of Physical Chemistry Letters, 2022, 13, 1908-1913.	2.1	4
112	Hydrogen isotope effects on the structural phase transition of NH3BH3. International Journal of Hydrogen Energy, 2011, 36, 7927-7931.	3.8	2
113	Thermal stability and structural studies on the mixtures of Mg(BH₄)₂ and glymes. Dalton Transactions, 2022, 51, 7268-7273.	1.6	2
114	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
115	A comparison of hydrogen release kinetics from 5- and 6-membered 1,2-BN-cycloalkanes. RSC Advances, 2021, 11, 34132-34136.	1.7	1
116	High-capacity hydrogen storage in lithium and sodium amidoboranes. , 2010, , 276-279.		0