Tibor SzilvÃ;si

List of Publications by Year in descending order

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119 papers 3,791 citations

34 h-index 54 g-index

128 all docs

 $\begin{array}{c} 128 \\ \\ \text{docs citations} \end{array}$

128 times ranked 2702 citing authors

#	Article	IF	Citations
1	Direct time-domain observation of attosecond final-state lifetimes in photoemission from solids. Science, 2016, 353, 62-67.	12.6	181
2	A Bis(silylene)â€Substituted <i>ortho</i> à€Carborane as a Superior Ligand in the Nickelâ€Catalyzed Amination of Arenes. Angewandte Chemie - International Edition, 2016, 55, 12868-12872.	13.8	141
3	A Fragile Zwitterionic Phosphasilene as a Transfer Agent of the Elusive Parent Phosphinidene (:PH). Journal of the American Chemical Society, 2013, 135, 11795-11798.	13.7	120
4	Can low-valent silicon compounds be better transition metal ligands than phosphines and NHCs?. RSC Advances, 2015, 5, 5077-5086.	3.6	106
5	From a Phosphaketenylâ€Functionalized Germylene to 1,3â€Digermaâ€2,4â€diphosphacyclobutadiene. Angewandte Chemie - International Edition, 2016, 55, 4781-4785.	13.8	103
6	From an Fe ₂ P ₃ complex to FeP nanoparticles as efficient electrocatalysts for water-splitting. Chemical Science, 2018, 9, 8590-8597.	7.4	103
7	A monotopic aluminum telluride with an Al=Te double bond stabilized by N-heterocyclic carbenes. Nature Communications, 2015, 6, 10037.	12.8	88
8	Peripheral mechanism of a carbonyl hydrosilylation catalysed by an SiNSi iron pincer complex. Chemical Science, 2015, 6, 7143-7149.	7.4	86
9	Unexpected Photodegradation of a Phosphaketenylâ€Substituted Germyliumylidene Borate Complex. Angewandte Chemie - International Edition, 2017, 56, 4333-4336.	13.8	85
10	CO ₂ Fixation and Catalytic Reduction by a Neutral Aluminum Double Bond. Angewandte Chemie - International Edition, 2019, 58, 10961-10965.	13.8	75
11	An NHC-Stabilized Silicon Analogue of Acylium Ion: Synthesis, Structure, Reactivity, and Theoretical Studies. Journal of the American Chemical Society, 2015, 137, 5828-5836.	13.7	74
12	Twist of a Silicon–Silicon Double Bond: Selective <i>Anti</i> Ininodisilene. Journal of the American Chemical Society, 2017, 139, 9156-9159.	13.7	73
13	From a Zwitterionic Phosphasilene to Base Stabilized Silyliumylidene-Phosphide and Bis(silylene) Complexes. Journal of the American Chemical Society, 2013, 135, 17958-17968.	13.7	68
14	A Donorâ€Stabilized Zwitterionic "Halfâ€Parent―Phosphasilene and Its Unusual Reactivity towards Small Molecules. Chemistry - A European Journal, 2014, 20, 1947-1956.	3.3	65
15	Synthesis and Unexpected Reactivity of Germyliumylidene Hydride [:GeH] ⁺ Stabilized by a Bis(<i>N</i> -heterocyclic carbene)borate Ligand. Journal of the American Chemical Society, 2014, 136, 11300-11303.	13.7	64
16	An Elusive Hydridoaluminum(I) Complex for Facile C–H and C–O Bond Activation of Ethers and Access to Its Isolable Hydridogallium(I) Analogue: Syntheses, Structures, and Theoretical Studies. Journal of the American Chemical Society, 2014, 136, 9732-9742.	13.7	64
17	A Neutral Tetraphosphacyclobutadiene Ligand in Cobalt(I) Complexes. Angewandte Chemie - International Edition, 2015, 54, 1250-1254.	13.8	63
18	An Intramolecular Silylene Borane Capable of Facile Activation of Small Molecules, Including Metalâ€Free Dehydrogenation of Water. Angewandte Chemie - International Edition, 2017, 56, 3699-3702.	13.8	63

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19	A facile access to a novel NHC-stabilized silyliumylidene ion and $\hat{\text{Ca}}\in \text{H}$ activation of phenylacetylene. Chemical Communications, 2014, 50, 12619-12622.	4.1	62
20	Isolation of an Nâ∈Heterocyclic Carbene Complex of a Borasilene. Chemistry - A European Journal, 2019, 25, 11036-11041.	3.3	62
21	Isolation and Structure of Germyleneâ€Germyliumylidenes Stabilized by Nâ€Heterocyclic Imines. Angewandte Chemie - International Edition, 2016, 55, 11619-11624.	13.8	59
22	Precise Activation of Ammonia and Carbon Dioxide by an Iminodisilene. Angewandte Chemie - International Edition, 2018, 57, 14575-14579.	13.8	57
23	From a Phosphaketenylâ€Functionalized Germylene to 1,3â€Digermaâ€2,4â€diphosphacyclobutadiene. Angewandte Chemie, 2016, 128, 4859-4863.	2.0	55
24	Distinguishing attosecond electron–electron scattering and screening in transition metals. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E5300-E5307.	7.1	55
25	A Bis(silylene)â€Substituted <i>ortho</i> â€Carborane as a Superior Ligand in the Nickelâ€Catalyzed Amination of Arenes. Angewandte Chemie, 2016, 128, 13060-13064.	2.0	52
26	A bis(silylene)-stabilized diphosphorus compound and its reactivity as a monophosphorus anion transfer reagent. Nature Chemistry, 2020, 12, 801-807.	13.6	52
27	Internal Catalytic Effect of Bulky NHC Ligands in Suzuki–Miyaura Cross-Coupling Reaction. ACS Catalysis, 2013, 3, 1984-1991.	11.2	47
28	Unexpected Photodegradation of a Phosphaketenylâ€Substituted Germyliumylidene Borate Complex. Angewandte Chemie, 2017, 129, 4397-4400.	2.0	47
29	Theoretical Assessment of Low-Valent Germanium Compounds as Transition Metal Ligands: Can They Be Better than Phosphines or NHCs?. Organometallics, 2017, 36, 1591-1600.	2.3	44
30	Tuning the Optical Gap of Nanometer-Size Diamond Cages by Sulfurization: A Time-Dependent Density Functional Study. Physical Review Letters, 2012, 108, 267401.	7.8	41
31	Redoxâ€Triggered Orientational Responses of Liquid Crystals to Chlorine Gas. Angewandte Chemie - International Edition, 2018, 57, 9665-9669.	13.8	39
32	Heavier Carbonyl Olefination: The Sila-Wittig Reaction. Journal of the American Chemical Society, 2019, 141, 16991-16996.	13.7	38
33	The correlation theory of the chemical bond. Scientific Reports, 2017, 7, 2237.	3.3	37
34	Threeâ€Coordinate Boron(III) and Diboron(II) Dications. Chemistry - A European Journal, 2018, 24, 4283-4288.	3.3	35
35	The Quest for Stable Silaaldehydes: Synthesis and Reactivity of a Masked Silacarbonyl. Chemistry - A European Journal, 2019, 25, 1198-1202.	3.3	34
36	Design of Chemoresponsive Liquid Crystals through Integration of Computational Chemistry and Experimental Studies. Chemistry of Materials, 2017, 29, 3563-3571.	6.7	33

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37	Silylene–Nickel Promoted Cleavage of Bâ^'O Bonds: From Catechol Borane to the Hydroborylene Ligand. Angewandte Chemie - International Edition, 2017, 56, 7470-7474.	13.8	33
38	From an Isolable Acyclic Phosphinosilylene Adduct to Donorâ€Stabilized SiE Compounds (E=O, S, Se). Chemistry - A European Journal, 2015, 21, 18930-18933.	3.3	32
39	Bis(silylene)â€Stabilized Monovalent Nitrogen Complexes. Angewandte Chemie - International Edition, 2020, 59, 22043-22047.	13.8	31
40	New Route to Access an Acylâ€Functionalized Phosphasilene and a Fourâ€Membered Siâ€Pâ€Câ€O Heterocycle. Chemistry - A European Journal, 2014, 20, 9312-9318.	3.3	29
41	A Persistent 1,2â€Dihydrophosphasilene Adduct. Angewandte Chemie - International Edition, 2015, 54, 15060-15063.	13.8	29
42	Facile rotation around a silicon–phosphorus double bond enabled through coordination to tungsten. Chemical Communications, 2015, 51, 11272-11275.	4.1	29
43	Improving the Catalytic Activity in the Rhodiumâ€Mediated Hydroformylation of Styrene by a Bis(Nâ€heterocyclic silylene) Ligand. European Journal of Inorganic Chemistry, 2017, 2017, 1284-1291.	2.0	29
44	Molecular Tailoring: Reaction Path Control with Bulky Substituents. Organometallics, 2012, 31, 3207-3212.	2.3	28
45	Platinum(II) complexes incorporating racemic and optically active 1-alkyl-3-phospholene P-ligands: Synthesis, stereostructure, NMR properties and catalytic activity. Journal of Organometallic Chemistry, 2014, 751, 306-313.	1.8	28
46	Reversible metathesis of ammonia in an acyclic germylene–Ni ⁰ complex. Chemical Science, 2021, 12, 5582-5590.	7.4	28
47	Neutral "Cp-Free―Silyl-Lanthanide(II) Complexes: Synthesis, Structure, and Bonding Analysis. Inorganic Chemistry, 2015, 54, 7065-7072.	4.0	27
48	Systematic Study of N-Heterocyclic Carbene Coordinate Hydrosilylene Transition-Metal Complexes. Inorganic Chemistry, 2017, 56, 10061-10069.	4.0	27
49	Computational Chemistryâ€Guided Design of Selective Chemoresponsive Liquid Crystals Using Pyridine and Pyrimidine Functional Groups. Advanced Functional Materials, 2018, 28, 1703581.	14.9	27
50	The role of anions in adsorbate-induced anchoring transitions of liquid crystals on surfaces with discrete cation binding sites. Soft Matter, 2018, 14, 797-805.	2.7	27
51	Open-Shell Lanthanide(II+) or -(III+) Complexes Bearing \ddot{I}_f -Silyl and Silylene Ligands: Synthesis, Structure, and Bonding Analysis. Inorganic Chemistry, 2015, 54, 3306-3315.	4.0	26
52	Isolation and Structure of Germyleneâ€Germyliumylidenes Stabilized by Nâ€Heterocyclic Imines. Angewandte Chemie, 2016, 128, 11791-11796.	2.0	26
53	A New Domain of Reactivity for Highâ€Valent Dinuclear [M(μâ€O) ₂ M′] Complexes in Oxidation Reactions. Angewandte Chemie - International Edition, 2017, 56, 297-301.	13.8	26
54	CO ₂ Fixation and Catalytic Reduction by a Neutral Aluminum Double Bond. Angewandte Chemie, 2019, 131, 11077-11081.	2.0	25

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55	Reaction of an Nâ€Heterocyclic Carbeneâ€Stabilized Silicon(II) Monohydride with Alkynes: [2+2+1] Cycloaddition versus Hydrogen Abstraction. Chemistry - A European Journal, 2015, 21, 1949-1954.	3.3	24
56	Alkaline-Earth-Metal-Induced Liberation of Rare Allotropes of Elemental Silicon and Germanium from N-Heterocyclic Metallylenes. Inorganic Chemistry, 2015, 54, 8840-8848.	4.0	24
57	Isolation and Reactivity of Chlorotetryliumylidenes Using a Bidentate Bis(N-heterocyclic imine) Ligand. Organometallics, 2020, 39, 4265-4272.	2.3	24
58	An Intramolecular Silylene Borane Capable of Facile Activation of Small Molecules, Including Metal-Free Dehydrogenation of Water. Angewandte Chemie, 2017, 129, 3753-3756.	2.0	23
59	Chalcogen-atom transfer and exchange reactions of NHC-stabilized heavier silaacylium ions. Dalton Transactions, 2017, 46, 16014-16018.	3.3	23
60	Synthesis of a Metalloâ€Iminosilane via a Silanone–Metal Ï€â€Complex. Angewandte Chemie - International Edition, 2017, 56, 14282-14286.	13.8	22
61	Synthesis and properties of hydroxy tail-terminated cyanobiphenyl liquid crystals. Liquid Crystals, 2019, 46, 397-407.	2.2	22
62	An Sâ€Oxygenated [NiFe] Complex Modelling Sulfenate Intermediates of an O ₂ â€Tolerant Hydrogenase. Angewandte Chemie - International Edition, 2017, 56, 2208-2211.	13.8	21
63	Precise Activation of Ammonia and Carbon Dioxide by an Iminodisilene. Angewandte Chemie, 2018, 130, 14783-14787.	2.0	20
64	Versatile Tautomerization of EH $<$ sub $>$ 2 $<$ /sub $>$ -Substituted Silylenes (E = N, P, As) in the Coordination Sphere of Nickel. Journal of the American Chemical Society, 2019, 141, 3304-3314.	13.7	20
65	Molecular tailoring: a possible synthetic route to hexasilabenzene. Dalton Transactions, 2014, 43, 1184-1190.	3.3	19
66	Using Functionalized Silyl Ligands To Suppress Solvent Coordination to Silyl Lanthanide(II) Complexes. Inorganic Chemistry, 2017, 56, 5328-5341.	4.0	19
67	Identifying the Rate-Limiting Elementary Steps of Nitrogen Fixation with Single-Site Fe Model Complexes. Inorganic Chemistry, 2018, 57, 8499-8508.	4.0	19
68	Transition Metal Carbonyl Complexes of an N-Heterocyclic Carbene Stabilized Silyliumylidene Ion. Inorganic Chemistry, 2019, 58, 14931-14937.	4.0	19
69	Amplification of Elementary Surface Reaction Steps on Transition Metal Surfaces Using Liquid Crystals: Dissociative Adsorption and Dehydrogenation. Journal of the American Chemical Society, 2019, 141, 16003-16013.	13.7	18
70	Synthesis and properties of fluorine tail-terminated cyanobiphenyls and terphenyls for chemoresponsive liquid crystals. Liquid Crystals, 2020, 47, 3-16.	2.2	17
71	The mechanism and energetics of insertion reactions of silylenes. Dalton Transactions, 2010, 39, 9347.	3.3	16
72	An Amplified Ylidic "Half-Parent―Iminosilane LSiâ•NH. Journal of the American Chemical Society, 2014, 136, 14207-14214.	13.7	16

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73	DMRG on Top of Plane-Wave Kohn–Sham Orbitals: A Case Study of Defected Boron Nitride. Journal of Chemical Theory and Computation, 2021, 17, 1143-1154.	5.3	16
74	Platinum(II) Complexes Incorporating Racemic and Optically Active 1-Aryl-3- phospholene P-Ligands as Potential Catalysts in Hydroformylation. Current Organic Chemistry, 2014, 18, 1529-1538.	1.6	15
75	Facile Rearrangement of a Bis(N-heterocyclic carbene)borate Chelate Ligand and Access to [:GeX]+Complexes (X = H, Cl). European Journal of Inorganic Chemistry, 2015, 2015, 2377-2380.	2.0	15
76	From zinco(<scp>ii</scp>) arsaketenes to silylene-stabilised zinco arsinidene complexes. Chemical Communications, 2018, 54, 6124-6127.	4.1	15
77	Accessing the main-group metal formyl scaffold through CO-activation in beryllium hydride complexes. Nature Communications, 2022, 13, 461.	12.8	14
78	Facile Access to Stable Silylium Ions Stabilized by N-Heterocyclic Imines. Molecules, 2016, 21, 1155.	3.8	13
79	Reactivity of an Nâ€Heterocyclic Carbene Stabilized Hydrosilylene towards a Ketone and CO2: Experimental and Theoretical Study. European Journal of Inorganic Chemistry, 2016, 2016, 2696-2703.	2.0	13
80	Demonstrating the Direct Relationship between Hydrogen Evolution Reaction and Catalyst Deactivation in Synthetic Fe Nitrogenases. ACS Catalysis, 2020, 10, 12555-12568.	11.2	13
81	Trends in computational molecular catalyst design. Dalton Transactions, 2021, 50, 10325-10339.	3.3	13
82	An Isolable Threeâ€Coordinate Germanone and Its Reactivity. Chemistry - A European Journal, 2021, 27, 15914-15917.	3.3	13
83	Fluorine Modification of the Surface of Diamondoids: A Time-Dependent Density Functional Study. Journal of Physical Chemistry C, 2014, 118, 4410-4415.	3.1	12
84	Transition Metal Complexes of a "Half-Parent―Phosphasilene Adduct Representing Silyleneâ†'Phosphinideneâ†'Metal Complexes. Organometallics, 2015, 34, 5703-5708.	2.3	12
85	On the mechanism of the reaction of white phosphorus with silylenes. Dalton Transactions, 2011, 40, 7193.	3.3	11
86	A study on the optical resolution of 1-isopropyl-3-methyl-3-phospholene 1-oxide and its use in the synthesis of borane and platinum complexes. Journal of Organometallic Chemistry, 2015, 797, 140-152.	1.8	11
87	Synthesis of a Metalloâ€lminosilane via a Silanone–Metal Ï€â€Complex. Angewandte Chemie, 2017, 129, 14470-14474.	2.0	11
88	Redoxâ€Triggered Orientational Responses of Liquid Crystals to Chlorine Gas. Angewandte Chemie, 2018, 130, 9813-9817.	2.0	11
89	Unique Insertion Mechanisms of Bis-dehydro- \hat{l}^2 -diketiminato Silylene. Organometallics, 2011, 30, 5344-5351.	2.3	10
90	Molecular Tailoring: Substituent Design for Hexagermabenzene. Organometallics, 2013, 32, 4733-4740.	2.3	10

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91	Synthesis, Characterization, and Application of Platinum(II) Complexes Incorporating Racemic and Optically Active 4-Chloro-5-Methyl-1-Phenyl-1,2,3,6-Tetrahydrophosphinine Ligand. Heteroatom Chemistry, 2016, 27, 91-101.	0.7	10
92	The role of iron-oxide aerosols and sunlight in the atmospheric reduction of Hg(II) species: A DFT+U study. Applied Catalysis B: Environmental, 2018, 234, 347-356.	20.2	10
93	Metal nitrene-like reactivity of a Siî€N bond towards CO ₂ . Chemical Communications, 2018, 54, 9352-9355.	4.1	10
94	New room temperature nematogens by cyano tail termination of alkoxy and alkylcyanobiphenyls and their anchoring behavior on metal salt-decorated surface. Liquid Crystals, 2020, 47, 540-556.	2.2	10
95	An automated cluster surface scanning method for exploring reaction paths on metal-cluster surfaces. Computational Materials Science, 2021, 186, 110010.	3.0	10
96	Silylene–Nickel Promoted Cleavage of Bâ^'O Bonds: From Catechol Borane to the Hydroborylene Ligand. Angewandte Chemie, 2017, 129, 7578-7582.	2.0	9
97	Quantum chemical calculations to determine partitioning coefficients for HgCl2 on iron-oxide aerosols. Science of the Total Environment, 2018, 636, 580-587.	8.0	9
98	Bis(silylene)â€Stabilized Monovalent Nitrogen Complexes. Angewandte Chemie, 2020, 132, 22227-22231.	2.0	9
99	Designing chemically selective liquid crystalline materials that respond to oxidizing gases. Journal of Materials Chemistry C, 2021, 9, 6507-6517.	5.5	9
100	A New Domain of Reactivity for Highâ€Valent Dinuclear [M(μâ€O) 2 M′] Complexes in Oxidation Reactions. Angewandte Chemie, 2017, 129, 303-307.	2.0	8
101	Exploring Hydrogen Evolution Accompanying Nitrogen Reduction on Biomimetic Nitrogenase Analogs: Can Fe–NxHyIntermediates Be Active Under Turnover Conditions?. Inorganic Chemistry, 2019, 58, 7969-7977.	4.0	8
102	Binding of Organophosphorus Nerve Agents and Their Simulants to Metal Salts. ACS Applied Materials & Samp; Interfaces, 2020, 12, 30941-30953.	8.0	8
103	Influence of multifluorophenyloxy terminus on the mesomorphism of the alkoxy and alkyl cyanobiphenyl compounds in search of new ambient nematic liquid crystals and mixtures. Liquid Crystals, 2021, 48, 672-688.	2.2	8
104	Coupling the chemical reactivity of bimetallic surfaces to the orientations of liquid crystals. Materials Horizons, 2021, 8, 2050-2056.	12.2	8
105	Benchmarking Semiempirical QM Methods for Calculating the Dipole Moment of Organic Molecules. Journal of Physical Chemistry A, 2022, 126, 1905-1921.	2.5	8
106	Facile Access to Dative, Single, and Double Siliconâ^'Metal Bonds Through Mâ^'Cl Insertion Reactions of Baseâ€Stabilized Si ^{II} Cations. Chemistry - A European Journal, 2020, 26, 6271-6278.	3.3	7
107	Identification of stable adsorption sites and diffusion paths on nanocluster surfaces: an automated scanning algorithm. Npj Computational Materials, 2019, 5, .	8.7	6
108	Why do N-heterocyclic carbenes and silylenes activate white phosphorus differently?. Structural Chemistry, 2015, 26, 1335-1342.	2.0	5

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109	Computational Chemistry-Based Evaluation of Metal Salts and Metal Oxides for Application in Mercury-Capture Technologies. Industrial & Engineering Chemistry Research, 2020, 59, 9015-9022.	3.7	4
110	Design of Chemoresponsive Soft Matter Using Hydrogen-Bonded Liquid Crystals. Materials, 2021, 14, 1055.	2.9	4
111	Investigations of LiP(SiMe ₂ CH ₂ SiMe ₃)–P <i>t</i> Bu ₂ , the Surprising Byproduct in the Metalation of (Me ₃ Si) _{Si)₂P–P<i>t</i>Bu₂. European Journal of Inorganic Chemistry, 2017, 2017, 5521-5528.}	2.0	3
112	H ₂ and N ₂ Binding Affinities Are Coupled in Synthetic Fe Nitrogenases Limiting N ₂ Fixation. Organometallics, 2022, 41, 1134-1146.	2.3	3
113	From <i>As</i> â€Zincoarsasilene (LZnâ€As=SiL′) to Arsaethynolato (As≡Câ^²O) and Arsaketenylido (O=C=A Zinc Complexes. Angewandte Chemie - International Edition, 2019, 58, 3382-3386.	.s) 13.8	2
114	Experimental and Computational Study of the Properties of Imidazole Compounds with Branched and Cycloalkyl Substituents. Liquids, 2022, 2, 14-25.	2.5	2
115	Rþcktitelbild: Silylene–Nickel Promoted Cleavage of Bâ~O Bonds: From Catechol Borane to the Hydroborylene Ligand (Angew. Chem. 26/2017). Angewandte Chemie, 2017, 129, 7788-7788.	2.0	0
116	Theoretical Evidence for the Utilization of Lowâ€Valent Mainâ€Group Complexes as Rareâ€Synthon Equivalents. Chemistry - A European Journal, 2017, 23, 17908-17914.	3.3	0
117	Frontispiece: Theoretical Evidence for the Utilization of Lowâ€Valent Mainâ€Group Complexes as Rareâ€Synthon Equivalents. Chemistry - A European Journal, 2017, 23, .	3.3	0
118	From As â€Zincoarsasilene (LZnâ€As=SiL′) to Arsaethynolato (As≡Câ^'O) and Arsaketenylido (O=C=As) Zinc Complexes. Angewandte Chemie, 2019, 131, 3420-3424.	2.0	0
119	Properties of Imidazolium Ionic Liquids with Glycerol-Derived Functional Groups. Journal of Chemical & Engineering Data, 2022, 67, 1905-1914.	1.9	0