

# Felipe Fantuzzi

## List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	cAAC-Stabilized 9,10-diboraanthracenes Acenes with Open-Shell Singlet Biradical Ground States. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 19338-19343.	13.8	54
2	Lewis-Base Stabilization of the Parent Al(I) Hydride under Ambient Conditions. <i>Journal of the American Chemical Society</i> , 2019, 141, 16954-16960.	13.7	45
3	Nature of the Chemical Bond and Origin of the Inverted Dipole Moment in Boron Fluoride: A Generalized Valence Bond Approach. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5335-5343.	2.5	35
4	A Neutral Beryllium(I) Radical. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 20776-20780.	13.8	33
5	Description of Polar Chemical Bonds from the Quantum Mechanical Interference Perspective. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2322-2332.	5.3	27
6	Chemical bonding in the pentagonal-pyramidal benzene dication and analogous isoelectronic hexa-coordinate species. <i>Computational and Theoretical Chemistry</i> , 2017, 1116, 225-233.	2.5	24
7	Isolation and Reactivity of an Antiaromatic s-Block Metal Compound. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 3812-3819.	13.8	24
8	Photodissociation of methyl formate in circumstellar environment: stability under soft X-rays. <i>Monthly Notices of the Royal Astronomical Society</i> , 2011, 417, 2631-2641.	4.4	23
9	Interference Energy in C-H and C-C Bonds of Saturated Hydrocarbons: Dependence on the Type of Chain and Relationship to Bond Dissociation Energy. <i>Journal of Physical Chemistry A</i> , 2013, 117, 4025-4034.	2.5	22
10	The non-covalent nature of the molecular structure of the benzene molecule. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 11024-11030.	2.8	22
11	Ruthenium(II)-Catalyzed Double Annulation of Quinones: Step-Economical Access to Valuable Bioactive Compounds. <i>Chemistry - A European Journal</i> , 2020, 26, 10981-10986.	3.3	22
12	Highly Colored Boron-Doped Thiazolothiazoles from the Reductive Dimerization of Boron Isothiocyanates. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 6446-6450.	13.8	22
13	Diborane(4) Azides: Surprisingly Stable Sources of Transient Iminoboranes. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 15480-15486.	13.8	21
14	The role of quantum-mechanical interference and quasi-classical effects in conjugated hydrocarbons. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 5479.	2.8	20
15	The Nature of the Chemical Bond from a Quantum Mechanical Interference Perspective. <i>ChemistrySelect</i> , 2017, 2, 604-619.	1.5	20
16	Reduction and Rearrangement of a Boron(I) Carbonyl Complex. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 2963-2968.	13.8	20
17	Adducts of the Parent Boraphosphaketene H <sub>2</sub> BPCO and their Decarbonylative Insertion Chemistry. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 13666-13670.	13.8	20
18	An Unsymmetrical, Cyclic Diborene Based on a Chelating CAAC Ligand and its Small-Molecule Activation and Rearrangement Chemistry. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	13.8	20

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19	The Nature of the Singlet and Triplet States of Cyclobutadiene as Revealed by Quantum Interference. <i>ChemPhysChem</i> , 2016, 17, 288-295.	2.1	19
20	Reduction of a dihydroboryl cation to a boryl anion and its air-stable, neutral hydroboryl radical through hydrogen shuttling. <i>Chemical Science</i> , 2020, 11, 551-555.	7.4	19
21	The Dimethylbismuth Cation: Entry Into Dative Bi~Bi Bonding and Unconventional Methyl Exchange. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 24388-24394.	13.8	19
22	On the metastability of doubly charged homonuclear diatomics. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 19352-19359.	2.8	17
23	Hydrogenated Benzene in Circumstellar Environments: Insights into the Photostability of Super-hydrogenated PAHs. <i>Astrophysical Journal</i> , 2018, 854, 61.	4.5	17
24	cAAC-stabilisierte 9,10-Diboraanthracene - offenschalige Singulettbiradikale. <i>Angewandte Chemie</i> , 2020, 132, 19502-19507.	2.0	17
25	Twisting versus Delocalization in CAAC- and NHC-Stabilized Boron-Based Biradicals: The Roles of Sterics and Electronics. <i>Chemistry - A European Journal</i> , 2021, 27, 5160-5170.	3.3	17
26	Rhodium(III)-Catalyzed C-H/N-H Alkyne Annulation of Nonsymmetric 2-Aryl (Benz)imidazole Derivatives: Photophysical and Mechanistic Insights. <i>Journal of Organic Chemistry</i> , 2021, 86, 264-278.	3.2	16
27	Destruction and multiple ionization of PAHs by X-rays in circumnuclear regions of AGNs. <i>Monthly Notices of the Royal Astronomical Society</i> , 2019, 488, 451-469.	4.4	15
28	Oxidation, Coordination, and Nickel-Mediated Deconstruction of a Highly Electron-Rich Diboron Analogue of 1,3,5-Hexatriene. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 15717-15725.	13.8	14
29	SINGLE AND DOUBLE PHOTOIONIZATION AND PHOTODISSOCIATION OF TOLUENE BY SOFT X-RAYS IN A CIRCUMSTELLAR ENVIRONMENT. <i>Astrophysical Journal</i> , 2016, 821, 4.	4.5	12
30	Doubly and Triply Charged Species Formed from Chlorobenzene Reveal Unusual C-Cl Multiple Bonding. <i>Journal of the American Chemical Society</i> , 2018, 140, 4288-4292.	13.7	12
31	Bond-Strengthening Backdonation in Aminoborylene-Stabilized Aminoborylenes: At the Intersection of Borylenes and Diborenes. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 12893-12897.	13.8	12
32	Functionalization of N <sub>2</sub> via Formal 1,3-Haloboration of a Tungsten(0) f-Dinitrogen Complex. <i>Chemistry - A European Journal</i> , 2020, 26, 16019-16027.	3.3	12
33	Production of Long-Lived Benzene Dications from Electron Impact in the 20-2000 eV Energy Range Combined with the Search for Global Minimum Structures. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9261-9271.	2.5	11
34	Intensiv farbige Bor-dotierte Thiazolthiazole durch reduktive Dimerisierung von Borisothiocyanaten. <i>Angewandte Chemie</i> , 2021, 133, 6519-6524.	2.0	11
35	Cyclo-Dipnictadialanes. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 24318-24325.	13.8	11
36	Accurate Polarization-Resolved Absorption Spectra of Organic Semiconductor Thin Films Using First-Principles Quantum-Chemical Methods: Pentacene as a Case Study. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 3726-3731.	4.6	11

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37	Theoretical and experimental investigation on the stability of C=1â€“6Hâ” and C=1â€“4H+ clusters. Chemical Physics, 2013, 410, 109-117.	1.9	10
38	Prediction of Boronâ€“Boron Tripleâ€Bond Polymers Stabilized by Janusâ€Type Bis(Nâ€heterocyclic) Carbenes. Chemistry - A European Journal, 2015, 21, 7814-7819.	3.3	10
39	Unexpected reversal of stability in strained systems containing one-electron bonds. Physical Chemistry Chemical Physics, 2019, 21, 24984-24992.	2.8	10
40	One- and two-electron reduction of triarylborane-based helical donorâ€acceptor compounds. Chemical Science, 2021, 12, 11864-11872.	7.4	10
41	Diboryne Nanostructures Stabilized by Multitopic N-Heterocyclic Carbenes: A Computational Study. Inorganic Chemistry, 2018, 57, 3931-3940.	4.0	9
42	Reactivity of cyano- and isothiocyanatoborylenes: metal coordination, one-electron oxidation and boron-centred Brâ”sted basicity. Chemical Science, 2021, 12, 7937-7942.	7.4	9
43	Isolation of Neutral, Monoâ€-, and Dicationic B 2 P 2 Rings by Diphosphorus Addition to a Boronâ”Boron Triple Bond. Angewandte Chemie - International Edition, 2021, 60, 13661-13665.	13.8	9
44	Tuneable reduction of cymantrenylboranes to diborenes or borylene-derived boratafulvenes. Chemical Communications, 2020, 56, 14809-14812.	4.1	8
45	Boranediyâ€- and Diborane(4)â€1,2â€diylâ€Bridged Platinum Aâ€Frame Complexes. Chemistry - A European Journal, 2020, 26, 8518-8523.	3.3	8
46	Fragmentation of isocyanic acid, HNCO, following core excitation and ionization. Journal of Chemical Physics, 2021, 154, 114302.	3.0	8
47	Platinumâ€templated Coupling of B=N Units: Synthesis of BNB N Analogues of 1,3â€Dienes and a Butatriene. Angewandte Chemie - International Edition, 2021, 60, 16864-16868.	13.8	8
48	Positive molecular ions and ionâ€neutral complexes in the gas phase: Structure and stability of C<sub>2</sub>H<sub>4</sub>O<sub>2</sub><sup>+Â·</sup> and C<sub>2</sub>H<sub>4</sub>O<sub>2</sub><sup>2+</sup> isomers. International Journal of Quantum Chemistry, 2012, 112, 3303-3311.	2.0	7
49	Gas-phase spectroscopic characterization of neutral and ionic polycyclic aromatic phosphorus heterocycles (PAPHs). Monthly Notices of the Royal Astronomical Society, 2020, 500, 2564-2576.	4.4	7
50	Diboran(4)azide als stabile Quelle fÃ¼r kurzlebige Iminoborane. Angewandte Chemie, 2020, 132, 15608-15614.	2.0	7
51	Unexpected formation of a dodecanuclear {Coll6Cull6} nanowheel under ambient conditions: magneto-structural correlations. Dalton Transactions, 2021, 50, 12430-12434.	3.3	7
52	Structure, Stability, and Spectroscopic Properties of Small Acetonitrile Cation Clusters. Journal of Physical Chemistry A, 2020, 124, 6845-6855.	2.5	6
53	Isolierung und ReaktivitÃt eines sâ€Blockâ€Metallâ€Antiaromaten. Angewandte Chemie, 2021, 133, 3856-3863.	2.0	6
54	Reduktion und Umlagerung eines Bor(I)â€Carbonylkomplexes. Angewandte Chemie, 2021, 133, 3000-3005.	2.0	6

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55	Addukte des Stammboraphosphaketens H <sub>2</sub> BPCO und deren Insertionsreaktionen mittels Decarbonylierung. <i>Angewandte Chemie</i> , 2021, 133, 13780-13784.	2.0	6
56	Taming the Antiferromagnetic Beast: Computational Design of Ultrashort Mn <sup>II</sup> -Mn Bonds Stabilized by N-heterocyclic Carbenes. <i>Chemistry - A European Journal</i> , 2021, 27, 12126-12136.	3.3	6
57	An Unsymmetrical, Cyclic Diborene Based on a Chelating CAAC Ligand and its Small-Molecule Activation and Rearrangement Chemistry. <i>Angewandte Chemie</i> , 0, , .	2.0	6
58	Splitting of multiple hydrogen molecules by bioinspired diniobium metal complexes: a DFT study. <i>Dalton Transactions</i> , 2021, 50, 840-849.	3.3	5
59	Ein neutrales Beryllium(I)-Radikal. <i>Angewandte Chemie</i> , 2021, 133, 20944-20948.	2.0	5
60	Multiply charged naphthalene and its C <sub>10</sub> H <sub>8</sub> isomers: bonding, spectroscopy, and implications in AGN environments. <i>Monthly Notices of the Royal Astronomical Society</i> , 2022, 512, 4669-4682.	4.4	5
61	Probing the Potential of Hitherto Unexplored Base-Stabilized Borylenes in Dinitrogen Binding. <i>Chemistry - A European Journal</i> , 2022, 28, .	3.3	5
62	Modulation of the Naked-Eye and Fluorescence Color of a Protonated Boron-doped Thiazolothiazole by Anion-dependent Hydrogen Bonding. <i>Chemistry - A European Journal</i> , 0, , .	3.3	5
63	Selective mono- and dimetallation of a group 3 sandwich complex. <i>Chemical Communications</i> , 2019, 55, 9677-9680.	4.1	4
64	Bindungsstärkende $\pi$ - $\sigma$ -Bindung in Aminoborylen-stabilisierten Aminoborylenen: an der Grenze zwischen Borylenen und Diborenen. <i>Angewandte Chemie</i> , 2019, 131, 13025-13029.	2.0	4
65	Mechanistic Insights into the Formation of Lithium Fluoride Nanotubes. <i>Chemistry - A European Journal</i> , 2019, 25, 5269-5279.	3.3	4
66	Dissociative single and double photoionization of biphenyl (C <sub>12</sub> H <sub>10</sub> ) by soft X-rays in planetary nebulae. <i>Monthly Notices of the Royal Astronomical Society</i> , 2020, 499, 6066-6083.	4.4	4
67	Probing the Potential of Hitherto Unexplored Base-Stabilized Borylenes in Dinitrogen Binding. <i>Chemistry - A European Journal</i> , 2022, 28, e202200833.	3.3	4
68	Understanding, Modulating, and Leveraging Transannular M $\pi$ -Z Interactions. <i>Inorganic Chemistry</i> , 2021, 60, 12790-12800.	4.0	3
69	Dialkynylboranes(4) and the selectable reactivity of their C-H, C-C and B-B bonds. <i>Chemical Communications</i> , 2021, 57, 2645-2648.	4.1	3
70	Azidoborolate anions and azidoborole adducts: isolable forms of an unstable borole azide. <i>Chemical Communications</i> , 2022, 58, 4735-4738.	4.1	3
71	Can a Wanzlick-like equilibrium exist between dicoordinate borylenes and diborenes?. <i>Chemical Science</i> , 0, , .	7.4	3
72	Electrophilic activation of difunctional aminoboranes: B-N coupling versus intramolecular Cl/Me exchange. <i>Chemical Communications</i> , 2022, 58, 4464-4467.	4.1	3

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73	Oxidation, Coordination, and Nickel-Mediated Deconstruction of a Highly Electron-Rich Diboron Analogue of 1,3,5-Hexatriene. <i>Angewandte Chemie</i> , 2020, 132, 15847-15855.	2.0	2
74	<i>Ab initio</i> study of structural and electronic properties of lithium fluoride nanotubes. <i>Journal of Applied Physics</i> , 2021, 129, .	2.5	2
75	Isolierung neutraler, mono- und dikationischer B <sub>2</sub> P <sub>2</sub> -Ringe durch Addition eines Diphosphans an eine Bor-Bor-Dreifachbindung. <i>Angewandte Chemie</i> , 2021, 133, 13774-13779.	2.0	2
76	Platin-vermittelte Kupplung von B=N-Einheiten: Synthese von BNB-Analoga von 1,3-Dienen und Butatrien. <i>Angewandte Chemie</i> , 2021, 133, 17000-17004.	2.0	2
77	Diphosphino-Functionalized 1,8-Naphthyridines: a Multifaceted Ligand Platform for Boranes and Diboranes. <i>Chemistry - A European Journal</i> , 2021, 27, 15751-15756.	3.3	2
78	Controlled Synthesis of Oligomers Containing Main-Chain B(sp <sup>2</sup> )-B(sp <sup>2</sup> ) Bonds. <i>Chemistry - A European Journal</i> , 2021, 27, 16043-16048.	3.3	2
79	1,2-Dialkynyldiboranes(4): B-B versus C-C bond reactivity. <i>Dalton Transactions</i> , 2022, 51, 6197-6203.	3.3	2
80	Mercury(II) Chloride. <i>Synlett</i> , 2014, 25, 1043-1044.	1.8	1
81	Diverse ring-opening reactions of rhodium $\lambda^4$ -azaborete complexes. <i>Chemical Science</i> , 2020, 11, 9134-9140.	7.4	1
82	Cyclo-Dipnictadialanes. <i>Angewandte Chemie</i> , 2021, 133, 24520.	2.0	1
83	Are disulfide bonds resilient to double ionization? Insights from coincidence spectroscopy and <i>ab initio</i> calculations. <i>RSC Advances</i> , 2020, 10, 35039-35048.	3.6	0
84	Twisting versus Delocalization in CAAC- and NHC-Stabilized Boron-Based Biradicals: The Roles of Sterics and Electronics. <i>Chemistry - A European Journal</i> , 2021, 27, 5056-5056.	3.3	0
85	Frontispiece: The Dimethylbismuth Cation: Entry Into Dative Bi-Bi Bonding and Unconventional Methyl Exchange. <i>Angewandte Chemie - International Edition</i> , 2021, 60, .	13.8	0