

Electron Flow in Reaction Mechanisms“Revealed from

Angewandte Chemie - International Edition

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Citation Report

#	ARTICLE	IF	CITATIONS
1	Mechanistic Insight into the Facilitation of $\beta$ -Lactam Fragmentation through Metal Assistance. Chemistry - A European Journal, 2015, 21, 16781-16785.	1.7	25
2	Exploring electron pair behaviour in chemical bonds using the extracule density. Physical Chemistry Chemical Physics, 2015, 17, 20194-20204.	1.3	9
3	The Stabilizing Effects in Gold Carbene Complexes. Angewandte Chemie - International Edition, 2015, 54, 10336-10340.	7.2	103
4	Theoretical Insight into the Hydrogen Evolution Activity of Open-Ended Carbon Nanotubes. Journal of Physical Chemistry Letters, 2015, 6, 3956-3960.	2.1	31
5	Dinuclear planar chiral ferrocenyl gold( <i>i</i> ) & gold( <i>ii</i> ) complexes. Chemical Communications, 2015, 51, 16806-16809.	2.2	16
7	Gold(I) Vinylidene Complexes as Reactive Intermediates and Their Tendency to $\pi$ -Backbond. Chemistry - A European Journal, 2016, 22, 2892-2895.	1.7	65
8	Structural diversity, spectral characterization and computational studies of Cu(I) complexes with pyridylamide ligands. Inorganica Chimica Acta, 2016, 446, 150-160.	1.2	5
9	Curly arrows meet electron density transfers in chemical reaction mechanisms: from electron localization function (ELF) analysis to valence-shell electron-pair repulsion (VSEPR) inspired interpretation. Chemical Communications, 2016, 52, 8183-8195.	2.2	66
10	Elucidating Hyperconjugation from Electronegativity to Predict Drug Conformational Energy in a High Throughput Manner. Journal of Chemical Information and Modeling, 2016, 56, 788-801.	2.5	9
11	Photochemical Reductive C-C Coupling with a Guanidine Electron Donor. European Journal of Organic Chemistry, 2016, 2016, 5045-5054.	1.2	12
12	Why metal-oxos react with dihydroanthracene and cyclohexadiene at comparable rates, despite having different C-H bond strengths. A computational study. Chemical Communications, 2016, 52, 10509-10512.	2.2	28
13	NHC-CAAC Heterodimers with Three Stable Oxidation States. Angewandte Chemie - International Edition, 2016, 55, 12886-12890.	7.2	68
14	NHC-CAAC Heterodimers with Three Stable Oxidation States. Angewandte Chemie, 2016, 128, 13078-13082.	1.6	23
15	Synthesis and Characterization of Copper Complexes with Cu <sup>I</sup> Cu <sup>I</sup> , Cu <sup>1.5</sup> Cu <sup>1.5</sup> m and Cu <sup>II</sup> Cu <sup>II</sup> Core Structures Supported by a Flexible Dipyridylamide Ligand. Inorganic Chemistry, 2016, 55, 11462-11472.	1.9	15
16	Molybdenum dinitrogen complexes facially coordinated by linear tridentate PEP ligands (E = N or P): impact of the central E donor in trans-position to N <sub>2</sub> . Dalton Transactions, 2016, 45, 14801-14813.	1.6	21
17	Computergestützte Syntheseplanung: Das Ende vom Anfang. Angewandte Chemie, 2016, 128, 6004-6040.	1.6	35
18	Computer-Assisted Synthetic Planning: The End of the Beginning. Angewandte Chemie - International Edition, 2016, 55, 5904-5937.	7.2	395
19	Correlation effects in strong-field ionization of heteronuclear diatomic molecules. Physical Review A, 2016, 93, .	1.0	15

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21	Ein Aluminiumâ€“Fluoridâ€“Komplex mit gekoppelter Ammoniumâ€“Einheit als auÃƒergewÃƒhnlich aktiver kooperativer Katalysator in der asymmetrischen Carboxycyanierung von Aldehyden. <i>Angewandte Chemie</i> , 2017, 129, 4115-4119.	1.6	12
22	An Aluminum Fluoride Complex with an Appended Ammonium Salt as an Exceptionally Active Cooperative Catalyst for the Asymmetric Carboxycyanation of Aldehydes. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 4056-4060.	7.2	32
23	Fluoride-Mediated Desulfonylative Intramolecular Cyclization to Fused and Bridged Bicyclic Compounds: A Complex Mechanism. <i>Journal of Organic Chemistry</i> , 2017, 82, 2579-2588.	1.7	3
24	Anomalous effect of non-alternant hydrocarbons on carbocation and carbanion electronic configurations. <i>Chemical Science</i> , 2017, 8, 4231-4241.	3.7	10
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26	On the outside looking in: rethinking the molecular mechanism of 1,3-dipolar cycloadditions from the perspective of bonding evolution theory. The reaction between cyclic nitrones and ethyl acrylate. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 18288-18302.	1.3	31
27	Effect of Substituents on the Bond Strength of Air-Stable Dicyanomethyl Radical Thermochromes. <i>Journal of Organic Chemistry</i> , 2017, 82, 6497-6501.	1.7	42
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29	When Bifunctional Catalyst Encounters Dual MLC Modes: DFT Study on the Mechanistic Preference in Ru-PNNH Pincer Complex Catalyzed Dehydrogenative Coupling Reaction. <i>ACS Catalysis</i> , 2017, 7, 786-795.	5.5	41
30	Theory and Applications of Generalized Pipekâ€“Mezey Wannier Functions. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 460-474.	2.3	32
31	The Two Faces of Tetramethylcyclam in Iron Chemistry: Distinct Feâ€“Oâ€“M Complexes Derived from [Fe <sup>IV</sup> (O <sub>anti</sub> <sup>syn</sup> )(TMC)] <sup>2+</sup> Isomers. <i>Inorganic Chemistry</i> , 2017, 56, 518-527.	1.9	14
32	Curly arrows, electron flow, and reaction mechanisms from the perspective of the bonding evolution theory. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 29031-29046.	1.3	36
33	Detection and Characterization of Hydride Ligands in Iron Complexes by High-Resolution Hard X-ray Spectroscopy and Implications for Catalytic Processes. <i>Inorganic Chemistry</i> , 2017, 56, 13300-13310.	1.9	18
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35	Hydrogenâ€“Atom Transfer Oxidation with H <sub>2</sub> O <sub>2</sub> Catalyzed by		

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38	Mechanistic investigations of the 2-coumaranone chemiluminescence. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 22852-22859.	1.3	17
39	Computing the arrows of chemical reactions. <i>ChemTexts</i> , 2017, 3, 1.	1.0	9
40	Synthetic nitrogen fixation with mononuclear molybdenum complexes: Electronic-structural and mechanistic insights from DFT. <i>Coordination Chemistry Reviews</i> , 2017, 345, 263-280.	9.5	19
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45	A systematic examination of classical and multi-center bonding in heteroborane clusters. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4666-4675.	1.3	26
46	How to tame a palladium terminal imido. <i>Journal of Organometallic Chemistry</i> , 2018, 864, 26-36.	0.8	14
47	ÃœbergangsmetallÃœKomplexierung eines Tetrahalogendiborans. <i>Angewandte Chemie</i> , 2018, 130, 419-423.	1.6	7
48	Efficient Treatment of Local Meta-generalized Gradient Density Functionals via Auxiliary Density Expansion: The Density Fitting J + X Approximation. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1297-1303.	2.3	10
49	Facile reactions of gold( <i>scp</i> ) complexes with tri( <i>tert</i> -butyl)azadiboriridine. <i>Dalton Transactions</i> , 2018, 47, 5181-5188.	1.6	11
50	How to tame a palladium terminal oxo. <i>Chemical Science</i> , 2018, 9, 1155-1167.	3.7	24
51	Transitionâ€”Metal ÃœLigation of a Tetrahalodiborane. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 412-416.	7.2	18
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53	The tardy dance of molecular orbitals. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25718.	1.0	3
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57	The Interhalogen Cations $[\text{Br}_2\text{F}_5]^+$ and $[\text{Br}_3\text{F}_8]^+$ . <i>Angewandte Chemie - International Edition</i> , 2018, 57, 14640-14644.	7.2	15
58	Mechanism of Ti-Catalyzed Oxidative Nitrene Transfer in [2 + 2 + 1] Pyrrole Synthesis from Alkynes and Azobenzene. <i>Journal of the American Chemical Society</i> , 2018, 140, 7267-7281.	6.6	76
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60	Transferability in Machine Learning for Electronic Structure via the Molecular Orbital Basis. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4772-4779.	2.3	149
61	cPCET versus HAT: A Direct Theoretical Method for Distinguishing X-H Bond Activation Mechanisms. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 11913-11917.	7.2	77
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67	From Dialkyltitanium Species to Titanacyclopropanes: An Ab Initio Study. <i>Organometallics</i> , 2019, 38, 4171-4182.	1.1	5
68	Ï Noninnocence: Masked Phenyl Cation Transfer at Formal Ni <sup>IV</sup> . <i>Angewandte Chemie</i> , 2019, 131, 13267-13273.	1.6	8
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72	Stabilization of Classical $[\text{B}_2\text{H}_5]^+$ : Structure and Bonding of $[(\text{Cp}^*\text{Ta})_2(\text{B}_2\text{H}_5)(\text{I}/4\text{H})\text{L}_2]$ ( $\text{Cp}^* = \text{I}^5\text{C}_5\text{Me}_5$ ; $\text{L} = \text{SCH}_2\text{S}$ ). <i>Angewandte Chemie - International Edition</i> , 2019, 58, 17684-17689.	7.2	24
73	Analytical Gradient Theory for Strongly Contracted (SC) and Partially Contracted (PC) N-Electron Valence State Perturbation Theory (NEVPT2). <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5417-5425.	2.3	18

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74	Phosphaaluminirenes: Synthons for Main Group Heterocycles. <i>Journal of the American Chemical Society</i> , 2019, 141, 16971-16982.	6.6	30
75	A DFT study of Co( <i>i</i> ) and Ni( <i>ii</i> ) pincer complex-catalyzed hydrogenation of ketones: intriguing mechanism dichotomy by ligand field variation. <i>Catalysis Science and Technology</i> , 2019, 9, 125-135.	2.1	17
76	Noninnocence: Masked Phenyl Cation Transfer at Formal Ni <sup>IV</sup> . <i>Angewandte Chemie - International Edition</i> , 2019, 58, 13133-13139.	7.2	27
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82	Cationic Gold(I) Diarylallenyldene Complexes: Bonding Features and Ligand Effects. <i>ChemPhysChem</i> , 2019, 20, 1671-1679.	1.0	18
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86	Visualizing Complex-Valued Molecular Orbitals. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3223-3228.	1.1	13
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90	Facile Conversion of syn {Fe IV (O)(TMC)} <sup>2+</sup> into the anti Isomer via Meunier's Oxo-Hydroxo Tautomerism Mechanism. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 1995-1999.	7.2	9
91	Resonance Natural Bond Orbitals: Efficient Semilocalized Orbitals for Computing and Visualizing Reactive Chemical Processes. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 916-921.	2.3	13

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92	Asymmetric Carboxycyanation of Aldehydes by Cooperative AlF/Onium Salt Catalysts: from Cyanoformate to KCN as Cyanide Source. <i>Chemistry - A European Journal</i> , 2019, 25, 1515-1524.	1.7	17
93	Nâ€Heterocyclic Carbene Stabilized Dicarbondiphosphides: Strong Neutral Fourâ€Membered Heterocyclic 6â€Electron Donors. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 4288-4293.	7.2	21
94	Analytical Gradient Theory for Quasidegenerate $\langle i \rangle N \langle /i \rangle$ -Electron Valence State Perturbation Theory (QD-NEVPT2). <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 326-339.	2.3	19
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99	Localized Bond Orbital Analysis of the Bonds of O <sub>2</sub> . <i>Journal of Physical Chemistry A</i> , 2020, 124, 9771-9776.	1.1	3
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101	A Truxenoneâ€Based Covalent Organic Framework as an Allâ€Solidâ€State Lithiumâ€Ion Battery Cathode with High Capacity. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 20385-20389.	7.2	110
102	What Makes a Good (Computed) Energy Profile?. <i>Topics in Organometallic Chemistry</i> , 2020, , 1-38.	0.7	15
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110	A Room-Temperature Stable Distonic Radical Cation. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 23830-23835.	7.2	13
111	Ligand-Mediated Spin-State Changes in a Cobalt-Dipyrroin-Bisphenol Complex. <i>Inorganic Chemistry</i> , 2020, 59, 12903-12912.	1.9	14
112	A Room-Temperature Stable Distonic Radical Cation. <i>Angewandte Chemie</i> , 2020, 132, 24038-24043.	1.6	3
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123	Cs[Cl <sub>3</sub> F <sub>10</sub> ]: Eine Verbindung mit propellerförmigem [Cl <sub>3</sub> F <sub>10</sub> ] <sup>-</sup> Anion, die im außergewöhnlichen A <sup>5+</sup> B <sup>5+</sup> Strukturtyp kristallisiert. <i>Angewandte Chemie</i> , 2020, 132, 18272-18276.	1.6	1
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126	A mechanistic insight into rhodium-doped gold clusters as a better hydrogenation catalyst. <i>Nanoscale</i> , 2020, 12, 5125-5138.	2.8	6
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129	Anomalous Electronic Properties of Iodous Materials: Application to High-Spin Reactive Intermediates and Conjugated Polymers. <i>Journal of Organic Chemistry</i> , 2020, 85, 4145-4152.	1.7	4
130	Fast Evaluation of Two-Center Integrals over Gaussian Charge Distributions and Gaussian Orbitals with General Interaction Kernels. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2570-2583.	2.3	12
131	Superelectrophilic Gallium(III) Homodimers in Gallium Chloride-Mediated Methylation of Benzene: A Theoretical Study. <i>ACS Catalysis</i> , 2020, 10, 3027-3033.	5.5	13
132	Can We Safely Obtain Formal Oxidation States from Centroids of Localized Orbitals?. <i>Molecules</i> , 2020, 25, 234.	1.7	14
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