

Diego M Andrada

List of Publications by Year in descending order

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83
papers

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citations

126907

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161849

54
g-index

89
all docs

89
docs citations

89
times ranked

2430
citing authors

#	ARTICLE	IF	CITATIONS
1	Energy decomposition analysis. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1345.	14.6	369
2	Acyclic Germynes: Congeners of Allenes with a Central Germanium Atom. Journal of the American Chemical Society, 2013, 135, 12422-12428.	13.7	172
3	Donor-acceptor bonding in novel low-coordinated compounds of boron and group-14 atoms C ₄ H ₄ Sn. Chemical Society Reviews, 2016, 45, 1129-1144.	38.1	162
4	Formation and Characterization of the Boron Dicarbonyl Complex [B(CO) ₂] ⁺ . Angewandte Chemie - International Edition, 2015, 54, 11078-11083.	13.8	107
5	The Structure of the Carbene Stabilized Si ₂ H ₂ May Be Equally Well Described with Coordinate Bonds as with Classical Double Bonds. Journal of the American Chemical Society, 2016, 138, 10429-10432.	13.7	105
6	Stabilization of Heterodiatomic SiC Through Ligand Donation: Theoretical Investigation of SiC(L) ₂ (L=NHC ^{Me} , CAAC ^{Me} , PMe ₃). Angewandte Chemie - International Edition, 2015, 54, 12319-12324.	13.8	102
7	(L) ₂ C ₂ P ₂ : Dicarbonyldiphosphide Stabilized by Heterocyclic Carbenes or Cyclic Diamido Carbenes. Angewandte Chemie - International Edition, 2017, 56, 5744-5749.	13.8	102
8	The Bonding Situation in Metalated Ylides. Chemistry - A European Journal, 2017, 23, 4422-4434.	3.3	92
9	Dative and Electron-Sharing Bonding in C ₂ F ₄ . Chemistry - A European Journal, 2018, 24, 9083-9089.	3.3	73
10	Carbon Monoxide Bonding With BeO and BeCO ₃ : Surprisingly High CO Stretching Frequency of OCBeco ₃ . Angewandte Chemie - International Edition, 2015, 54, 124-128.	13.8	70
11	Direct estimate of the internal π -donation to the carbene centre within N-heterocyclic carbenes and related molecules. Beilstein Journal of Organic Chemistry, 2015, 11, 2727-2736.	2.2	64
12	The [B ₃ (NN) ₃] ⁺ and [B ₃ (CO) ₃] ⁺ Complexes Featuring the Smallest π -Aromatic Species B ₃ ⁺ . Angewandte Chemie - International Edition, 2016, 55, 2078-2082.	13.8	64
13	Experimental and Theoretical Studies of the Infrared Spectra and Bonding Properties of NgBeCO ₃ and a Comparison with NgBeO (Ng = He, Ne, Ar, Kr, Xe). Journal of Physical Chemistry A, 2015, 119, 2543-2552.	2.5	62
14	Energy components in energy decomposition analysis (EDA) are path functions; why does it matter?. Physical Chemistry Chemical Physics, 2020, 22, 22459-22464.	2.8	60
15	A Catalyst with Two-coordinate Nickel: Theoretical and Catalytic Studies. European Journal of Inorganic Chemistry, 2014, 2014, 818-823.	2.0	57
16	Isolation of Bridging and Terminal Coinage Metal-Nitrene Complexes. Journal of the American Chemical Society, 2014, 136, 3800-3802.	13.7	57
17	Carbodicarbenes: Unexpected π -Accepting Ability during Reactivity with Small Molecules. Journal of the American Chemical Society, 2017, 139, 12830-12836.	13.7	57
18	A Stable Neutral Radical in the Coordination Sphere of Aluminum. Angewandte Chemie - International Edition, 2017, 56, 397-400.	13.8	56

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19	Facile access to silyl-functionalized N-heterocyclic olefins with HSiCl ₃ . <i>Chemical Communications</i> , 2013, 49, 9440.	4.1	55
20	(L) ₂ C ₂ P ₂ : Dicarbonyldiphosphide Stabilized by N-Heterocyclic Carbenes or Cyclic Diamido Carbenes. <i>Angewandte Chemie</i> , 2017, 129, 5838-5843.	2.0	55
21	A Triatomic Silicon(0) Cluster Stabilized by a Cyclic Alkyl(amino) Carbene. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 3158-3161.	13.8	54
22	An Electrophilic Carbene-Anchored Silylene-Phosphinidene. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 4219-4223.	13.8	54
23	Carbene-Dichlorosilylene Stabilized Phosphinidenes Exhibiting Strong Intramolecular Charge Transfer Transition. <i>Journal of the American Chemical Society</i> , 2015, 137, 150-153.	13.7	50
24	Comparison of Hydrogen and Gold Bonding in [XHX] ⁺ , [XAuX] ⁺ , and Isoelectronic [NgHNg] ⁺ , [NgAuNg] ⁺ (X=Halogen, Ng=Noble Gas). <i>Chemistry - A European Journal</i> , 2016, 22, 11317-11328.	3.3	50
25	Theoretical study of the molecular aspect of the suspected novichok agent A234 of the Skripal poisoning. <i>Royal Society Open Science</i> , 2019, 6, 181831.	2.4	45
26	Stabilisierung von heterodiatomarem SiC durch Donorliganden – theoretische Untersuchung von SiC(L) ₂ (L=NHCMe, CAACMe, PMe ₃). <i>Angewandte Chemie</i> , 2015, 127, 12494-12500.	2.0	44
27	A Modular Access to Divinyldiphosphenes with a Strikingly Small HOMO-LUMO Energy Gap. <i>Chemistry - A European Journal</i> , 2019, 25, 8127-8134.	3.3	40
28	DFT Study of Thermal 1,3-Dipolar Cycloaddition Reactions between Alkynyl Metal(0) Fischer Carbene Complexes and 3-H-1,2-Dithiole-3-thione Derivatives. <i>Organometallics</i> , 2011, 30, 466-476.	2.3	38
29	Steric versus Electronic Effects in the Structure of Heteroatom (S and O)-Substituted Free and Metal (Cr and W)-Complexed Carbenes. <i>Organometallics</i> , 2007, 26, 5854-5858.	2.3	36
30	Cyclic trinuclear copper, silver, and gold complexes: a theoretical insight. <i>Dalton Transactions</i> , 2015, 44, 377-385.	3.3	36
31	An open route to asymmetric substituted Al-Al bonds using Al- and Al-precursors. <i>Chemical Communications</i> , 2017, 53, 2543-2546.	4.1	35
32	Bonding situation in silicon complexes [(L) ₂ (Si ₂)] and [(L) ₂ (Si)] with NHC and cAAC ligands. <i>Journal of Organometallic Chemistry</i> , 2015, 792, 139-148.	1.8	33
33	Synthesis, Characterization, and Theoretical Investigation of Two-Coordinate Palladium(0) and Platinum(0) Complexes Utilizing σ -Accepting Carbenes. <i>Chemistry - A European Journal</i> , 2015, 21, 9312-9318.	3.3	33
34	Normal-to-abnormal rearrangement of an N-heterocyclic carbene with a silylene transition metal complex. <i>Dalton Transactions</i> , 2017, 46, 7791-7799.	3.3	32
35	Dative versus electron-sharing bonding in N-oxides and phosphane oxides R ₃ EO and relative energies of the R ₂ EOR isomers (E = N, P; R = H, F, Cl, Me, Ph). A theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 11856-11866.	2.8	32
36	A theoretical study of the hydrolysis mechanism of A-234; the suspected novichok agent in the Skripal attack. <i>RSC Advances</i> , 2020, 10, 27884-27893.	3.6	31

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37	Mono- and di-cationic hydrido boron compounds. Dalton Transactions, 2015, 44, 14359-14367.	3.3	29
38	Preorganized Anion Traps for Exploiting Anion-π Interactions: An Experimental and Computational Study. Chemistry - A European Journal, 2013, 19, 16988-17000.	3.3	27
39	Proton Affinities of Cationic Carbene Adducts [AC(PPh) ₃] ₂ ⁺ (A=Halogen, Hydrogen, Methyl) and Unusual Electronic Structures of the Cations and Dications [AC(H)(PPh) ₃] ₂ ²⁺ . Chemistry - A European Journal, 2016, 22, 8536-8546.	3.3	27
40	Path-dependency of energy decomposition analysis & the elusive nature of bonding. Physical Chemistry Chemical Physics, 2022, 24, 2344-2348.	2.8	27
41	Benchmarking lithium amide versus amine bonding by charge density and energy decomposition analysis arguments. Chemical Science, 2018, 9, 3111-3121.	7.4	26
42	Organosilicon Radicals with Si-H and Si-Me Bonds from Commodity Precursors. Journal of the American Chemical Society, 2017, 139, 11028-11031.	13.7	25
43	The oxidation state in low-valent beryllium and magnesium compounds. Chemical Science, 2022, 13, 6583-6591.	7.4	25
44	Effects of Metal Coordination on the π-System of the 2,5-Bis-((pyrrolidino)-methyl)-pyrrole Pincer Ligand. Inorganic Chemistry, 2013, 52, 9539-9548.	4.0	23
45	Observation of Main-Group Tricarbonyls [B(CO) ₃] and [C(CO) ₃] ⁺ Featuring a Tilted One-Electron Donor Carbonyl Ligand. Chemistry - A European Journal, 2016, 22, 2376-2385.	3.3	23
46	Carbene stabilized interconnected bis-germylene and its silicon analogue with small methyl substituents. Dalton Transactions, 2017, 46, 7947-7952.	3.3	23
47	Synthesis, Structure, and Bonding Analysis of Tin(II) Dihalide and Cyclopentadienyltin(II) Halide (Alkyl)(amino)carbene Complexes. Organometallics, 2019, 38, 1052-1061.	2.3	23
48	Beyond the Classical Electron Sharing and Dative Bond Picture: Case of the Spin-Polarized Bond. Angewandte Chemie - International Edition, 2021, 60, 1498-1502.	13.8	23
49	A C ₂ Fragment as Four-Electron π Donor. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2017, 643, 1096-1099.	1.2	20
50	A bis(aluminocenophane) with a short aluminum-aluminum single bond. Dalton Transactions, 2019, 48, 14953-14957.	3.3	20
51	Isolation of a 16-Electron 1,4-Diphosphine-1,4-diide with a Planar C ₄ P ₂ Ring. Chemistry - A European Journal, 2021, 27, 3055-3064.	3.3	20
52	Mechanism of the Aminolysis of Fischer Alkoxy and Thiocarbene Complexes: A DFT Study. Journal of Organic Chemistry, 2010, 75, 5821-5836.	3.2	19
53	Bonding analysis of ylidone complexes EL ₂ (E = Ca-Pb) with phosphine and carbene ligands. Canadian Journal of Chemistry, 2016, 94, 1006-1014.	1.1	19
54	Ruthenophanes: Evaluating Cation-π Interactions in [Ru(η ⁶ -C ₁₆ H ₁₂ R ₄)(NH ₃) ₃] ^{2+/3+} Complexes. A Computational Insight. Organometallics, 2014, 33, 2301-2312.	2.3	17

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55	Silavinylidene Stabilized by an N-Heterocyclic Carbene: A Theoretically Predicted Stable Molecule. Chemistry - A European Journal, 2014, 20, 9216-9220.	3.3	17
56	Photoremoval of Protecting Groups: Mechanistic Aspects of 1,3-Dithiane Conversion to a Carbonyl Group. Journal of Organic Chemistry, 2015, 80, 2733-2739.	3.2	17
57	Heterocumulene Sulfinyl Radical OCNSO. Angewandte Chemie - International Edition, 2017, 56, 2140-2144.	13.8	17
58	Isolation of 1,4-Diarsinine Cl_2 Diide and 1,4-Diarsinine Derivatives. Angewandte Chemie - International Edition, 2021, 60, 15849-15853.	13.8	17
59	Electrophilic terminal arsinidene-iron(0) complexes with a two-coordinated arsenic atom. Chemical Communications, 2019, 55, 14669-14672.	4.1	15
60	ExcelAutomat: a tool for systematic processing of files as applied to quantum chemical calculations. Journal of Computer-Aided Molecular Design, 2017, 31, 667-673.	2.9	14
61	Dative versus electron-sharing bonding in <i>N</i> -imides and phosphane imides R_3ENX and relative energies of the $R_2EN(X)R$ isomers (E = N, P; R = H, Cl, Me, Ph; X = H, F, Cl). Molecular Physics, 2019, 117, 1306-1314.	1.7	14
62	Bonding Situation in Stannocene and Plumbocene N-Heterocyclic Carbene Complexes. Organometallics, 2020, 39, 516-527.	2.3	14
63	A Cyclic Iminoborane-NHC Adduct: Synthesis, Reactivity, and Bonding Analysis. Inorganic Chemistry, 2021, 60, 14202-14211.	4.0	13
64	Strong Intermolecular Interactions Shaping a Small Piano-Stool Complex. Angewandte Chemie - International Edition, 2013, 52, 10365-10369.	13.8	12
65	Understanding the Heteroatom Effect on the Ullmann Copper-Catalyzed Cross-Coupling of X-Arylation (X = NH, O, S) Mechanism. Catalysts, 2017, 7, 388.	3.5	12
66	Metalloradical Cations and Dications Based on Divinyldiphosphene and Divinyldiarsene Ligands. Chemistry - A European Journal, 2021, 27, 5803-5809.	3.3	12
67	Chemical Bonding in Silicon Carbonyl Complexes. Chemistry - A European Journal, 2021, 27, 10601-10609.	3.3	12
68	Metathesis Reactions of a NHC-Stabilized Phosphaborene. Angewandte Chemie - International Edition, 2022, 61, .	13.8	11
69	Ruthenium(II) complexes of N-heterocyclic carbenes derived from imidazolium-linked cyclophanes. Dalton Transactions, 2014, 43, 14710-14719.	3.3	10
70	Aminosilanetrithiol $RSi(SH)_3$: an experimental and quantum-chemical study. Chemical Communications, 2014, 50, 4628-4630.	4.1	9
71	Unveiling the Electronic Structure of the Bi(+1)/Bi(+3) Redox Couple on NCN and NNN Pincer Complexes. Inorganic Chemistry, 2021, 60, 17657-17668.	4.0	9
72	Isolation of Elusive Electrophilic Phosphinidene Complexes with σ -Donor N-Heterocyclic Vinyl Substituents. Journal of Organic Chemistry, 2020, 85, 14351-14359.	3.2	6

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73	Über die klassische Elektronenpaar- und die dative Bindung hinaus: Die Spin-polarisierte Bindung. <i>Angewandte Chemie</i> , 2021, 133, 1520-1524.	2.0	6
74	Dicarbonyls of Carbon and Methylidyne Cations. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2903-2910.	2.5	5
75	Isolierung von 1,4-Diarsinin- und 1,4-Diarsinin-Derivaten. <i>Angewandte Chemie</i> , 2021, 133, 1598–15987.5		
76	Role of the hydrophobicity on the thermodynamic and kinetic acidity of Fischer thiocarbene complexes. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6616.	2.8	4
77	Diarylpnictogenyldialkylalanesâ€”Synthesis, Structures, Bonding Analysis, and CO ₂ Capture. <i>Inorganic Chemistry</i> , 2022, 61, 1672-1684.	4.0	4
78	Decoding the reaction mechanism of the cyclocondensation of ethyl acetate ₂ (⁴) Tj ETQq0 0 0 rgBT /Overl evolution theory. <i>Journal of Computational Chemistry</i> , 2022, , .	3.3	4
79	Nucleophilic substitution in ionizable Fischer thiocarbene complexes: steric effect of the alkyl substituent on the heteroatom. <i>Dalton Transactions</i> , 2015, 44, 5520-5534.	3.3	3
80	BiCl ₃ -Facilitated removal of methoxymethyl-ether/ester derivatives and DFT study of â€”Oâ€”Câ€”Oâ€” bond cleavage. <i>New Journal of Chemistry</i> , 2021, 45, 7109-7116.	2.8	3
81	Surprisingly stable Siâ€”CO species. <i>Nature Chemistry</i> , 2020, 12, 1089-1091.	13.6	2
82	Metathesis Reactions of a NHC-Stabilized Phosphaborene. <i>Angewandte Chemie</i> , 0, , .	2.0	2
83	Cage-size effects on the encapsulation of ² P ₂ by fullerenes. <i>Journal of Computational Chemistry</i> , 2022, , .	3.3	1