Diego M Andrada

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/8385557/publications.pdf

Version: 2024-02-01

83 papers	3,324 citations	126907 33 h-index	161849 54 g-index
89 all docs	89 docs citations	89 times ranked	2430 citing authors

#	Article	IF	Citations
1	Diarylpnictogenyldialkylalanesâ”€Synthesis, Structures, Bonding Analysis, and CO₂ Capture. Inorganic Chemistry, 2022, 61, 1672-1684.	4.0	4
2	Path-dependency of energy decomposition analysis & the elusive nature of bonding. Physical Chemistry Chemical Physics, 2022, 24, 2344-2348.	2.8	27
3	Decoding the reaction mechanism of the cyclocondensation of ethyl acetate2â€oxoâ€2â€(<scp> 4â€oxoâ€4) Tj ETQq1 1 0.784314 rgB evolution theory. Journal of Computational Chemistry, 2022, , .	3.3	4
4	The oxidation state in low-valent beryllium and magnesium compounds. Chemical Science, 2022, 13, 6583-6591.	7.4	25
5	Cageâ€size effects on the encapsulation of <scp> P ₂ </scp> by fullerenes. Journal of Computational Chemistry, 2022, , .	3.3	1
6	Metathesis Reactions of a NHCâ€Stabilized Phosphaborene. Angewandte Chemie - International Edition, 2022, 61, .	13.8	11
7	Isolation of a 16Ïâ€Electrons 1,4â€Diphosphinineâ€1,4â€diide with a Planar C₄P₂ Ring. Chemistry - A European Journal, 2021, 27, 3055-3064.	3.3	20
8	Ãœber die klassische Elektronenpaarâ€•und die dative Bindung hinaus: Die Spinâ€polarisierte Bindung. Angewandte Chemie, 2021, 133, 1520-1524.	2.0	6
9	Beyond the Classical Electronâ€Sharing and Dative Bond Picture: Case of the Spinâ€Polarized Bond. Angewandte Chemie - International Edition, 2021, 60, 1498-1502.	13.8	23
10	BiCl₃-Facilitated removal of methoxymethyl-ether/ester derivatives and DFT study of â€“Oâ€“Câ€“Oâ€“ bond cleavage. New Journal of Chemistry, 2021, 45, 7109-7116.	2.8	3
11	Metalloradical Cations and Dications Based on Divinyldiphosphene and Divinyldiarsene Ligands. Chemistry - A European Journal, 2021, 27, 5803-5809.	3.3	12
12	Chemical Bonding in Silicon Carbonyl Complexes. Chemistry - A European Journal, 2021, 27, 10601-10609.	3.3	12
13	Isolierung von 1,4â€Diarsininâ€1,4â€diidâ€•und 1,4â€Diarsininâ€Derivaten. Angewandte Chemie, 2021, 133, 15982-15987.	2.0	5
14	Isolation of 1,4â€Diarsinineâ€1,4â€diide and 1,4â€Diarsinine Derivatives. Angewandte Chemie - International Edition, 2021, 60, 15849-15853.	13.8	17
15	A Cyclic Iminoborane-NHC Adduct: Synthesis, Reactivity, and Bonding Analysis. Inorganic Chemistry, 2021, 60, 14202-14211.	4.0	13
16	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
17	Surprisingly stable Siâ€“CO species. Nature Chemistry, 2020, 12, 1089-1091.	13.6	2
18	A theoretical study of the hydrolysis mechanism of A-234; the suspected novichok agent in the Skripal attack. RSC Advances, 2020, 10, 27884-27893.	3.6	31

#	Article	IF	Citations
19	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
20	Isolation of Elusive Electrophilic Phosphinidene Complexes with Ï€-Donor N-Heterocyclic Vinyl Substituents. Journal of Organic Chemistry, 2020, 85, 14351-14359.	3.2	6
21	Bonding Situation in Stannocene and Plumbocene N-Heterocyclic Carbene Complexes. Organometallics, 2020, 39, 516-527.	2.3	14
22	A Modular Access to Divinyldiphosphenes with a Strikingly Small HOMOâ€“LUMO Energy Gap. Chemistry - A European Journal, 2019, 25, 8127-8134.	3.3	40
23	Theoretical study of the molecular aspect of the suspected novichok agent A234 of the Skripal poisoning. Royal Society Open Science, 2019, 6, 181831.	2.4	45
24	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
25	Electrophilic terminal arsinidene-iron(0) complexes with a two-coordinated arsenic atom. Chemical Communications, 2019, 55, 14669-14672.	4.1	15
26	A bis(aluminocenophane) with a short aluminumâ€“aluminum single bond. Dalton Transactions, 2019, 48, 14953-14957.	3.3	20
27	Dative versus electron-sharing bonding in N-imides and phosphane imides R₃ENX and relative energies of the R₂EN(X)R isomers (E = N, P; R = H, Cl, Me, Ph; X = H, F, Cl). Molecular Physics, 2019, 117, 1306-1314.	1.7	14
28	Benchmarking lithium amideversusamine bonding by charge density and energy decomposition analysis arguments. Chemical Science, 2018, 9, 3111-3121.	7.4	26
29	Dative and Electronâ€Sharing Bonding in C₂F₄. Chemistry - A European Journal, 2018, 24, 9083-9089.	3.3	73
30	Dativeversuselectron-sharing bonding in N-oxides and phosphane oxides R₃EO and relative energies of the R₂EOR isomers (E = N, P; R = H, F, Cl, Me, Ph). A theoretical study. Physical Chemistry Chemical Physics, 2018, 20, 11856-11866.	2.8	32
31	Energy decomposition analysis. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1345.	14.6	369
32	Heterocumulene Sulfinyl Radical OCNSO. Angewandte Chemie - International Edition, 2017, 56, 2140-2144.	13.8	17
33	The Bonding Situation in Metalated Ylides. Chemistry - A European Journal, 2017, 23, 4422-4434.	3.3	92
34	An open route to asymmetric substituted Alâ€“Al bonds using Al(<scp>i</scp>)- and Al(<scp>iii</scp>)-precursors. Chemical Communications, 2017, 53, 2543-2546.	4.1	35
35	(L)₂C₂P₂: Dicarbondiphosphide Stabilized by Nâ€Heterocyclic Carbenes or Cyclic Diamido Carbenes. Angewandte Chemie - International Edition, 2017, 56, 5744-5749.	13.8	102
36	(L)₂C₂P₂: Dicarbondiphosphide Stabilized by Nâ€Heterocyclic Carbenes or Cyclic Diamido Carbenes. Angewandte Chemie, 2017, 129, 5838-5843.	2.0	55

#	Article	IF	Citations
37	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
38	Normal-to-abnormal rearrangement of an N-heterocyclic carbene with a silylene transition metal complex. Dalton Transactions, 2017, 46, 7791-7799.	3.3	32
39	Carbene stabilized interconnected bis-germylene and its silicon analogue with small methyl substituents. Dalton Transactions, 2017, 46, 7947-7952.	3.3	23
40	Dicarbonyls of Carbon and Methylidyne Cations. Journal of Physical Chemistry A, 2017, 121, 2903-2910.	2.5	5
41	An Electrophilic Carbeneâ€Anchored Silyleneâ€“Phosphinidene. Angewandte Chemie - International Edition, 2017, 56, 4219-4223.	13.8	54
42	A Stable Neutral Radical in the Coordination Sphere of Aluminum. Angewandte Chemie - International Edition, 2017, 56, 397-400.	13.8	56
43	Organosilicon Radicals with Siâ€“H and Siâ€“Me Bonds from Commodity Precursors. Journal of the American Chemical Society, 2017, 139, 11028-11031.	13.7	25
44	Carbodicarbenes: Unexpected Ï€-Accepting Ability during Reactivity with Small Molecules. Journal of the American Chemical Society, 2017, 139, 12830-12836.	13.7	57
45	A C₂ Fragment as Fourâ€Electron Ïƒ Donor. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2017, 643, 1096-1099.	1.2	20
46	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
47	Proton Affinities of Cationic Carbone Adducts [AC(PPh₃)₂]⁺ (A=Halogen, Hydrogen, Methyl) and Unusual Electronic Structures of the Cations and Dications [AC(H)(PPh₃)₂]²⁺. Chemistry - A European Journal, 2016, 22, 8536-8546.	3.3	27
48	The [B₃(NN)₃]⁺ and [B₃(CO)₃]⁺ Complexes Featuring the Smallest Ï€â€Aromatic Species B₃⁺. Angewandte Chemie - International Edition, 2016, 55, 2078-2082.	13.8	64
49	The Structure of the Carbene Stabilized Si₂H₂ 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
50	Comparison of Hydrogen and Gold Bonding in [XHX]^{â^'}, [XAuX]^{â^'}, and Isoelectronic [NgHNg]⁺, [NgAuNg]⁺ (X=Halogen, Ng=Noble Gas). Chemistry - A European Journal, 2016, 22, 11317-11328.	3.3	50
51	Bonding analysis of ylidone complexes EL₂ (E = Câ€“Pb) with phosphine and carbene ligands L. Canadian Journal of Chemistry, 2016, 94, 1006-1014.	1.1	19
52	Observation of Mainâ€Group Tricarbonyls [B(CO)₃] and [C(CO)₃]⁺ Featuring a Tilted Oneâ€Electron Donor Carbonyl Ligand. Chemistry - A European Journal, 2016, 22, 2376-2385.	3.3	23
53	A Triatomic Silicon(0) Cluster Stabilized by a Cyclic Alkyl(amino) Carbene. Angewandte Chemie - International Edition, 2016, 55, 3158-3161.	13.8	54
54	Donorâ€“acceptor bonding in novel low-coordinated compounds of boron and group-14 atoms Câ€“Sn. Chemical Society Reviews, 2016, 45, 1129-1144.	38.1	162

#	Article	IF	Citations
55	Stabilization of Heterodiatomic SiC Through Ligand Donation: Theoretical Investigation of SiC(L)₂ (L=NHC^{Me}, CAAC^{Me}, PMe₃). Angewandte Chemie - International Edition, 2015, 54, 12319-12324.	13.8	102
56	Stabilisierung von heterodiatomarem SiC durch Donorliganden â€“ theoretische Untersuchung von SiC(L)₂ (L=NHC^{Me}, CAAC^{Me}, PMe₃). Angewandte Chemie, 2015, 127, 12494-12500.	2.0	44
57	Formation and Characterization of the Boron Dicarbonyl Complex [B(CO)₂]^{â^'}. Angewandte Chemie - International Edition, 2015, 54, 11078-11083.	13.8	107
58	Direct estimate of the internal Ï€-donation to the carbene centre within N-heterocyclic carbenes and related molecules. Beilstein Journal of Organic Chemistry, 2015, 11, 2727-2736.	2.2	64
59	Carbene-Dichlorosilylene Stabilized Phosphinidenes Exhibiting Strong Intramolecular Charge Transfer Transition. Journal of the American Chemical Society, 2015, 137, 150-153.	13.7	50
60	Carbon Monoxide Bonding With BeO and BeCO₃: Surprisingly High CO Stretching Frequency of OCBeCO₃. Angewandte Chemie - International Edition, 2015, 54, 124-128.	13.8	70
61	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
62	Mono- and di-cationic hydrido boron compounds. Dalton Transactions, 2015, 44, 14359-14367.	3.3	29
63	Nucleophilic substitution in ionizable Fischer thiocarbene complexes: steric effect of the alkyl substituent on the heteroatom. Dalton Transactions, 2015, 44, 5520-5534.	3.3	3
64	Bonding situation in silicon complexes [(L) 2 (Si 2)] and [(L) 2 (Si)] with NHC and cAAC ligands. Journal of Organometallic Chemistry, 2015, 792, 139-148.	1.8	33
65	Synthesis, Characterization, and Theoretical Investigation of Twoâ€Coordinate Palladium(0) and Platinum(0) Complexes Utilizing Ï€â€Accepting Carbenes. Chemistry - A European Journal, 2015, 21, 9312-9318.	3.3	33
66	Cyclic trinuclear copper(<scp>i</scp>), silver(<scp>i</scp>), and gold(<scp>i</scp>) complexes: a theoretical insight. Dalton Transactions, 2015, 44, 377-385.	3.3	36
67	Experimental and Theoretical Studies of the Infrared Spectra and Bonding Properties of NgBeCO₃ and a Comparison with NgBeO (Ng = He, Ne, Ar, Kr, Xe). Journal of Physical Chemistry A, 2015, 119, 2543-2552.	2.5	62
68	A Catalyst with Twoâ€Coordinate Nickel: Theoretical and Catalytic Studies. European Journal of Inorganic Chemistry, 2014, 2014, 818-823.	2.0	57
69	Aminosilanetrithiol RSi(SH)₃: an experimental and quantum-chemical study. Chemical Communications, 2014, 50, 4628-4630.	4.1	9
70	Ruthenium(<scp>ii</scp>) complexes of N-heterocyclic carbenes derived from imidazolium-linked cyclophanes. Dalton Transactions, 2014, 43, 14710-14719.	3.3	10
71	Ruthenophanes: Evaluating Cationâ^Ï€ Interactions in [Ru(Î·6-C16H12R4)(NH3)3]2+/3+Complexes. A Computational Insight. Organometallics, 2014, 33, 2301-2312.	2.3	17
72	Isolation of Bridging and Terminal Coinage Metalâ€“Nitrene Complexes. Journal of the American Chemical Society, 2014, 136, 3800-3802.	13.7	57

#	Article	IF	Citations
73	Silavinylidene Stabilized by an Nâ€Heterocyclic Carbene: A Theoretically Predicted Stable Molecule. Chemistry - A European Journal, 2014, 20, 9216-9220.	3.3	17
74	Effects of Metal Coordination on the Ï€-System of the 2,5-Bis-{(pyrrolidino)-methyl}-pyrrole Pincer Ligand. Inorganic Chemistry, 2013, 52, 9539-9548.	4.0	23
75	Strong Intermolecular Interactions Shaping a Small Pianoâ€Stool Complex. Angewandte Chemie - International Edition, 2013, 52, 10365-10369.	13.8	12
76	Acyclic Germylones: Congeners of Allenes with a Central Germanium Atom. Journal of the American Chemical Society, 2013, 135, 12422-12428.	13.7	172
77	Facile access to silyl-functionalized N-heterocyclic olefins with HSiCl3. Chemical Communications, 2013, 49, 9440.	4.1	55
78	Preorganized Anion Traps for Exploiting Anionâ€“Ï€ Interactions: An Experimental and Computational Study. Chemistry - A European Journal, 2013, 19, 16988-17000.	3.3	27
79	DFT Study of Thermal 1,3-Dipolar Cycloaddition Reactions between Alkynyl Metal(0) Fischer Carbene Complexes and 3H-1,2-Dithiole-3-thione Derivatives. Organometallics, 2011, 30, 466-476.	2.3	38
80	Role of the hydrophobicity on the thermodynamic and kinetic acidity of Fischer thiocarbene complexes. Physical Chemistry Chemical Physics, 2010, 12, 6616.	2.8	4
81	Mechanism of the Aminolysis of Fischer Alkoxy and Thiocarbene Complexes: A DFT Study. Journal of Organic Chemistry, 2010, 75, 5821-5836.	3.2	19
82	Steric versus Electronic Effects in the Structure of Heteroatom (S and O)-Substituted Free and Metal (Cr and W)-Complexed Carbenes. Organometallics, 2007, 26, 5854-5858.	2.3	36
83	Metathesis Reactions of a NHCâ€Stabilized Phosphaborene. Angewandte Chemie, 0, , .	2.0	2