Julia Contreras-Garcia

List of Publications by Year
in descending order

110 papers	15,485 citations	117625 34 h-index	30087 103 g-index
117 all docs	117 docs citations	117 times ranked	11801 citing authors

#	Article	IF	Citations
1	Dependence of hydrocarbon sigma CC bond strength on bond angles: The concepts of â€œinvertedâ€• â€œdirectâ€•and â€œsuperdirectâ€•bonds. Computational and Theoretical Chemistry, 2022, 1207, 113505.	2.5	3
2	Importance of non-covalent interactions in a nitrile anion metal-complex based on pyridine ligands: A theoretical and experimental approach. Journal of Molecular Structure, 2022, 1261, 132885.	3.6	1
3	<scp>NCIPLOT</scp> and the analysis of noncovalent interactions using the reduced density gradient. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1497.	14.6	56
4	Energetics of Electron Pairs in Electrophilic Aromatic Substitutions. Molecules, 2021, 26, 513.	3.8	4
5	Understanding Topological Insulators in Real Space. Molecules, 2021, 26, 2965.	3.8	1
6	Kickâ€“Fukui: A Fukui Function-Guided Method for Molecular Structure Prediction. Journal of Chemical Information and Modeling, 2021, 61, 3955-3963.	5.4	14
7	NCI: looking at solute/solvent interactions. Electronic Structure, 2021, 3, 034006.	2.8	1
8	Strong correlation between electronic bonding network and critical temperature in hydrogen-based superconductors. Nature Communications, 2021, 12, 5381.	12.8	39
9	Unveiling the role of the lone electron pair in sesquioxides at high pressure: compressibility of Î²-Sb₂O₃. Dalton Transactions, 2021, 50, 5493-5505.	3.3	7
10	The role of Si vacancies in the segregation of O, C, and N at silicon grain boundaries: An ab initio study. Journal of Chemical Physics, 2021, 155, 174704.	3.0	5
11	Cluster Assembled Silicon-Lithium Nanostructures: A Nanowire Confined Inside a Carbon Nanotube. Frontiers in Chemistry, 2021, 9, 767421.	3.6	1
12	The â€œInverted Bondsâ€•Revisited: Analysis of â€œIn Silicoâ€•Models and of [1.1.1]Propellane by Using Orbital Forces. Chemistry - A European Journal, 2020, 26, 6839-6845.	3.3	10
13	How does the acidic milieu interfere in the capability of ruthenium nitrosyl complexes to release nitric oxide?. New Journal of Chemistry, 2020, 44, 773-779.	2.8	6
14	A Bond Charge Model Ansatz for Intrinsic Bond Energies: Application to Câ€“C Bonds. Journal of Physical Chemistry A, 2020, 124, 176-184.	2.5	2
15	Real-Space Approach to the Reaction Force: Understanding the Origin of Synchronicity/Nonsynchronicity in Multibond Chemical Reactions. Journal of Physical Chemistry A, 2020, 124, 1959-1972.	2.5	12
16	Steric clash in real space: biphenyl revisited. Physical Chemistry Chemical Physics, 2020, 22, 21251-21256.	2.8	16
17	NCIPLOT4: Fast, Robust, and Quantitative Analysis of Noncovalent Interactions. Journal of Chemical Theory and Computation, 2020, 16, 4150-4158.	5.3	151
18	Making Base-Assisted Câ€“H Bond Activation by Cp*Co(III) Effective: A Noncovalent Interaction-Inclusive Theoretical Insight and Experimental Validation. Organometallics, 2020, 39, 2609-2629.	2.3	13

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19	Characterization and Decomposition of the Natural van der Waals SnSb₂Te₄ under Compression. Inorganic Chemistry, 2020, 59, 9900-9918.	4.0	31
20	New Way for Probing Bond Strength. Journal of Physical Chemistry A, 2020, 124, 1850-1860.	2.5	121
21	Borates or phosphates? That is the question. Acta Crystallographica Section A: Foundations and Advances, 2020, 76, 197-205.	0.1	2
22	X-Ray Diffraction and Theoretical Calculationâ€“Supported Formation of Polymorphic Cocrystals Discovered Through Thermal Methods: A Case Study. Journal of Pharmaceutical Sciences, 2019, 108, 3340-3347.	3.3	19
23	Nine questions on energy decomposition analysis. Journal of Computational Chemistry, 2019, 40, 2248-2283.	3.3	113
24	High pressure theoretical and experimental analysis of the bandgap of BaMoO4, PbMoO4, and CdMoO4. Applied Physics Letters, 2019, 115, .	3.3	24
25	Labeling IL-18 with alkaloids: toward the use of cytokines as carrier molecules in chemotherapy. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	1
26	Localizing electron density errors in density functional theory. Physical Chemistry Chemical Physics, 2019, 21, 20927-20938.	2.8	9
27	A chemical theory of topological insulators. Chemical Communications, 2019, 55, 12281-12287.	4.1	16
28	NCI-ELMO: A New Method To Quickly and Accurately Detect Noncovalent Interactions in Biosystems. Journal of Chemical Theory and Computation, 2019, 15, 6456-6470.	5.3	21
29	Overcoming Distrust in Solid State Simulations: Adding Error Bars to Computational Data. Journal of Physical Chemistry C, 2019, 123, 4767-4772.	3.1	10
30	A first step towards quantum energy potentials of electron pairs. Physical Chemistry Chemical Physics, 2019, 21, 4215-4223.	2.8	11
31	Valenceâ€Shell Electronâ€Pair Repulsion Theory Revisited: An Explanation for Core Polarization. Chemistry - A European Journal, 2019, 25, 10938-10945.	3.3	7
32	The Pauli principle and the confinement of electron pairs in a double well: Aspects of electronic bonding under pressure. Journal of Chemical Physics, 2019, 150, 204304.	3.0	9
33	A regression approach to accurate interaction energies using topological descriptors. Computational and Theoretical Chemistry, 2019, 1159, 23-26.	2.5	16
34	Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, 10881-10905.	3.3	108
35	New electron delocalization tools to describe the aromaticity in porphyrinoids. Physical Chemistry Chemical Physics, 2018, 20, 2787-2796.	2.8	86
36	The Independent Gradient Model: A New Approach for Probing Strong and Weak Interactions in Molecules from Wave Function Calculations. ChemPhysChem, 2018, 19, 724-735.	2.1	263

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37	Bending Carbon Nanoforms for Supramolecular Recognition: A Topological Study on Hemifullerene-Based Aggregates. Journal of Physical Chemistry A, 2018, 122, 1124-1137.	2.5	5
38	Building Fluorinated Hybrid Crystals: Understanding the Role of Noncovalent Interactions. Crystal Growth and Design, 2018, 18, 6901-6910.	3.0	14
39	Perspective: Chemical Information Encoded in Electron Density. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2018, 34, 567-580.	4.9	4
40	Accurately extracting the signature of intermolecular interactions present in the NCI plot of the reduced density gradient versus electron density. Physical Chemistry Chemical Physics, 2017, 19, 17928-17936.	2.8	1,068
41	Microscopic analysis of AgCl polymorphism. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	0
42	Tuning Azoheteroarene Photoswitch Performance through Heteroaryl Design. Journal of the American Chemical Society, 2017, 139, 1261-1274.	13.7	244
43	On understanding the chemical origin of band gaps. Journal of Molecular Modeling, 2017, 23, 271.	1.8	9
44	Binding of Thioflavin T and Related Probes to Polymorphic Models of Amyloid-Î² Fibrils. Journal of Physical Chemistry B, 2017, 121, 8926-8934.	2.6	34
45	A topological study of chemical bonds under pressure: solid hydrogen as a model case. Physical Chemistry Chemical Physics, 2017, 19, 26381-26395.	2.8	7
46	Revealing strong interactions with the reduced density gradient: a benchmark for covalent, ionic and charge-shift bonds. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	82
47	Using electron density to understand co-crystal structures. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C798-C798.	0.1	0
48	Effects of the CO2 Guest Molecule on the sI Clathrate Hydrate Structure. Materials, 2016, 9, 777.	2.9	33
49	Alkali Ion Incorporation into V₂O₅: a Noncovalent Interactions Analysis. Journal of Physical Chemistry C, 2016, 120, 4259-4265.	3.1	17
50	A Complete NCI Perspective: From New Bonds to Reactivity. Challenges and Advances in Computational Chemistry and Physics, 2016, , 491-527.	0.6	24
51	A benchmark for the non-covalent interaction (NCI) index orâ€¦ is it really all in the geometry?. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	124
52	Ordered helium trapping and bonding in compressed arsenolite: Synthesis of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">A</mml:mi><mml:msub><mml:mi mathvariant="normal">s</mml:mi><mml:mn>4</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>6</mml:mn></mml:msub><mml:mo>Â·</mml:mo><mml:mn>2</mml:mn><mml:mi>He</mml:mi></mml:mrow></mml:math>	3.2	29
53	Phase stability of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î²</mml:mi><mml:mo>â€²</mml:mo><mml:mi mathvariant="normal">B</mml:mi><mml:msub><mml:mi mathvariant="normal">i</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> under compression: Optical and elastic properties and electron density topology analysis. Physical Review B,	3.2	16
54	Understanding conductivity in molecular switches: a real space approach in octaphyrins. Physical Chemistry Chemical Physics, 2016, 18, 11829-11838.	2.8	10

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55	Unravelling Proteinâ€“DNA Interactions at Molecular Level: A DFT and NCI Study. Journal of Chemical Theory and Computation, 2016, 12, 523-534.	5.3	35
56	How strong are the metalloceneâ€“metallocene interactions? Cases of ferrocene, ruthenocene, and osmocene. Physical Chemistry Chemical Physics, 2016, 18, 550-556.	2.8	34
57	Understanding the molecular switching properties of octaphyrins. Physical Chemistry Chemical Physics, 2016, 18, 11885-11900.	2.8	29
58	Exploiting the cyclodextrins ability for antioxidants encapsulation: A computational approach to carnosol and carnosic acid embedding. Computational and Theoretical Chemistry, 2016, 1077, 65-73.	2.5	21
59	Interpretation of the reduced density gradient. Molecular Physics, 2016, 114, 1406-1414.	1.7	103
60	Chemical Bonding under Pressure. , 2015, , 131-157.		0
61	Guestâ€“host interactions in gas clathrate hydrates under pressure. High Pressure Research, 2015, 35, 49-56.	1.2	9
62	The role of dispersion forces in metal-supported self-assembled monolayers. Computational and Theoretical Chemistry, 2015, 1053, 322-327.	2.5	12
63	The Missing Entry in the Agosticâ€“Anagostic Series: Rh(I)â€“Î·¹-C Interactions in P(CH)P Pincer Complexes. Inorganic Chemistry, 2015, 54, 2960-2969.	4.0	46
64	From ELF to Compressibility in Solids. International Journal of Molecular Sciences, 2015, 16, 8151-8167.	4.1	10
65	Six questions on topology in theoretical chemistry. Computational and Theoretical Chemistry, 2015, 1053, 2-16.	2.5	99
66	Understanding the Fundamental Role of Ï€Ï€, ÏƒÏƒ, and ÏƒÏ€ Dispersion Interactions in Shaping Carbonâ€Based Materials. Chemistry - A European Journal, 2014, 20, 4931-4941.	3.3	109
67	Following the Molecular Mechanism for the NH₃ + LiH â†' LiNH₂ + H₂ Chemical Reaction: A Study Based on the Joint Use of the Quantum Theory of Atoms in Molecules (QTAIM) and Noncovalent Interaction (NCI) Index. Journal of Physical Chemistry A, 2014, 118, 1663-1672.	2.5	61
68	Unraveling non-covalent interactions within flexible biomolecules: from electron density topology to gas phase spectroscopy. Physical Chemistry Chemical Physics, 2014, 16, 9876.	2.8	156
69	The Houkâ€“List transition states for organocatalytic mechanisms revisited. Chemical Science, 2014, 5, 2057-2071.	7.4	154
70	Revisiting H₂O Nucleation around Au⁺ and Hg²⁺: The Peculiar â€œPseudo-Softâ€•Character of the Gold Cation. Journal of Chemical Theory and Computation, 2014, 10, 1900-1909.	5.3	7
71	Labelling Herceptin with a novel oxaliplatin derivative: a computational approach towards the selective drug delivery. Journal of Molecular Modeling, 2014, 20, 2401.	1.8	24
72	Characterizing Molecular Interactions in Chemical Systems. IEEE Transactions on Visualization and Computer Graphics, 2014, 20, 2476-2485.	4.4	63

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73	Stochastic Voyages into Uncharted Chemical Space Produce a Representative Library of All Possible Drug-Like Compounds. Journal of the American Chemical Society, 2013, 135, 7296-7303.	13.7	214
74	Are Bond Critical Points Really Critical for Hydrogen Bonding?. Journal of Chemical Theory and Computation, 2013, 9, 3263-3266.	5.3	414
75	Delocalization error of density-functional approximations: A distinct manifestation in hydrogen molecular chains. Journal of Chemical Physics, 2012, 137, 214106.	3.0	66
76	Revealing non-covalent interactions in solids: NCI plots revisited. Physical Chemistry Chemical Physics, 2012, 14, 12165.	2.8	279
77	Local pressures in Zn chalcogenide polymorphs. Europhysics Letters, 2012, 98, 56002.	2.0	14
78	Revealing Nonâ€covalent Interactions in Molecular Crystals through Their Experimental Electron Densities. Chemistry - A European Journal, 2012, 18, 15523-15536.	3.3	173
79	Density-Functional Errors in Alkanes: A Real-Space Perspective. Journal of Chemical Theory and Computation, 2012, 8, 2676-2681.	5.3	16
80	Coupling Quantum Interpretative Techniques: Another Look at Chemical Mechanisms in Organic Reactions. Journal of Chemical Theory and Computation, 2012, 8, 3993-3997.	5.3	104
81	Highly selective mercury(ii) cations detection in mixedâ€“aqueous media by a ferrocene-based fluorescent receptor. Dalton Transactions, 2012, 41, 4437.	3.3	27
82	Ionic interactions: Comparative topological approach. Computational and Theoretical Chemistry, 2012, 998, 193-201.	2.5	41
83	Silverâ€Catalysed Enantioselective Addition of Oï£¿H and Nï£¿H Bonds to Allenes: A New Model for Stereoselectivity Based on Noncovalent Interactions. Chemistry - A European Journal, 2012, 18, 11317-11324.	3.3	54
84	Analysis of Hydrogen-Bond Interaction Potentials from the Electron Density: Integration of Noncovalent Interaction Regions. Journal of Physical Chemistry A, 2011, 115, 12983-12990.	2.5	339
85	Bonding Changes Along Solid-Solid Phase Transitions Using the Electron Localization Function Approach. , 2011, , 625-658.		3
86	NCIPLOT: A Program for Plotting Noncovalent Interaction Regions. Journal of Chemical Theory and Computation, 2011, 7, 625-632.	5.3	2,897
87	On Bonding in Ionic Crystals. Journal of Physical Chemistry C, 2011, 115, 257-263.	3.1	13
88	Electron delocalization and bond formation under the ELF framework. Theoretical Chemistry Accounts, 2011, 128, 411-418.	1.4	29
89	Optical and electronic properties of dense sodium. Physical Review B, 2011, 83, .	3.2	48
90	Communication: A density functional with accurate fractional-charge and fractional-spin behaviour for s-electrons. Journal of Chemical Physics, 2011, 135, 081103.	3.0	31

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91	Non-covalent interactions descriptor using experimental electron densities. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C448-C449.	0.3	0
92	Revealing Noncovalent Interactions. Journal of the American Chemical Society, 2010, 132, 6498-6506.	13.7	6,465
93	Synthesis and chemical diversity analysis of bicyclo[3.3.1]non-3-en-2-ones. Tetrahedron, 2010, 66, 5852-5862.	1.9	17
94	From molecular to polymeric CO2: bonding transformations under pressure. High Pressure Research, 2009, 29, 113-117.	1.2	1
95	Universal compressibility behaviour of ions in ionic crystals. High Pressure Research, 2009, 29, 97-102.	1.2	4
96	A new polymorph with a layered structure É›-CaTe2O5. Solid State Sciences, 2009, 11, 289-293.	3.2	12
97	Bases for Understanding Polymerization under Pressure: The Practical Case of CO₂. Journal of Physical Chemistry B, 2009, 113, 1068-1073.	2.6	13
98	A Quantum Chemical Interpretation of Compressibility in Solids. Journal of Chemical Theory and Computation, 2009, 5, 2108-2114.	5.3	30
99	Bonding changes across the Î±-cristobaliteâ†'stishovite transition path in silica. High Pressure Research, 2009, 29, 93-96.	1.2	5
100	Quantum-mechanical calculations of zircon to scheelite transition pathways inZrSiO4. Physical Review B, 2009, 79, .	3.2	27
101	Potassium under Pressure: A Pseudobinary Ionic Compound. Physical Review Letters, 2009, 103, 115501.	7.8	100
102	The bulk modulus of cubic spinel selenides: an experimental and theoretical study. High Pressure Research, 2009, 29, 72-75.	1.2	8
103	Computation of Local and Global Properties of the Electron Localization Function Topology in Crystals. Journal of Chemical Theory and Computation, 2009, 5, 164-173.	5.3	26
104	Useful applications of the electron localization function in high-pressure crystal chemistry. Journal of Physics and Chemistry of Solids, 2008, 69, 2204-2207.	4.0	25
105	On the mechanism of the zircon-reidite pressure induced transformation. Journal of Physics and Chemistry of Solids, 2008, 69, 2277-2280.	4.0	28
106	Origin of incommensurate modulations in the high-pressure phosphorus IV phase. Physical Review B, 2008, 78, .	3.2	24
107	How Electron Localization Function Quantifies and Pictures Chemical Changes in a Solid: The B3 â†' B1 Pressure Induced Phase Transition in BeO. Journal of Physical Chemistry B, 2008, 112, 9787-9794.	2.6	26
108	Visualizing Correlation Regions: The Case of the Ammonia Crystal. Chemistry Methods, 0, , .	3.8	2

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109	Effect of strain on interactions of Î£ 3{111} silicon grain boundary with oxygen impurities from firstâ€principles. Physica Status Solidi (B): Basic Research, 0, , 2100377.	1.5	3
110	Insight into the inclusion of heteroatom impurities in Silicon structures. Physical Chemistry Chemical Physics, 0, , .	2.8	0