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	Revealing Noncovalent Interactions. Journal of the American Chemical Society, 2010, 132, 6498-6506.	13.7	6,465
2	NCIPLOT: A Program for Plotting Noncovalent Interaction Regions. Journal of Chemical Theory and Computation, 2011, 7, 625-632.	5.3	2,897
3	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
4	Are Bond Critical Points Really Critical for Hydrogen Bonding?. Journal of Chemical Theory and Computation, 2013, 9, 3263-3266.	5.3	414
5	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
6	Revealing non-covalent interactions in solids: NCI plots revisited. Physical Chemistry Chemical Physics, 2012, 14, 12165.	2.8	279
7	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
8	Tuning Azoheteroarene Photoswitch Performance through Heteroaryl Design. Journal of the American Chemical Society, 2017, 139, 1261-1274.	13.7	244
9	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
10	Revealing Nonâ€covalent Interactions in Molecular Crystals through Their Experimental Electron Densities. Chemistry - A European Journal, 2012, 18, 15523-15536.	3.3	173
11	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
12	The Houkâ€“List transition states for organocatalytic mechanisms revisited. Chemical Science, 2014, 5, 2057-2071.	7.4	154
13	NCIPLOT4: Fast, Robust, and Quantitative Analysis of Noncovalent Interactions. Journal of Chemical Theory and Computation, 2020, 16, 4150-4158.	5.3	151
14	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
15	New Way for Probing Bond Strength. Journal of Physical Chemistry A, 2020, 124, 1850-1860.	2.5	121
16	Nine questions on energy decomposition analysis. Journal of Computational Chemistry, 2019, 40, 2248-2283.	3.3	113
17	Understanding the Fundamental Role of Ï€/Ï€, Ïƒ/Ïƒ, and Ïƒ/Ï€ Dispersion Interactions in Shaping Carbonâ€Based Materials. Chemistry - A European Journal, 2014, 20, 4931-4941.	3.3	109
18	Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, 10881-10905.	3.3	108

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19	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
20	Interpretation of the reduced density gradient. Molecular Physics, 2016, 114, 1406-1414.	1.7	103
21	Potassium under Pressure: A Pseudobinary Ionic Compound. Physical Review Letters, 2009, 103, 115501.	7.8	100
22	Six questions on topology in theoretical chemistry. Computational and Theoretical Chemistry, 2015, 1053, 2-16.	2.5	99
23	New electron delocalization tools to describe the aromaticity in porphyrinoids. Physical Chemistry Chemical Physics, 2018, 20, 2787-2796.	2.8	86
24	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
25	Delocalization error of density-functional approximations: A distinct manifestation in hydrogen molecular chains. Journal of Chemical Physics, 2012, 137, 214106.	3.0	66
26	Characterizing Molecular Interactions in Chemical Systems. IEEE Transactions on Visualization and Computer Graphics, 2014, 20, 2476-2485.	4.4	63
27	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
28	<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
29	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
30	Optical and electronic properties of dense sodium. Physical Review B, 2011, 83, .	3.2	48
31	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
32	Ionic interactions: Comparative topological approach. Computational and Theoretical Chemistry, 2012, 998, 193-201.	2.5	41
33	Strong correlation between electronic bonding network and critical temperature in hydrogen-based superconductors. Nature Communications, 2021, 12, 5381.	12.8	39
34	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
35	How strong are the metalloceneâ€"metallocene interactions? Cases of ferrocene, ruthenocene, and osmocene. Physical Chemistry Chemical Physics, 2016, 18, 550-556.	2.8	34
36	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

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37	Effects of the CO2 Guest Molecule on the sI Clathrate Hydrate Structure. Materials, 2016, 9, 777.	2.9	33
38	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
39	Characterization and Decomposition of the Natural van der Waals SnSb₂Te₄ under Compression. Inorganic Chemistry, 2020, 59, 9900-9918.	4.0	31
40	A Quantum Chemical Interpretation of Compressibility in Solids. Journal of Chemical Theory and Computation, 2009, 5, 2108-2114.	5.3	30
41	Electron delocalization and bond formation under the ELF framework. Theoretical Chemistry Accounts, 2011, 128, 411-418.	1.4	29
42	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>. Physical Review B, 2016, 93, .	3.2	29
43	Understanding the molecular switching properties of octaphyrins. Physical Chemistry Chemical Physics, 2016, 18, 11885-11900.	2.8	29
44	On the mechanism of the zircon-reidite pressure induced transformation. Journal of Physics and Chemistry of Solids, 2008, 69, 2277-2280.	4.0	28
45	Quantum-mechanical calculations of zircon to scheelite transition pathways inZrSiO4. Physical Review B, 2009, 79, .	3.2	27
46	Highly selective mercury(ii) cations detection in mixedâ€“aqueous media by a ferrocene-based fluorescent receptor. Dalton Transactions, 2012, 41, 4437.	3.3	27
47	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
48	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
49	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
50	Origin of incommensurate modulations in the high-pressure phosphorus IV phase. Physical Review B, 2008, 78, .	3.2	24
51	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
52	A Complete NCI Perspective: From New Bonds to Reactivity. Challenges and Advances in Computational Chemistry and Physics, 2016, , 491-527.	0.6	24
53	High pressure theoretical and experimental analysis of the bandgap of BaMoO4, PbMoO4, and CdMoO4. Applied Physics Letters, 2019, 115, .	3.3	24
54	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

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55	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
56	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
57	Synthesis and chemical diversity analysis of bicyclo[3.3.1]non-3-en-2-ones. Tetrahedron, 2010, 66, 5852-5862.	1.9	17
58	Alkali Ion Incorporation into V₂O₅: a Noncovalent Interactions Analysis. Journal of Physical Chemistry C, 2016, 120, 4259-4265.	3.1	17
59	Density-Functional Errors in Alkanes: A Real-Space Perspective. Journal of Chemical Theory and Computation, 2012, 8, 2676-2681.	5.3	16
60	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î²</mml:mi><mml:mo>â^'</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
61	A chemical theory of topological insulators. Chemical Communications, 2019, 55, 12281-12287.	4.1	16
62	A regression approach to accurate interaction energies using topological descriptors. Computational and Theoretical Chemistry, 2019, 1159, 23-26.	2.5	16
63	Steric clash in real space: biphenyl revisited. Physical Chemistry Chemical Physics, 2020, 22, 21251-21256.	2.8	16
64	Local pressures in Zn chalcogenide polymorphs. Europhysics Letters, 2012, 98, 56002.	2.0	14
65	Building Fluorinated Hybrid Crystals: Understanding the Role of Noncovalent Interactions. Crystal Growth and Design, 2018, 18, 6901-6910.	3.0	14
66	Kickâ€“Fukui: A Fukui Function-Guided Method for Molecular Structure Prediction. Journal of Chemical Information and Modeling, 2021, 61, 3955-3963.	5.4	14
67	Bases for Understanding Polymerization under Pressure: The Practical Case of CO₂. Journal of Physical Chemistry B, 2009, 113, 1068-1073.	2.6	13
68	On Bonding in Ionic Crystals. Journal of Physical Chemistry C, 2011, 115, 257-263.	3.1	13
69	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
70	A new polymorph with a layered structure É›-CaTe2O5. Solid State Sciences, 2009, 11, 289-293.	3.2	12
71	The role of dispersion forces in metal-supported self-assembled monolayers. Computational and Theoretical Chemistry, 2015, 1053, 322-327.	2.5	12
72	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

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73	A first step towards quantum energy potentials of electron pairs. Physical Chemistry Chemical Physics, 2019, 21, 4215-4223.	2.8	11
74	From ELF to Compressibility in Solids. International Journal of Molecular Sciences, 2015, 16, 8151-8167.	4.1	10
75	Understanding conductivity in molecular switches: a real space approach in octaphyrins. Physical Chemistry Chemical Physics, 2016, 18, 11829-11838.	2.8	10
76	Overcoming Distrust in Solid State Simulations: Adding Error Bars to Computational Data. Journal of Physical Chemistry C, 2019, 123, 4767-4772.	3.1	10
77	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
78	Guestâ€“host interactions in gas clathrate hydrates under pressure. High Pressure Research, 2015, 35, 49-56.	1.2	9
79	On understanding the chemical origin of band gaps. Journal of Molecular Modeling, 2017, 23, 271.	1.8	9
80	Localizing electron density errors in density functional theory. Physical Chemistry Chemical Physics, 2019, 21, 20927-20938.	2.8	9
81	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
82	The bulk modulus of cubic spinel selenides: an experimental and theoretical study. High Pressure Research, 2009, 29, 72-75.	1.2	8
83	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
84	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
85	Valenceâ€Shell Electronâ€Pair Repulsion Theory Revisited: An Explanation for Core Polarization. Chemistry - A European Journal, 2019, 25, 10938-10945.	3.3	7
86	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
87	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
88	Bonding changes across the Î±-cristobaliteâ†'stishovite transition path in silica. High Pressure Research, 2009, 29, 93-96.	1.2	5
89	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
90	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

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91	Universal compressibility behaviour of ions in ionic crystals. High Pressure Research, 2009, 29, 97-102.	1.2	4
92	Energetics of Electron Pairs in Electrophilic Aromatic Substitutions. Molecules, 2021, 26, 513.	3.8	4
93	Perspective: Chemical Information Encoded in Electron Density. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2018, 34, 567-580.	4.9	4
94	Bonding Changes Along Solid-Solid Phase Transitions Using the Electron Localization Function Approach. , 2011, , 625-658.		3
95	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
96	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
97	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
98	Visualizing Correlation Regions: The Case of the Ammonia Crystal. Chemistry Methods, 0, , .	3.8	2
99	Borates or phosphates? That is the question. Acta Crystallographica Section A: Foundations and Advances, 2020, 76, 197-205.	0.1	2
100	From molecular to polymeric CO2: bonding transformations under pressure. High Pressure Research, 2009, 29, 113-117.	1.2	1
101	Labeling IL-18 with alkaloids: toward the use of cytokines as carrier molecules in chemotherapy. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	1
102	Understanding Topological Insulators in Real Space. Molecules, 2021, 26, 2965.	3.8	1
103	NCI: looking at solute/solvent interactions. Electronic Structure, 2021, 3, 034006.	2.8	1
104	Cluster Assembled Silicon-Lithium Nanostructures: A Nanowire Confined Inside a Carbon Nanotube. Frontiers in Chemistry, 2021, 9, 767421.	3.6	1
105	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
106	Chemical Bonding under Pressure. , 2015, , 131-157.		0
107	Microscopic analysis of AgCl polymorphism. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	0
108	Non-covalent interactions descriptor using experimental electron densities. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C448-C449.	0.3	0

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109	Using electron density to understand co-crystal structures. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C798-C798.	0.1	0
110	Insight into the inclusion of heteroatom impurities in Silicon structures. Physical Chemistry Chemical Physics, 0, , .	2.8	0