Giovanni Bistoni

List of Publications by Year
in descending order

63 papers	2,628 citations	147801 31 h-index	197818 49 g-index
65 all docs	65 docs citations	65 times ranked	2419 citing authors

#	Article	IF	Citations
1	Decomposition of Intermolecular Interaction Energies within the Local Pair Natural Orbital Coupled Cluster Framework. Journal of Chemical Theory and Computation, 2016, 12, 4778-4792.	5.3	231
2	How Ï€ back-donation quantitatively controls the CO stretching response in classical and non-classical metal carbonyl complexes. Chemical Science, 2016, 7, 1174-1184.	7.4	158
3	Chemistry and Quantum Mechanics in 2019: Give Us Insight <i>and</i> Numbers. Journal of the American Chemical Society, 2019, 141, 2814-2824.	13.7	93
4	Understanding the Role of Dispersion in Frustrated Lewis Pairs and Classical Lewis Adducts: A Domainâ€Based Local Pair Natural Orbital Coupled Cluster Study. Chemistry - A European Journal, 2017, 23, 865-873.	3.3	91
5	Local Energy Decomposition of Open-Shell Molecular Systems in the Domain-Based Local Pair Natural Orbital Coupled Cluster Framework. Journal of Chemical Theory and Computation, 2019, 15, 1616-1632.	5.3	86
6	Effect of Electron Correlation on Intermolecular Interactions: A Pair Natural Orbitals Coupled Cluster Based Local Energy Decomposition Study. Journal of Chemical Theory and Computation, 2019, 15, 215-228.	5.3	84
7	The Chemical Bond in Gold(I) Complexes with N-Heterocyclic Carbenes. Organometallics, 2014, 33, 4200-4208.	2.3	73
8	Local energy decomposition analysis of hydrogen-bonded dimers within a domain-based pair natural orbital coupled cluster study. Beilstein Journal of Organic Chemistry, 2018, 14, 919-929.	2.2	72
9	Charge-displacement analysis via natural orbitals for chemical valence: Charge transfer effects in coordination chemistry. Journal of Chemical Physics, 2015, 142, 084112.	3.0	69
10	When the Tolman Electronic Parameter Fails: A Comparative DFT and Charge Displacement Study of [(L)Ni(CO)₃]^{0/â€“} and [(L)Au(CO)]^{0/+}. Inorganic Chemistry, 2014, 53, 9907-9916.	4.0	67
11	Unveiling the Photophysical Properties of Boron-dipyrromethene Dyes Using a New Accurate Excited State Coupled Cluster Method. Journal of Chemical Theory and Computation, 2020, 16, 564-575.	5.3	64
12	Disentanglement of Donation and Backâ€Donation Effects on Experimental Observables: A Case Study of Goldâ€“Ethyne Complexes. Angewandte Chemie - International Edition, 2013, 52, 11599-11602.	13.8	61
13	Unveiling the Delicate Balance of Steric and Dispersion Interactions in Organocatalysis Using High-Level Computational Methods. Journal of the American Chemical Society, 2020, 142, 3613-3625.	13.7	58
14	NHC-Gold-Alkyne Complexes: Influence of the Carbene Backbone on the Ion Pair Structure. Organometallics, 2013, 32, 4444-4447.	2.3	56
15	Finding chemical concepts in the Hilbert space: Coupled cluster analyses of noncovalent interactions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1442.	14.6	56
16	Formation of Agostic Structures Driven by London Dispersion. Angewandte Chemie - International Edition, 2018, 57, 4760-4764.	13.8	55
17	London dispersion effects in the coordination and activation of alkanes in Ïƒ-complexes: a local energy decomposition study. Physical Chemistry Chemical Physics, 2019, 21, 11569-11577.	2.8	54
18	Selectively Measuring Ï€â€…Backâ€Donation in Gold(I) Complexes by NMR Spectroscopy. Chemistry - A European Journal, 2015, 21, 2467-2473.	3.3	53

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19	Scalable and Highly Diastereo- and Enantioselective Catalytic Dielsâ€“Alder Reaction of Î±,Î²-Unsaturated Methyl Esters. Journal of the American Chemical Society, 2018, 140, 12671-12676.	13.7	52
20	Ï€ Activation of Alkynes in Homogeneous and Heterogeneous Gold Catalysis. Journal of Physical Chemistry A, 2016, 120, 5239-5247.	2.5	49
21	London Dispersion Interactions in Pnictogen Cations [ECl₂]⁺ and [E=E]²⁺ (E=P, As, Sb) Supported by Anionic <i>N</i>â€Heterocyclic Carbenes. Chemistry - A European Journal, 2018, 24, 18922-18932.	3.3	47
22	Modulating the Bonding Properties of Nâ€Heterocyclic Carbenes (NHCs): A Systematic Chargeâ€Displacement Analysis. Chemistry - A European Journal, 2017, 23, 7558-7569.	3.3	45
23	Treating Subvalence Correlation Effects in Domain Based Pair Natural Orbital Coupled Cluster Calculations: An Out-of-the-Box Approach. Journal of Chemical Theory and Computation, 2017, 13, 3220-3227.	5.3	45
24	Extrapolation to the Limit of a Complete Pair Natural Orbital Space in Local Coupled-Cluster Calculations. Journal of Chemical Theory and Computation, 2020, 16, 6142-6149.	5.3	45
25	The furan microsolvation blind challenge for quantum chemical methods: First steps. Journal of Chemical Physics, 2018, 148, 014301.	3.0	44
26	Pair natural orbital and canonical coupled cluster reaction enthalpies involving light to heavy alkali and alkaline earth metals: the importance of sub-valence correlation. Physical Chemistry Chemical Physics, 2017, 19, 9374-9391.	2.8	43
27	A New Ligand Design Based on London Dispersion Empowers Chiral Bismuthâ€“Rhodium Paddlewheel Catalysts. Journal of the American Chemical Society, 2021, 143, 5666-5673.	13.7	42
28	Strong Electron-Donating Ligands Accelerate the Protodeauration Step in Gold(I)-Catalyzed Reactions: A <i>Quantitative</i> Understanding of the Ligand Effect. Organometallics, 2016, 35, 2275-2285.	2.3	41
29	¹³Câ€…NMR Spectroscopy of Nâ€Heterocyclic Carbenes Can Selectively Probe Ïƒ Donation in Gold(I) Complexes. Chemistry - A European Journal, 2017, 23, 2722-2728.	3.3	38
30	Toward Accurate QM/MM Reaction Barriers with Large QM Regions Using Domain Based Pair Natural Orbital Coupled Cluster Theory. Journal of Chemical Theory and Computation, 2018, 14, 3524-3531.	5.3	37
31	HFLD: A Nonempirical London Dispersion-Corrected Hartreeâ€“Fock Method for the Quantification and Analysis of Noncovalent Interaction Energies of Large Molecular Systems. Journal of Chemical Theory and Computation, 2019, 15, 5894-5907.	5.3	36
32	Local energy decomposition of coupledâ€cluster interaction energies: Interpretation, benchmarks, and comparison with symmetryâ€adapted perturbation theory. International Journal of Quantum Chemistry, 2021, 121, e26339.	2.0	36
33	Computational Design of Near-Infrared Fluorescent Organic Dyes Using an Accurate New Wave Function Approach. Journal of Physical Chemistry Letters, 2019, 10, 4822-4828.	4.6	33
34	Hydrogenative Metathesis of Enynes via Piano-Stool Ruthenium Carbene Complexes Formed by Alkyne gem-Hydrogenation. Journal of the American Chemical Society, 2020, 142, 18541-18553.	13.7	30
35	Strong and Confined Acids Control Five Stereogenic Centers in Catalytic Asymmetric Dielsâ€“Alder Reactions of Cyclohexadienones with Cyclopentadiene. Angewandte Chemie - International Edition, 2020, 59, 12347-12351.	13.8	30
36	Quantitative assessment of the carbocation/carbene character of the goldâ€“carbene bond. Dalton Transactions, 2015, 44, 13999-14007.	3.3	29

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37	A Combined Spectroscopic and Computational Study on the Mechanism of Iron-Catalyzed Aminofunctionalization of Olefins Using Hydroxylamine Derived Nâ€"O Reagent as the â€œAminoâ€•Source and â€œOxidantâ€• Journal of the American Chemical Society, 2022, 144, 2637-2656.	13.7	29
38	Relationship between the anion/cation relative orientation and the catalytic activity of nitrogen acyclic carbeneâ€"gold catalysts. Catalysis Science and Technology, 2015, 5, 1558-1567.	4.1	28
39	The first microsolvation step for furans: New experiments and benchmarking strategies. Journal of Chemical Physics, 2020, 152, 164303.	3.0	28
40	Advances in Charge Displacement Analysis. Journal of Chemical Theory and Computation, 2016, 12, 1236-1244.	5.3	27
41	Anomalous ligand effect in gold(i)-catalyzed intramolecular hydroamination of alkynes. Chemical Communications, 2015, 51, 5990-5993.	4.1	24
42	Formyltetrahydrofolate Decarbonylase Synthesizes the Active Site CO Ligand of O₂-Tolerant [NiFe] Hydrogenase. Journal of the American Chemical Society, 2020, 142, 1457-1464.	13.7	24
43	Charge-Displacement Analysis of the Interaction in the Ammoniaâ€"Noble Gas Complexes. Journal of Physical Chemistry A, 2011, 115, 14657-14666.	2.5	23
44	From Serendipity to Rational Design: Heteroleptic Dirhodium Amidate Complexes for Diastereodivergent Asymmetric Cyclopropanation. Journal of the American Chemical Society, 2022, 144, 7465-7478.	13.7	23
45	Harnessing the ambiphilicity of silyl nitronates in a catalytic asymmetric approach to aliphatic Î²3-amino acids. Nature Catalysis, 2021, 4, 1043-1049.	34.4	20
46	Physical Nature of Differential Spin-State Stabilization of Carbenes by Hydrogen and Halogen Bonding: A Domain-Based Pair Natural Orbital Coupled Cluster Study. Journal of Physical Chemistry A, 2019, 123, 5081-5090.	2.5	19
47	Redesigning donorâ€"acceptor Stenhouse adduct photoswitches through a joint experimental and computational study. Chemical Science, 2021, 12, 2916-2924.	7.4	18
48	Taming phosphorus mononitride. Nature Chemistry, 2022, 14, 928-934.	13.6	18
49	Dispersion Forces Drive the Formation of Uraniumâ€"Alkane Adducts. Journal of the American Chemical Society, 2020, 142, 1864-1870.	13.7	17
50	Addressing the System-Size Dependence of the Local Approximation Error in Coupled-Cluster Calculations. Journal of Physical Chemistry A, 2021, 125, 9932-9939.	2.5	17
51	Triple Resonance Experiments for the Rapid Detection of ¹⁰³Rh NMR Shifts: A Combined Experimental and Theoretical Study into Dirhodium and Bismuthâ€"Rhodium Paddlewheel Complexes. Journal of the American Chemical Society, 2021, 143, 12473-12479.	13.7	16
52	Unraveling individual <scp>hostâ€"guest</scp> interactions in molecular recognition from first principles quantum mechanics: Insights into the nature of nicotinic acetylcholine receptor agonist binding. Journal of Computational Chemistry, 2021, 42, 293-302.	3.3	12
53	Unveiling the complex pattern of intermolecular interactions responsible for the stability of the DNA duplex. Chemical Science, 2021, 12, 12785-12793.	7.4	11
54	Understanding the Nature and Properties of Hydrogenâ€"Hydrogen Bonds: The Stability of a Bulky Phosphatetrahedrane as a Case Study. Journal of Physical Chemistry A, 2021, 125, 6151-6157.	2.5	10

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55	An induced-fit model for asymmetric organocatalytic reactions: a case study of the activation of olefins <i>via</i> chiral BrÃ¸nsted acid catalysts. Chemical Science, 2022, 13, 8848-8859.	7.4	8
56	Formation of Agostic Structures Driven by London Dispersion. Angewandte Chemie, 2018, 130, 4850-4854.	2.0	7
57	Starke und sterisch begrenzte SÃuren kontrollieren fÃ¼nf stereogene Zentren in der katalytischen asymmetrischen Dielsâ€Alderâ€Reaktion von Cyclohexadienonen mit Cyclopentadien. Angewandte Chemie, 2020, 132, 12446-12450.	2.0	7
58	Fragment-Based Local Coupled Cluster Embedding Approach for the Quantification and Analysis of Noncovalent Interactions: Exploring the Many-Body Expansion of the Local Coupled Cluster Energy. Journal of Chemical Theory and Computation, 2021, 17, 3348-3359.	5.3	7
59	Open-Shell Variant of the London Dispersion-Corrected Hartreeâ€“Fock Method (HFLD) for the Quantification and Analysis of Noncovalent Interaction Energies. Journal of Chemical Theory and Computation, 2022, 18, 2292-2307.	5.3	7
60	Electronic Structure Calculations and Experimental Studies on the Thermal Initiation of the Twin Polymerization Process. ChemPlusChem, 2017, 82, 1396-1407.	2.8	4
61	Orbital Decomposition of the Carbon Chemical Shielding Tensor in Gold(I) Nâ€Heterocyclic Carbene Complexes. European Journal of Inorganic Chemistry, 2020, 2020, 1177-1183.	2.0	4
62	Can Domain-Based Local Pair Natural Orbitals Approaches Accurately Predict Phosphorescence Energies?. Physical Chemistry Chemical Physics, 0, , .	2.8	3
63	Charge Transfer in Beryllium Bonds and Cooperativity of Beryllium and Halogen Bonds. A New Perspective. Challenges and Advances in Computational Chemistry and Physics, 2016, , 461-489.	0.6	1