Leonardo Belpassi

List of Publications by Year
in descending order

120	4,059	101543 36	138484 58
papers	citations	h-index	g-index

127	127	127	3138
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The Chemical Bond between Au(I) and the Noble Gases. Comparative Study of NgAuF and NgAu⁺ (Ng = Ar, Kr, Xe) by Density Functional and Coupled Cluster Methods. Journal of the American Chemical Society, 2008, 130, 1048-1060.	13.7	260
2	Influence of the dye molecular structure on the TiO₂conduction band in dye-sensitized solar cells: disentangling charge transfer and electrostatic effects. Energy and Environmental Science, 2013, 6, 183-193.	30.8	247
3	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
4	Ion Pairing in Cationic Olefinâ^'Gold(I) Complexes. Journal of the American Chemical Society, 2009, 131, 3170-3171.	13.7	134
5	Revealing Charge-Transfer Effects in Gas-Phase Water Chemistry. Accounts of Chemical Research, 2012, 45, 1571-1580.	15.6	107
6	Solvent-, Silver-, and Acid-Free NHC-Au-X Catalyzed Hydration of Alkynes. The Pivotal Role of the Counterion. ACS Catalysis, 2016, 6, 7363-7376.	11.2	106
7	Counterion Effect in the Reaction Mechanism of NHC Gold(I)-Catalyzed Alkoxylation of Alkynes: Computational Insight into Experiment. ACS Catalysis, 2015, 5, 803-814.	11.2	98
8	A Phosphine Gold(I) Ï€-Alkyne Complex: Tuning the Metalâ^'Alkyne Bond Character and Counterion Position by the Choice of the Ancillary Ligand. Inorganic Chemistry, 2010, 49, 3080-3082.	4.0	92
9	On the Dewarâ€“Chattâ€“Duncanson Model for Catalytic Gold(I) Complexes. Chemistry - A European Journal, 2010, 16, 7231-7240.	3.3	91
10	Charge-Transfer Energy in the Waterâ^'Hydrogen Molecular Aggregate Revealed by Molecular-Beam Scattering Experiments, Charge Displacement Analysis, and ab Initio Calculations. Journal of the American Chemical Society, 2010, 132, 13046-13058.	13.7	80
11	Ligand Effects on Bonding and Ion Pairing in Cationic Gold(I) Catalysts Bearing Unsaturated Hydrocarbons. European Journal of Inorganic Chemistry, 2013, 2013, 4121-4135.	2.0	73
12	The Chemical Bond in Gold(I) Complexes with N-Heterocyclic Carbenes. Organometallics, 2014, 33, 4200-4208.	2.3	73
13	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
14	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
15	Unexpected Anion Effect in the Alkoxylation of Alkynes Catalyzed by Nâ€Heterocyclic Carbene (NHC) Cationic Gold Complexes. Chemistry - A European Journal, 2014, 20, 14594-14598.	3.3	63
16	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
17	Extensive Experimental and Computational Study of Counterion Effect in the Reaction Mechanism of NHC-Gold(I)-Catalyzed Alkoxylation of Alkynes. Organometallics, 2016, 35, 641-654.	2.3	61
18	Recent advances and perspectives in four-component Diracâ€“Kohnâ€“Sham calculations. Physical Chemistry Chemical Physics, 2011, 13, 12368.	2.8	59

#	Article	IF	Citations
19	An ab Initio Benchmark and DFT Validation Study on Gold(I)-Catalyzed Hydroamination of Alkynes. Journal of Chemical Theory and Computation, 2014, 10, 1021-1034.	5.3	57
20	NHC-Gold-Alkyne Complexes: Influence of the Carbene Backbone on the Ion Pair Structure. Organometallics, 2013, 32, 4444-4447.	2.3	56
21	Fluorinated Î²-Diketonate Diglyme Lanthanide Complexes as New Second-Order Nonlinear Optical Chromophores: The Role of f Electrons in the Dipolar and Octupolar Contribution to Quadratic Hyperpolarizability. Journal of the American Chemical Society, 2010, 132, 4966-4970.	13.7	55
22	A Quantitative View of Charge Transfer in the Hydrogen Bond: The Water Dimer Case. ChemPhysChem, 2014, 15, 2682-2687.	2.1	55
23	Molecular-Beam Scattering Experiments and Theoretical Calculations Probing Charge Transfer in Weakly Bound Complexes of Water. Journal of Physical Chemistry A, 2009, 113, 15223-15232.	2.5	53
24	Selectively Measuring Ï€â€…Backâ€Donation in Gold(I) Complexes by NMR Spectroscopy. Chemistry - A European Journal, 2015, 21, 2467-2473.	3.3	53
25	Experimental Evidence of Chemical Components in the Bonding of Helium and Neon with Neutral Molecules. Chemistry - A European Journal, 2015, 21, 6234-6240.	3.3	53
26	Experimental and theoretical evidence of charge transfer in weakly bound complexes of water. Physical Chemistry Chemical Physics, 2009, 11, 9970.	2.8	52
27	Ï€ Activation of Alkynes in Homogeneous and Heterogeneous Gold Catalysis. Journal of Physical Chemistry A, 2016, 120, 5239-5247.	2.5	49
28	Nuclear electric quadrupole moment of gold. Journal of Chemical Physics, 2007, 126, 064314.	3.0	46
29	Unraveling the Anion/Ligand Interplay in the Reaction Mechanism of Gold(I)-Catalyzed Alkoxylation of Alkynes. Organometallics, 2017, 36, 2364-2376.	2.3	45
30	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
31	Ion pairing in NHC gold(I) olefin complexes: A combined experimental/theoretical study. Journal of Organometallic Chemistry, 2010, 695, 2679-2686.	1.8	42
32	Density Relaxation in Time-Dependent Density Functional Theory: Combining Relaxed Density Natural Orbitals and Multireference Perturbation Theories for an Improved Description of Excited States. Journal of Chemical Theory and Computation, 2014, 10, 4014-4024.	5.3	41
33	Strong Electron-Donating Ligands Accelerate the Protodeauration Step in Gold(I)-Catalyzed Reactions: A Quantitative Understanding of the Ligand Effect. Organometallics, 2016, 35, 2275-2285.	2.3	41
34	A combined NMR/DFT study on the ion pair structure of [(PR¹₂R²)Au(Î·²-3-hexyne)]BF₄complexes. Dalton Transactions, 2013, 42, 4122-4131.	3.3	40
35	Hydration and alkoxylation of alkynes catalyzed by NHCâ€“Auâ€“OTf. Green Chemistry, 2018, 20, 2125-2134.	9.0	40
36	Catching the role of anisotropic electronic distribution and charge transfer in halogen bonded complexes of noble gases. Journal of Chemical Physics, 2015, 142, 184304.	3.0	39

#	Article	IF	Citations
37	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
38	Electron density fitting for the Coulomb problem in relativistic density-functional theory. Journal of Chemical Physics, 2006, 124, 124104.	3.0	36
39	The Electronic Structure of Alkali Aurides. A Four-Component Diracâ^'Kohnâ^'Sham Study. Journal of Physical Chemistry A, 2006, 110, 4543-4554.	2.5	33
40	Dioxygen insertion into the gold(<scp>i</scp>)â€“hydride bond: spin orbit coupling effects in the spotlight for oxidative addition. Chemical Science, 2016, 7, 7034-7039.	7.4	33
41	Selective Emergence of the Halogen Bond in Ground and Excited States of Nobleâ€Gasâ€“Chlorine Systems. Angewandte Chemie - International Edition, 2019, 58, 4195-4199.	13.8	33
42	Spectroscopic properties of cyclometallated iridium complexes by TDDFT. Computational and Theoretical Chemistry, 2009, 914, 74-86.	1.5	31
43	Nature and Stability of Weak Halogen Bonds in the Gas Phase: Molecular Beam Scattering Experiments and Ab Initio Charge Displacement Calculations. Crystal Growth and Design, 2011, 11, 4279-4283.	3.0	30
44	Quantitative assessment of the carbocation/carbene character of the goldâ€“carbene bond. Dalton Transactions, 2015, 44, 13999-14007.	3.3	29
45	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
46	An Efficient Parallel All-Electron Four-Component Diracâ^'Kohnâ^'Sham Program Using a Distributed Matrix Approach. Journal of Chemical Theory and Computation, 2010, 6, 384-394.	5.3	27
47	Advances in Charge Displacement Analysis. Journal of Chemical Theory and Computation, 2016, 12, 1236-1244.	5.3	27
48	Charge-displacement analysis for excited states. Journal of Chemical Physics, 2014, 140, 054110.	3.0	26
49	Reactivity of a Gold-Aluminyl Complex with Carbon Dioxide: A Nucleophilic Gold?. Journal of the American Chemical Society, 2021, 143, 14433-14437.	13.7	26
50	Anomalous ligand effect in gold(i)-catalyzed intramolecular hydroamination of alkynes. Chemical Communications, 2015, 51, 5990-5993.	4.1	24
51	Helium Accepts Back-Donation In Highly Polar Complexes: New Insights into the Weak Chemical Bond. Journal of Physical Chemistry Letters, 2017, 8, 3334-3340.	4.6	24
52	Back-Donation in High-Valent d0 Metal Complexes: Does It Exist? The Case of NbV. Inorganic Chemistry, 2017, 56, 11266-11274.	4.0	24
53	Insight into the halogen-bond nature of noble gas-chlorine systems by molecular beam scattering experiments, ab initio calculations and charge displacement analysis. Physical Chemistry Chemical Physics, 2019, 21, 7330-7340.	2.8	24
54	BERTHA: Implementation of a four-component Diracâ€“Kohnâ€“Sham relativistic framework. Journal of Chemical Physics, 2020, 152, 164118.	3.0	24

#	Article	IF	Citations
55	Charge-Displacement Analysis of the Interaction in the Ammoniaâ€“Noble Gas Complexes. Journal of Physical Chemistry A, 2011, 115, 14657-14666.	2.5	23
56	Spinâ€Forbidden Reactions: Adiabatic Transition States Using Spinâ€“Orbit Coupled Density Functional Theory. Chemistry - A European Journal, 2018, 24, 5006-5015.	3.3	23
57	H₂Oâ€“CH₄and H₂Sâ€“CH₄complexes: a direct comparison through molecular beam experiments and ab initio calculations. Physical Chemistry Chemical Physics, 2015, 17, 30613-30623.	2.8	22
58	Charge-Displacement Analysis via Natural Orbitals for Chemical Valence in the Four-Component Relativistic Framework. Journal of Chemical Theory and Computation, 2018, 14, 1286-1296.	5.3	22
59	All-electron four-component Dirac-Kohn-Sham procedure for large molecules and clusters containing heavy elements. Physical Review B, 2008, 77, .	3.2	21
60	Molecular-beam study of the ammoniaâ€“noble gas systems: Characterization of the isotropic interaction and insights into the nature of the intermolecular potential. Journal of Chemical Physics, 2011, 135, 194301.	3.0	21
61	Efficient Parallel All-Electron Four-Component Diracâ€“Kohnâ€“Sham Program Using a Distributed Matrix Approach II. Journal of Chemical Theory and Computation, 2013, 9, 5356-5364.	5.3	21
62	Full Parallel Implementation of an All-Electron Four-Component Diracâ€“Kohnâ€“Sham Program. Journal of Chemical Theory and Computation, 2014, 10, 3766-3776.	5.3	21
63	Ligand Effect on Bonding in Gold(III) Carbonyl Complexes. Inorganic Chemistry, 2018, 57, 6161-6175.	4.0	21
64	Oligothiophenes Nanoâ€organized on a Cyclotetrasiloxane Scaffold as a Model of a Silicaâ€Bound Monolayer: Evidence for Intramolecular Excimer Formation. Chemistry - A European Journal, 2009, 15, 12791-12798.	3.3	20
65	Interaction of O₂ with CH₄, CF₄, and CCl₄ by Molecular Beam Scattering Experiments and Theoretical Calculations. Journal of Physical Chemistry A, 2016, 120, 5197-5207.	2.5	20
66	Computational strategies for a four-component Diracâ€“Kohnâ€“Sham program: Implementation and first applications. Journal of Chemical Physics, 2005, 122, 184109.	3.0	19
67	Poisson-transformed density fitting in relativistic four-component Diracâ€“Kohnâ€“Sham theory. Journal of Chemical Physics, 2008, 128, 124108.	3.0	19
68	The ligand effect on the oxidative addition of dioxygen to gold(<scp>i</scp>)â€“hydride complexes. Dalton Transactions, 2017, 46, 11679-11690.	3.3	19
69	Cyclization of 2-Alkynyldimethylaniline on Gold(I) Cationic and Neutral Complexes. Organometallics, 2016, 35, 595-604.	2.3	18
70	Cationic Gold(I) Diarylallenylidene Complexes: Bonding Features and Ligand Effects. ChemPhysChem, 2019, 20, 1671-1679.	2.1	18
71	Alkyne Activation with Gold(III) Complexes: A Quantitative Assessment of the Ligand Effect by Charge-Displacement Analysis. Inorganic Chemistry, 2019, 58, 3115-3129.	4.0	18
72	Diffusion NMR measurements on cationic linear gold(I) complexes. Polyhedron, 2015, 92, 52-59.	2.2	17

#	Article	IF	Citations
73	Goldâ€“superheavy-element interaction in diatomics and cluster adducts: A combined four-component Dirac-Kohn-Sham/charge-displacement study. Journal of Chemical Physics, 2015, 143, 024307.	3.0	17
74	The Chemical Bond and sâ€“d Hybridization in Coinage Metal(I) Cyanides. Inorganic Chemistry, 2019, 58, 11716-11729.	4.0	17
75	PyBERTHART: A Relativistic Real-Time Four-Component TDDFT Implementation Using Prototyping Techniques Based on Python. Journal of Chemical Theory and Computation, 2020, 16, 2410-2429.	5.3	17
76	Charge Displacement Analysisâ€”A Tool to Theoretically Characterize the Charge Transfer Contribution of Halogen Bonds. Molecules, 2020, 25, 300.	3.8	17
77	Leading Interaction Components in the Structure and Reactivity of Noble Gases Compounds. Molecules, 2020, 25, 2367.	3.8	17
78	The gold(<scp>iii</scp>)â€“CO bond: a missing piece in the gold carbonyl complex landscape. Chemical Communications, 2017, 53, 1603-1606.	4.1	16
79	Cooperative role of halogen and hydrogen bonding in the stabilization of water adducts with apolar molecules. New Journal of Chemistry, 2018, 42, 10603-10614.	2.8	16
80	Intermolecular Interaction in the NH₃â€“H₂ and H₂Oâ€“H₂ Complexes by Molecular Beam Scattering Experiments: The Role of Charge Transfer. Journal of Physical Chemistry A, 2013, 117, 12601-12607.	2.5	15
81	Intermolecular Interaction in the H₂Sâ€“H₂ Complex: Molecular Beam Scattering Experiments and Ab-Inito Calculations. Journal of Physical Chemistry A, 2014, 118, 6440-6450.	2.5	15
82	Parallelization of a relativistic DFT code. Future Generation Computer Systems, 2004, 20, 739-747.	7.5	14
83	An indirect approach to the determination of the nuclear quadrupole moment by four-component relativistic DFT in molecular calculations. Chemical Physics Letters, 2007, 442, 233-237.	2.6	14
84	Merging of E2 and E1cb Reaction Mechanisms: A Combined Theoretical and Experimental Study. European Journal of Organic Chemistry, 2009, 2009, 5501-5504.	2.4	13
85	Spinâ€“orbit coupling is the key to unraveling intriguing features of the halogen bond involving astatine. Physical Chemistry Chemical Physics, 2020, 22, 1897-1910.	2.8	13
86	On the role of charge transfer in the stabilization of weakly bound complexes involving water and hydrogen sulphide molecules. Chemical Physics, 2012, 398, 176-185.	1.9	12
87	Understanding the Reactivity of Mn-Oxo Porphyrins for Substrate Hydroxylation: Theoretical Predictions and Experimental Evidence Reconciled. Inorganic Chemistry, 2019, 58, 7345-7356.	4.0	12
88	Environmental Effects with Frozen-Density Embedding in Real-Time Time-Dependent Density Functional Theory Using Localized Basis Functions. Journal of Chemical Theory and Computation, 2020, 16, 5695-5711.	5.3	12
89	What Singles out Aluminyl Anions? A Comparative Computational Study of the Carbon Dioxide Insertion Reaction in Goldâ€“Aluminyl, â^'Gallyl, and â^'Indyl Complexes. Inorganic Chemistry, 2022, 61, 1704-1716.	4.0	11
90	Modelling Charge Transfer in Weak Chemical Bonds: Insights from the Chemistry of Helium. ChemPhysChem, 2018, 19, 1476-1485.	2.1	10

#	Article	IF	Citations
91	Spinâ€Forbidden Reactivity of Transition Metal Oxo Species: Exploring the Potential Energy Surfaces. Chemistry - A European Journal, 2020, 26, 3080-3089.	3.3	10
92	Hydration of alkynes catalyzed by [Au(X)(L)(ppy)]X in the green solvent Î³-valerolactone under acid-free conditions: the importance of the pre-equilibrium step. Catalysis Science and Technology, 2020, 10, 7757-7767.	4.1	10
93	Gold-Aluminyl and Gold-Diarylboryl Complexes: Bonding and Reactivity with Carbon Dioxide. Inorganic Chemistry, 2022, 61, 7327-7337.	4.0	10
94	Anab initioelectronic density study of the CH₄â€“Ar, CH₄â€“Xe, CH₄â€“H₂O and CH₄â€“H₂S complexes: insights into the nature of the intermolecular interaction. Molecular Physics, 2015, 113, 3992-3999.	1.7	9
95	The nature of the lead-iodine bond in PbI2: A case study for the modelling of lead halide perovskites. Computational and Theoretical Chemistry, 2019, 1164, 112558.	2.5	9
96	Disentanglement of orthogonal hydrogen and halogen bonds via natural orbital for chemical valence: A charge displacement analysis. Journal of Computational Chemistry, 2020, 41, 1185-1193.	3.3	8
97	Unraveling differences in aluminyl and carbene coordination chemistry: bonding in gold complexes and reactivity with carbon dioxide. Chemical Science, 2022, 13, 4623-4634.	7.4	8
98	An <scp>ETSâ€NOCV</scp>â€based computational strategies for the characterization of concerted transition states involving <scp>CO₂</scp>. Journal of Computational Chemistry, 2022, 43, 717-727.	3.3	7
99	Ubiquity of cis-Halide â†' Isocyanide Direct Interligand Interaction in Organometallic Complexes. Inorganic Chemistry, 2018, 57, 14554-14563.	4.0	6
100	Spin-resolved charge displacement analysis as an intuitive tool for the evaluation of cPCET and HAT scenarios. Chemical Communications, 2020, 56, 12146-12149.	4.1	6
101	Halogen bond interaction: Role of hybridization and induction. Chemical Physics Letters, 2021, 771, 138522.	2.6	6
102	Tuning the Gold(I)â€Carbon Ïƒ Bond in Goldâ€Alkynyl Complexes through Structural Modifications of the NHC Ancillary Ligand: Effect on Spectroscopic Observables and Reactivity. European Journal of Inorganic Chemistry, 2021, 2021, 2401-2416.	2.0	5
103	DFT studies of Î²-elimination reactions in water solution with different bases: Theory vs experiment. Computational and Theoretical Chemistry, 2010, 940, 103-114.	1.5	4
104	Chemical Bond Mechanism for Helium Revealed by Electronic Excitation. Journal of Physical Chemistry A, 2019, 123, 6572-6577.	2.5	4
105	Selective Emergence of the Halogen Bond in Ground and Excited States of Nobleâ€Gasâ€“Chlorine Systems. Angewandte Chemie, 2019, 131, 4239-4243.	2.0	4
106	Turn-off and -on fluorescence switching of a self-assembled sensor for mercury(II) induced by anionic micelles. Dyes and Pigments, 2020, 173, 107959.	3.7	4
107	Fluorescent signal transduction in a self-assembled Hg2+ chemosensor tuned by various interactions in micellar aqueous environment. Journal of Photochemistry and Photobiology A: Chemistry, 2020, 389, 112276.	3.9	4
108	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

#	Article	IF	Citations
109	The mechanism of the gold(<scp>i</scp>)-catalyzed Meyerâ€“Schuster rearrangement of 1-phenyl-2-propyn-1-ol via 4-endo-dig cyclization. Dalton Transactions, 2021, 50, 5154-5160.	3.3	4
110	Monitoring of the Pre-Equilibrium Step in the Alkyne Hydration Reaction Catalyzed by Au(III) Complexes: A Computational Study Based on Experimental Evidences. Molecules, 2021, 26, 2445.	3.8	4
111	Efficient Computation of Geometries for Gold Complexes. ChemPhysChem, 2021, 22, 1262-1268.	2.1	4
112	Experimental and theoretical investigation of the cycloisomerization of N-propargylcarboxamide catalyzed by NHC-Au-X in green solvents. Inorganica Chimica Acta, 2021, 522, 120372.	2.4	4
113	Relativistic quantum chemistry involving heavy atoms. Rendiconti Lincei, 2018, 29, 209-217.	2.2	3
114	Spectroscopic/Bond Property Relationship in Group 11 Dihydrides via Relativistic Four-Component Methods. Journal of Physical Chemistry A, 2020, 124, 10565-10579.	2.5	3
115	CHAPTER 26. Role of Ion Pairing in the Mechanisms of Au(i)-catalysed Reactions: Theory and Experiment. RSC Catalysis Series, 2019, , 564-578.	0.1	2
116	BERTHA and PyBERTHA: State of the Art for Full Four-Component Dirac-Kohn-Sham Calculations. Advances in Parallel Computing, 2020, , .	0.3	2
117	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
118	Ground and excited electronic states of AuH₂via detachment energies on AuH₂^{â^'} using state-of-the-art relativistic calculations. Physical Chemistry Chemical Physics, 2020, 22, 26742-26752.	2.8	1
119	Frontispiece: Spin-Forbidden Reactions: Adiabatic Transition States Using Spin-Orbit Coupled Density Functional Theory. Chemistry - A European Journal, 2018, 24, .	3.3	0
120	Donation and back-donation in cis- and trans-[(Î·5-C5H5)Fe(Î·1-CO)(Î¼-CO)]2 tautomers: Which relative is more generous? An ETS-NOCV bond analysis. Inorganica Chimica Acta, 2022, 536, 120897.	2.4	0