

Giuseppe Lanza

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Ligand Substituent, Anion, and Solvation Effects on Ion Pair Structure, Thermodynamic Stability, and Structural Mobility in σ -Constrained Geometry π -Olefin Polymerization Catalysts: An Ab Initio Quantum Chemical Investigation. <i>Journal of the American Chemical Society</i> , 2000, 122, 12764-12777.	13.7	140
2	Highly Electrophilic Olefin Polymerization Catalysts. Counteranion and Solvent Effects on Constrained Geometry Catalyst Ion Pair Structure and Reactivity. <i>Journal of the American Chemical Society</i> , 1998, 120, 8257-8258.	13.7	112
3	Energetic, Structural, and Dynamic Aspects of Ethylene Polymerization Mediated by Homogeneous Single-Site σ -Constrained Geometry Catalysts in the Presence of Cocatalyst and Solvation: An Investigation at the ab Initio Quantum Chemical Level. <i>Organometallics</i> , 2002, 21, 5594-5612.	2.3	109
4	Energetics and Mechanism of Organolanthanide-Mediated Aminoalkene Hydroamination/Cyclization. A Density Functional Theory Analysis. <i>Organometallics</i> , 2004, 23, 4097-4104.	2.3	109
5	Metal-Ligand Bonding and Bonding Energetics in Zerovalent Lanthanide, Group 3, Group 4, and Group 6 Bis(arene) Sandwich Complexes. A Combined Solution Thermochemical and ab Initio Quantum Chemical Investigation. <i>Journal of the American Chemical Society</i> , 1996, 118, 627-635.	13.7	80
6	Conformational Study and Hydrogen Bonds Detection on Elastin-Related Polypeptides Using X-ray Photoelectron Spectroscopy. <i>Biomacromolecules</i> , 2005, 6, 1299-1309.	5.4	63
7	Palladium(II)/Copper Halide/Solvent Combination for Selective Intramolecular Domino Reactions of Indolecarboxylic Acid Allylamides: An Unprecedented Arylation/Esterification Sequence. <i>Advanced Synthesis and Catalysis</i> , 2012, 354, 159-170.	4.3	59
8	Metal and Ancillary Ligand Structural Effects on Ethylene Insertion Processes at Cationic Group 4 Centers. A Systematic, Comparative Quantum Chemical Investigation at Various ab Initio Levels. <i>Organometallics</i> , 2001, 20, 4006-4017.	2.3	55
9	Charge Distribution and Second-Order Nonlinear Optical Response of Charged Centrosymmetric Chromophore Aggregates. An ab Initio Electronic Structure Study of <i>p</i> -Nitroaniline Dimers. <i>Journal of the American Chemical Society</i> , 1997, 119, 3003-3006.	13.7	48
10	Absolute Metal-Ligand σ Bond Enthalpies in Group 4 Metallocenes. A Thermochemical, Structural, Photoelectron Spectroscopic, and ab Initio Quantum Chemical Investigation. <i>Journal of the American Chemical Society</i> , 1999, 121, 355-366.	13.7	47
11	Removal of heavy metal ions from wastewaters using dendrimer-functionalized multi-walled carbon nanotubes. <i>Environmental Science and Pollution Research</i> , 2017, 24, 14735-14747.	5.3	45
12	A relativistic effective core potential ab initio study of molecular geometries and vibrational frequencies of lanthanide trihalides LnX ₃ (Ln = Gd, Lu; X = F, Cl). <i>Chemical Physics Letters</i> , 1996, 255, 341-346.	2.6	40
13	Energetics of Metal-Ligand Multiple Bonds. A Combined Solution Thermochemical and ab Initio Quantum Chemical Study of MO Bonding in Group 6 Metallocene Oxo Complexes. <i>Journal of the American Chemical Society</i> , 1998, 120, 3111-3122.	13.7	38
14	Equilibrium geometries and harmonic vibrational frequencies of lanthanum trihalides LaX ₃ (X \rightarrow F, Cl). A relativistic effective core potential ab initio MO study. <i>Chemical Physics Letters</i> , 1993, 214, 598-602.	2.6	36
15	Electronic Structure of Bis(2,4-pentanedionato-O,O η^2)oxovanadium(IV). A Photoelectron Spectroscopy, Electronic Spectroscopy, and ab Initio Molecular Orbital Study. <i>Inorganic Chemistry</i> , 1996, 35, 3885-3890.	4.0	31
16	Oxazole-Based Compounds As Anticancer Agents. <i>Current Medicinal Chemistry</i> , 2020, 26, 7337-7371.	2.4	30
17	Quasilinear Molecule par Excellence, SrCl ₂ : Structure from High-Temperature Gas-Phase Electron Diffraction and Quantum-Chemical Calculations of Computed Structures of SrCl ₂ ...Argon Complexes. <i>Chemistry - A European Journal</i> , 2006, 12, 8345-8357.	3.3	27
18	Ultra-short pulse laser ablation of Al ₇₀ Cu ₂₀ Fe ₁₀ alloy: Nanoparticles generation and thin films deposition. <i>Thin Solid Films</i> , 2009, 517, 1880-1886.	1.8	27

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19	Theoretical modeling of "constrained geometry catalysts" beyond the naked cation approach. Topics in Catalysis, 1999, 7, 45-60.	2.8	25
20	Electronic Structure, Molecular Geometry, and Bonding Energetics in Zerovalent Yttrium and Gadolinium Bis(arene) Sandwich Complexes. A Theoretical ab Initio Study. Organometallics, 1996, 15, 3985-3989.	2.3	24
21	Theoretical Study of the Molecular Properties of Cerium Trihalides and Tetrahalides CeX _n (n = 3, 4; X =) Tj ETQq1 1 0,784314,rgBT /O	2.5	24
22	On the effect of 4f electrons on the structural characteristics of lanthanide trihalides: Computational and electron diffraction study of dysprosium trichloride. Journal of Chemical Physics, 2008, 128, 074301.	3.0	24
23	Synthesis of spiro[isoindeole-1,5-isoaxazolidin]-3(2 <i>H</i>)-ones as potential inhibitors of the MDM2-p53 interaction. Beilstein Journal of Organic Chemistry, 2016, 12, 2793-2807.	2.2	23
24	Geometries and energies of small Gen (n= 2-6) clusters: an ab initio molecular orbital study. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 2961-2967.	1.7	22
25	Electronic Structure and Photoelectron Spectroscopy of the Monomeric Uranium(III) Alkyl [1.5-(CH ₃) ₅ C ₅] ₂ UCH[Si(CH ₃) ₃] ₂ . Organometallics, 1996, 15, 205-208.	2.3	22
26	Synthesis and biological activity of new arenediene-linked isoxazolidines. Bioorganic and Medicinal Chemistry, 2014, 22, 3379-3385.	3.0	22
27	Photoelectron Spectroscopy of f-Element Organometallic Complexes. 12. A Comparative Investigation of the Electronic Structure of Lanthanide Bis(polymethylcyclopentadienyl)hydrocarbyl Complexes by Relativistic ab Initio and DV-X.alpha. Calculations and Gas-Phase UV Photoelectron Spectroscopy. Organometallics, 1994, 13, 3810-3815.	2.3	21
28	Interfacial water at the trialanine hydrophilic surface: a DFT electronic structure and bottom-up investigation. Physical Chemistry Chemical Physics, 2015, 17, 17101-17111.	2.8	21
29	Growth of epitaxial TlBaCaCuO a-axis oriented films on LaAlO ₃ buffer layers grown on SrTiO ₃ (100) substrates. Journal of Alloys and Compounds, 1997, 251, 314-317.	5.5	19
30	Effect of Ba-Ca-Cu precursor matrix on the formation and properties of superconducting Tl ₂ Ba ₂ Ca _n -1Cu _n O _x films A combined metalorganic chemical vapour deposition and thallium vapour diffusion approach. Journal of Alloys and Compounds, 1997, 251, 332-336.	5.5	19
31	Ab Initio MP2 and Density Functional Theory Computational Study of AcAlaNH ₂ Peptide Hydration: A Bottom-Up Approach. ChemPhysChem, 2014, 15, 2785-2793.	2.1	18
32	Combined effects of solvation and aggregation propensity on the final supramolecular structures adopted by hydrophobic, glycine-rich, elastin-like polypeptides. Biopolymers, 2013, 99, 292-313.	2.4	16
33	1,2,4-Oxadiazole-5-ones as analogues of tamoxifen: synthesis and biological evaluation. Organic and Biomolecular Chemistry, 2019, 17, 4892-4905.	2.8	16
34	Competitive Formation of Enaminones and Amino-2(5 <i>H</i>)-furanones from the Isoxazolidine System: A Combined Synthetic and Quantum Chemical Study. European Journal of Organic Chemistry, 2010, 2010, 5897-5905.	2.4	15
35	Photoelectron spectroscopy of f element organometallic complexes. 11. An investigation of the electronic structure of some tris(.eta.5-cyclopentadienyl)thorium(IV) and -uranium(IV) complexes by relativistic effect core potential ab initio calculations and gas-phase UV photoelectron spectroscopy. The Journal of Physical Chemistry, 1993, 97, 11673-11676.	2.9	14
36	Theoretical Study of Anharmonic and Matrix Effects on the Molecular Structure and Vibrational Frequencies of GdF ₃ and GdCl ₃ . ChemPhysChem, 2004, 5, 120-123.	2.1	14

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37	Anharmonic, Temperature, and Matrix Effects on the Molecular Structure and Vibrational Frequencies of Lanthanide Trihalides LnX ₃ (Ln = La, Lu; X = F, Cl). <i>Journal of Physical Chemistry A</i> , 2005, 109, 2127-2138.	2.5	13
38	Effects of Hydration on the Zwitterion Trialanine Conformation by Electronic Structure Theory. <i>Journal of Physical Chemistry B</i> , 2016, 120, 11705-11719.	2.6	11
39	The High Selectivity of the Cp ₂ ZrHCl Reducing Agent for Imides: A Combined Experimental and Theoretical Study on ¹³ C-Lactam and Isoxazolidinone Derivatives. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 95-104.	2.4	9
40	Comprehensive and Accurate Ab Initio Energy Surface of Simple Alanine Peptides. <i>ChemPhysChem</i> , 2013, 14, 3284-3293.	2.1	9
41	Ab Initio Study on Spectroscopic Properties of GdF ₃ and GdCl ₃ . <i>Journal of Physical Chemistry A</i> , 2004, 108, 4949-4960.	2.5	8
42	How an Inert Gas Matrix Can Modify the Molecular Properties of Lanthanide Trifluoride. <i>ChemPhysChem</i> , 2009, 10, 507-511.	2.1	6
43	On the Stability of Polyalanine Secondary Structures: The Role of the Polyproline II Helix. <i>ChemPhysChem</i> , 2011, 12, 2724-2727.	2.1	6
44	Quantum Mechanics Approach to Hydration Energies and Structures of Alanine and Dialanine. <i>ChemPhysChem</i> , 2017, 18, 1586-1596.	2.1	6
45	The water molecule arrangement over the side chain of some aliphatic amino acids: A quantum chemical and bottom-up investigation. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26161.	2.0	6
46	Photoelectron spectroscopy of f-element organometallic complexes. 10. Investigation of the electronic structure and geometry of bis(eta-5-pentamethylcyclopentadienyl)phosphathoracyclobutane by relativistic ab initio, multipolar DV-X.alpha. calculations and gas-phase UV photoelectron spectroscopy. <i>Organometallics</i> , 1993, 12, 3326-3332.	2.3	5
47	Ab initio MO study of the molecular structure, vibrational frequencies and bond dissociation energy of bis(2,4-pentanedionato-O,O'-eta ²)oxovanadium(IV). <i>Journal of the Chemical Society, Faraday Transactions</i> , 1995, 91, 2709-2714.	1.7	5
48	Molecular properties of a representative glycine-rich sequence of elastin "BocVGGVGOEt: A combined FTIR experimental and quantum chemical investigation. <i>Computational and Theoretical Chemistry</i> , 2007, 812, 25-37.	1.5	5
49	Quantum Mechanics Study on Hydrophilic and Hydrophobic Interactions in the Trivalent "Water System. <i>Journal of Physical Chemistry B</i> , 2018, 122, 4289-4298.	2.6	5
50	5-(3-Phosphonated 1H-1,2,3-triazol-4-yl)isoxazolidines: synthesis, DFT studies and biological properties. <i>Arkivoc</i> , 2015, 2015, 253-269.	0.5	4
51	A theoretical study on the LaF ₃ molecule embedded in argon matrix. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 376-386.	2.0	3
52	Peptide Hydration Phenomena through a Combined Quantum Chemical and Bottom-Up Approach. <i>Zeitschrift Fur Physikalische Chemie</i> , 2016, 230, 1373-1393.	2.8	3
53	On the size, shape and energetics of the hydration shell around alkanes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 24852-24865.	2.8	3
54	Formation of 3-Aminofuran-2-(5H)-ones and 3-Amino-1H-pyrrole-2,5-diones by Rearrangement of Isoxazolidines. <i>Synlett</i> , 2011, 2011, 245-248.	1.8	2

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55	Ab initio Study on Spectroscopic Properties of GdF ₃ and GdCl ₃ . ChemInform, 2004, 35, no.	0.0	0