

Ignazio L Fragala

List of Publications by Year in descending order

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96
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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 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	Anchoring Molecular Magnets on the Si(100) Surface. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 4081-4084.	13.8	101
6	Engineering of molecular architectures of β^2 -diketonate precursors toward new advanced materials. <i>Coordination Chemistry Reviews</i> , 2007, 251, 1931-1950.	18.8	91
7	Surface structural-chemical characterization of a single-site d ⁰ heterogeneous arene hydrogenation catalyst having 100% active sites. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 413-418.	7.1	87
8	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
9	Organolanthanide-Catalyzed Hydroamination/Cyclization Reactions of Aminoalkynes. Computational Investigation of Mechanism, Lanthanide Identity, and Substituent Effects for a Very Exothermic C ^N Bond-Forming Process. <i>Organometallics</i> , 2006, 25, 5533-5539.	2.3	80
10	A novel route to the second-generation alkaline-earth metal precursors for metal-organic chemical vapour deposition: one-step synthesis of M(hfa) ₂ -tetraglyme (M=Ba, Sr, Ca and Th, U, Pu, Np, Pu, Am, Cm, Bk, Cf, Fm, Md, No, Lr) (Hf=1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100).	13.5	74
11	Energetics and Mechanism of Organolanthanide-Mediated Phosphinoalkene Hydrophosphination/Cyclization. A Density Functional Theory Analysis. <i>Organometallics</i> , 2005, 24, 4995-5003.	2.3	71
12	Photochemical Mechanism of the Formation of Nanometer-Sized Copper by UV Irradiation of Ethanol Bis(2,4-pentandionato)copper(II) Solutions. <i>Chemistry of Materials</i> , 2004, 16, 1260-1266.	6.7	68
13	Lanthanide second-generation precursors for MOCVD applications: Effects of the metal ionic radius and polyether length on coordination spheres and mass-transport properties. <i>Coordination Chemistry Reviews</i> , 2006, 250, 1605-1620.	18.8	68
14	Free-Standing Copper(II) Oxide Nanotube Arrays through an MOCVD Template Process. <i>Chemistry of Materials</i> , 2004, 16, 5559-5561.	6.7	67
15	Proximity and Cooperativity Effects in Binuclear d ⁰ Olefin Polymerization Catalysis. Theoretical Analysis of Structure and Reaction Mechanism. <i>Journal of the American Chemical Society</i> , 2009, 131, 3974-3984.	13.7	66
16	Links Between Single-Site Heterogeneous and Homogeneous Catalysis. DFT Analysis of Pathways for Organozirconium Catalyst Chemisorptive Activation and Olefin Polymerization on γ -Alumina. <i>Journal of the American Chemical Society</i> , 2008, 130, 16533-16546.	13.7	58
17	Molecular Recognition on a Cavitand-Functionalized Silicon Surface. <i>Journal of the American Chemical Society</i> , 2009, 131, 7447-7455.	13.7	58
18	Synthesis, Characterization, and Mass-Transport Properties of Two Novel Gadolinium(III) Hexafluoroacetylacetonate Polyether Adducts: A Promising Precursors for MOCVD of GdF ₃ Films. <i>Chemistry of Materials</i> , 1996, 8, 1292-1297.	6.7	55

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19	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
20	Selective monitoring of parts per million levels of CO by covalently immobilized metal complexes on glass. <i>Chemical Communications</i> , 2008, , 2900.	4.1	55
21	Fluorinated β^2 -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. <i>Journal of the American Chemical Society</i> , 2010, 132, 4966-4970.	13.7	55
22	New Thermally Stable and Highly Volatile Precursors for Lanthanum MOCVD: Synthesis and Characterization of Lanthanum β^2 -Diketonate Glyme Complexes. <i>Inorganic Chemistry</i> , 1995, 34, 6233-6234.	4.0	54
23	Is There a ZnO Face Stable to Atomic Hydrogen?. <i>Advanced Materials</i> , 2009, 21, 1700-1706.	21.0	53
24	A single photochemical route for the formation of both copper nanoparticles and patterned nanostructured films. <i>Journal of Materials Chemistry</i> , 2003, 13, 2409-2411.	6.7	52
25	Synthesis, Characterization, Crystal Structure and Mass Transport Properties of Lanthanum β^2 -Diketonate Glyme Complexes, Volatile Precursors for Metal-Organic Chemical Vapor Deposition Applications. <i>Chemistry of Materials</i> , 1998, 10, 3434-3444.	6.7	51
26	Dielectric properties of Pr ₂ O ₃ high-k films grown by metalorganic chemical vapor deposition on silicon. <i>Applied Physics Letters</i> , 2003, 83, 129-131.	3.3	51
27	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
28	Site-Specific Anchoring of Tetrairon(III) Single Molecule Magnets on Functionalized Si(100) Surfaces. <i>Chemistry of Materials</i> , 2008, 20, 2405-2411.	6.7	47
29	MOCVD Template Approach to the Fabrication of Free-Standing Nickel(II) Oxide Nanotube Arrays: Structural, Morphological, and Optical Properties Characterization. <i>Journal of Physical Chemistry C</i> , 2007, 111, 3211-3215.	3.1	46
30	Photoelectron spectra of bis-cyclopentadienyl metal dihalides. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 1980, 18, 61-73.	1.7	44
31	Grafting Cavitands on the Si(100) Surface. <i>Langmuir</i> , 2006, 22, 11126-11133.	3.5	41
32	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
33	A Novel Diamine Adduct of Zinc Bis(2-thenoyl-trifluoroacetate) as a Promising Precursor for MOCVD of Zinc Oxide Films. <i>Inorganic Chemistry</i> , 2005, 44, 9684-9689.	4.0	39
34	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
35	Equilibrium geometries and harmonic vibrational frequencies of lanthanum trihalides LaX ₃ (X = F, Cl). A relativistic effective core potential ab initio MO study. <i>Chemical Physics Letters</i> , 1993, 214, 598-602.	2.6	36
36	Morphological and structural control of nanostructured <100> oriented CeO ₂ films grown on random metallic substrates. <i>Journal of Materials Chemistry</i> , 2005, 15, 2328.	6.7	36

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37	Self-Assembly of Nanosize Coordination Cages on Si(100) Surfaces. Chemistry - A European Journal, 2007, 13, 6891-6898.	3.3	36
38	Tunable luminescent properties of a europium complex monolayer. Journal of Materials Chemistry, 2009, 19, 3507.	6.7	36
39	Relationship between the Nanostructures and the Optical Properties of CeO ₂ Thin Films. Journal of Physical Chemistry B, 2004, 108, 16357-16364.	2.6	35
40	Heteroepitaxy of LaAlO ₃ (100) on SrTiO ₃ (100): In Situ Growth of LaAlO ₃ Thin Films by Metal-Organic Chemical Vapor Deposition from a Liquid Single Source. Chemistry of Materials, 1998, 10, 3765-3768.	6.7	33
41	Metal-Organic Chemical Vapor Deposition of CeO ₂ @ 100° Oriented Films on No-Rolled Hastelloy C276. Chemistry of Materials, 2001, 13, 4402-4404.	6.7	33
42	Heteroepitaxial Growth of Nanostructured Cerium Dioxide Thin Films by MOCVD on a (001) TiO ₂ Substrate. Chemistry of Materials, 2003, 15, 1434-1440.	6.7	33
43	Calcium Copper-Titanate Thin Film Growth: Tailoring of the Operational Conditions through Nanocharacterization and Substrate Nature Effects. Journal of Physical Chemistry B, 2006, 110, 17460-17467.	2.6	33
44	Stereochemical Control Mechanisms in Propylene Polymerization Mediated by C ₁ -Symmetric CGC Titanium Catalyst Centers. Journal of the American Chemical Society, 2007, 129, 7327-7338.	13.7	33
45	Breakdown kinetics of Pr ₂ O ₃ films by conductive-atomic force microscopy. Applied Physics Letters, 2005, 87, 231913.	3.3	32
46	Synthesis, characterization and application of Ni(tta) ₂ ·tmeda to MOCVD of nickel oxide thin films. Dalton Transactions, 2006, , 1101-1106.	3.3	31
47	Synthesis, characterization and crystal structure of a new thermally stable and volatile precursor [bis(1,1,1,2,2,3,3,7,7,8,8,9,9-tetradecafluorononane-4,6-dionato) ₂ tetraglyme]barium(II) for MOCVD application. Journal of Materials Chemistry, 1994, 4, 1061-1066.	6.7	29
48	Recent Advances in Characterization of CaCu ₃ Ti ₄ O ₁₂ Thin Films by Spectroscopic Ellipsometric Metrology. Journal of the American Chemical Society, 2005, 127, 13772-13773.	13.7	28
49	MOCVD of CeF ₃ films on Si(100) substrates: synthesis, characterization and luminescence spectroscopy. Journal of Materials Chemistry, 2002, 12, 2816-2819.	6.7	27
50	Density Control of Dodecamanganese Clusters Anchored on Silicon(100). Chemistry - A European Journal, 2006, 12, 3558-3566.	3.3	26
51	Theoretical modeling of ϵ -constrained geometry catalysts—beyond the naked cation approach. Topics in Catalysis, 1999, 7, 45-60.	2.8	25
52	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
53	Theoretical Study of the Molecular Properties of Cerium Trihalides and Tetrahalides CeX _n (n = 3, 4; X = F, Cl, Br, I) <small>Tj ETQq1 1.0, 784314, rgBT / Over</small>	2.5	24
54	A volatile Pb(II) β -diketonate diglyme complex as a promising precursor for MOCVD of lead oxide films. Inorganica Chimica Acta, 2004, 357, 3927-3933.	2.4	24

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55	Atom-Efficient Carbon ¹⁸ Oxygen Bond Formation Processes. DFT Analysis of the Intramolecular Hydroalkoxylation/Cyclization of Alkynyl Alcohols Mediated by Lanthanide Catalysts. <i>Organometallics</i> , 2010, 29, 2004-2012.	2.3	23
56	Electronic Structure and Photoelectron Spectroscopy of the Monomeric Uranium(III) Alkyl [η -5-(CH ₃) ₅ C ₅] ₂ UCH[Si(CH ₃) ₃] ₂ â€¦â€¦. <i>Organometallics</i> , 1996, 15, 205-208.	2.3	22
57	MOCVD of Platinum (100) Films on Random Hastelloy C276. <i>Chemical Vapor Deposition</i> , 1999, 5, 59-61.	1.3	22
58	Chemical stability of CaCu ₃ Ti ₄ O ₁₂ thin films grown by MOCVD on different substrates. <i>Thin Solid Films</i> , 2007, 515, 6470-6473.	1.8	22
59	Synthesis, crystal structure and solid-state dynamics of the La(hfa) ₃ Â-Me(OCH ₂ CH ₂) ₄ OMe (Hhfaâ€¦=â€¦1,1,1,5,5,5-hexafluoropentane-2,4-dione) precursor for MOCVD applications. <i>Journal of the Chemical Society Dalton Transactions</i> , 1998, , 1509-1512.	1.1	19
60	Kinetic Study of MOCVD Fabrication of Copper(I) and Copper(II) Oxide Films. <i>Chemical Vapor Deposition</i> , 1999, 5, 21-27.	1.3	18
61	Multistep Anchoring Route of Luminescent (5-Amino-1,10-phenanthroline)tris(dibenzoylmethane)europium(III) on Si(100). <i>European Journal of Inorganic Chemistry</i> , 2010, 2010, 4121-4129.	2.0	17
62	Fabrication of polycrystalline LaAlO ₃ films on Si(100): An MOCVD application of the second-generation La(hfa) ₃ Â-diglyme precursor. <i>Chemical Vapor Deposition</i> , 1997, 3, 306-309.	1.3	16
63	Plasma-assisted metalorganic chemical vapor deposition growth of ZnO thin films. <i>Journal of Materials Research</i> , 2006, 21, 1632-1637.	2.6	16
64	Synthesis and characterization of La ₂ â€¦xBa _x CuO ₄ +Î thin film through a simple MOCVD approach. <i>Journal of Materials Chemistry</i> , 2005, 15, 4718.	6.7	15
65	Effects of high temperature annealing on MOCVD grown CaCu ₃ Ti ₄ O ₁₂ films on LaAlO ₃ substrates. <i>Surface and Coatings Technology</i> , 2007, 201, 9243-9247.	4.8	15
66	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. <i>The Journal of Physical Chemistry</i> , 1993, 97, 11673-11676.	2.9	14
67	Cathodoluminescence Investigation of Residual Stress in Er ³⁺ :YAlO ₃ Thin Films Grown on (110) SrTiO ₃ Substrate by Metal-Organic Chemical Vapor Deposition. <i>Journal of Physical Chemistry B</i> , 2006, 110, 23977-23981.	2.6	14
68	Covalent Functionalization of Silicon Surfaces with a Cavitand-Modified Salen. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 2124-2131.	2.0	14
69	Kinetics and Mechanisms of MOCVD Processes for the Fabrication of Sr-Containing Films From Sr(hfac) ₂ Tetraglyme Precursor. <i>Chemistry of Materials</i> , 2002, 14, 4307-4312.	6.7	12
70	A metal-organic chemical vapor deposition approach to double-sided Tl ₂ Ba ₂ Ca ₁ Cu ₂ O ₈ superconducting films on LaAlO ₃ (100) substrates. <i>Journal of Materials Chemistry</i> , 2002, 12, 3728-3732.	6.7	12
71	Effects of deposition temperature on the microstructural and electrical properties of praseodymium oxide-based films. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2005, 118, 117-121.	3.5	11
72	MOCVD Growth, Micro-Structural, and Superconducting Properties of a-Axis Oriented TlBaCaCuO Thin Films. <i>Chemistry of Materials</i> , 2004, 16, 608-613.	6.7	10

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73	Fascinating Role of the Number of f Electrons in Dipolar and Octupolar Contributions to Quadratic Hyperpolarizability of Trinuclear Lanthanides-Biscopper Schiff Base Complexes. <i>Inorganic Chemistry</i> , 2013, 52, 7550-7556.	4.0	10
74	Novel MOCVD approach to the low pressure in situ growth of TlBa ₂ CaCu ₂ O ₇ films. <i>Physica C: Superconductivity and Its Applications</i> , 2004, 408-410, 894-895.	1.2	9
75	In-situ Growth and Characterization of Highly Textured La _{0.9} Sr _{0.1} MnO ₃ Films on LaAlO ₃ (100) Substrates. <i>Chemical Vapor Deposition</i> , 2010, 16, 143-150.	1.3	9
76	Template-Free and Seedless Growth of Pt Nanocolumns: Imaging and Probing Their Nanoelectrical Properties. <i>ACS Nano</i> , 2007, 1, 183-190.	14.6	8
77	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
78	Ab initio MO study of the molecular structure, vibrational frequencies and bond dissociation energy of bis(2,4-pentanedionato-O,O ²⁻)oxovanadium(IV). <i>Journal of the Chemical Society, Faraday Transactions</i> , 1995, 91, 2709-2714.	1.7	5
79	Effects of the thermal annealing processes on praseodymium oxide based films grown on silicon substrates. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2005, 118, 192-196.	3.5	5
80	Comparison between First- and Second-Generation Praseodymium Precursors for the MOCVD Synthesis of Praseodymium Aluminate Thin Films. <i>Chemistry of Materials</i> , 2007, 19, 4442-4446.	6.7	5
81	Insight into Group 4 Metallocenium-Mediated Olefin Polymerization Reaction Coordinates Using a Metadynamics Approach. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3491-3497.	5.3	4
82	Photoelectron Spectroscopy of f-Element Organometallic Complexes. , 1985, , 327-360.		4
83	The Role of Intermolecular Interactions in Molecular Electronics. <i>Advances in Chemistry Series</i> , 1994, , 223-241.	0.6	3
84	Luminescent CeCl ₃ nanoparticles by Tris(1,1,1,5,5,5-hexafluoro-2,4-pentanedionato)cerium diglyme photolysis in chlorinated solvents. <i>Inorganica Chimica Acta</i> , 2006, 359, 4043-4052.	2.4	3
85	Tailoring nanostructure of ZnO thin films by plasma assisted and Au-catalyst assisted MOCVD. <i>Journal of Non-Crystalline Solids</i> , 2008, 354, 2821-2825.	3.1	3
86	XPS, FTIR-ATR, and AFM Structural Study of Silicon-Grafted Triol Monolayers for Controlled Anchoring of Single Molecule Magnets. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20696-20701.	3.1	2
87	MOCVD Growth of Rare Earth Oxides:The Case of the Praseodymium/Oxygen System. , 0, , 33-51.		1
88	Metal-organic chemical vapour deposition of Nd ₂ /3Cu ₃ Ti ₄ O ₁₂ films. <i>IOP Conference Series: Materials Science and Engineering</i> , 2010, 8, 012019.	0.6	1
89	Multifunctional Dy(hfa) ₃ glyme adducts: Synthesis and magnetic/luminescent behaviour. <i>Inorganica Chimica Acta</i> , 2022, 535, 120851.	2.4	1
90	Properties of Pr-based high k dielectric films obtained by Metal-Organic Chemical Vapor Deposition. <i>Materials Research Society Symposia Proceedings</i> , 2004, 811, 393.	0.1	0

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91	MOCVD Growth, Micro-Structural, and Superconducting Properties of a-Axis Oriented TlBaCaCuO Thin Films.. ChemInform, 2004, 35, no.	0.0	0
92	Electron Transport and Dielectric Breakdown Kinetics in Pr ₂ O ₃ High K Films. Advances in Science and Technology, 2006, 46, 21.	0.2	0
93	MOCVD Route to the Fabrication of Calcium Copper Titanate (CaCu ₃ Ti ₄ O ₁₂) Thin Films. Advances in Science and Technology, 2006, 45, 1194-1199.	0.2	0