Victor L Cruz

List of Publications by Year
in descending order

47	1,077	331670	434195
papers	citations	21 h-index	31 g-index

49	49	49	1173
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Structure of Bacteriocin AS-48: From Soluble State to Membrane Bound State. Journal of Molecular Biology, 2003, 334, 541-549.	4.2	92
2	Nickel 2-Iminopyridine N-Oxide (PymNox) Complexes: Cationic Counterparts of Salicylaldiminate-Based Neutral Ethylene Polymerization Catalysts. Organometallics, 2008, 27, 4711-4723.	2.3	64
3	Structureâ^'Activity Relationship Study of the Metallocene Catalyst Activity in Ethylene Polymerization. Organometallics, 2005, 24, 5095-5102.	2.3	58
4	3D-QSAR as a Tool for Understanding and Improving Single-Site Polymerization Catalysts. A Review. Organometallics, 2014, 33, 2944-2959.	2.3	56
5	3D-QSAR analysis of metallocene-based catalysts used in ethylene polymerisation. Polymer, 2004, 45, 2061-2072.	3.8	55
6	Theoretical Study on a Multicenter Model Based on Different Metal Oxidation States for the Bis(imino)pyridine Iron Catalysts in Ethylene Polymerization. Organometallics, 2009, 28, 5889-5895.	2.3	43
7	Bacteriocin AS-48 binding to model membranes and pore formation as revealed by coarse-grained simulations. Biochimica Et Biophysica Acta - Biomembranes, 2013, 1828, 2524-2531.	2.6	37
8	A theoretical study of the comonomer effect in the ethylene polymerization with zirconocene catalytic systems. Journal of Polymer Science Part A, 1998, 36, 1157-1167.	2.3	36
9	Surfaceâ€enhanced Raman spectra of dimethoate and omethoate. Journal of Raman Spectroscopy, 2011, 42, 980-985.	2.5	35
10	On the Nature of the Active Site in bis(imino)Pyridyl Iron, a Catalyst for Olefin Polymerization. Journal of Physical Chemistry C, 2008, 112, 5023-5028.	3.1	34
11	Water-Mediated Conformations of the Alanine Dipeptide as Revealed by Distributed Umbrella Sampling Simulations, Quantum Mechanics Based Calculations, and Experimental Data. Journal of Physical Chemistry B, 2011, 115, 4880-4886.	2.6	33
12	QSAR model for ethylene polymerisation catalysed by supported bis(imino)pyridine iron complexes. Polymer, 2007, 48, 7672-7678.	3.8	30
13	3D-QSAR study of ansa-metallocene catalytic behavior in ethylene polymerization. Polymer, 2007, 48, 4663-4674.	3.8	30
14	A computational study of iron-based Gibsonâ€"Brookhart catalysts for the copolymerisation of ethylene and 1-hexene. Polymer, 2002, 43, 3635-3645.	3.8	28
15	An experimental and computational evaluation of ethylene/styrene copolymerization with a homogeneous single-site titanium(IV)-constrained geometry catalyst. Journal of Polymer Science Part A, 2005, 43, 711-725.	2.3	28
16	Ab initio calculation of ethylene insertion in zirconocene catalyst systems: A comparative study between bridged and unbridged complexes. Polymer, 1996, 37, 1663-1667.	3.8	27
17	A theoretical study of ethyleneâ€"styrene copolymerization by using half-sandwich Cp-based titanium catalysts. Polymer, 2002, 43, 7017-7026.	3.8	27
18	Polymerization Activity Prediction of Zirconocene Single-Site Catalysts Using 3D Quantitative Structureâ€"Activity Relationship Modeling. Organometallics, 2012, 31, 1673-1679.	2.3	26

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19	Effect of a second ethylene molecule on the insertion of ethylene in zirconocene catalyst systems: A QM semiempirical study. Journal of Polymer Science Part A, 2000, 38, 571-582.	2.3	23
20	The unit cell expansion of branched polyethylene as detected by Raman spectroscopy: an experimental and simulation approach. Journal of Materials Science, 2007, 42, 1046-1049.	3.7	23
21	Ab initio study of hydrogenolysis as a chain transfer mechanism in olefin polymerization catalyzed by metallocenes. Polymer, 2000, 41, 6161-6169.	3.8	22
22	Copolymerization of ethylene and styrene by homogeneous metallocene catalysts. 1. Theoretical studies with rac-ethylenebis-(tetrahydroindenyl)MCl2 [M=Ti, Zr] systems. Polymer, 2003, 44, 295-306.	3.8	21
23	Ethylene/styrene copolymerisation by homogeneous metallocene catalysts: experimental and molecular simulations using rac-ethylenebis(tetrahydroindenyl)MCl2 [M=Ti,Zr] systems. Polymer, 2004, 45, 9029-9038.	3.8	21
24	Computational studies of the Brookhart's type catalysts for ethylene polymerisation. Part 2: ethylene insertion and chain transfer mechanisms. Polymer, 2003, 44, 2169-2176.	3.8	20
25	Ethylene-styrene copolymerization with constrained geometry catalysts: A density functional study. Journal of Chemical Physics, 2005, 122, 074901.	3.0	17
26	[1,2,3]Triazolo[1,5-a]pyridines. A theoretical (DFT) study of the ringâ€“chain isomerization. Tetrahedron, 2008, 64, 11150-11158.	1.9	17
27	DFT study of hydrogenolysis as a chain transfer mechanism in olefin polymerisation catalysed by nickel-diimine-type catalysts. Polymer, 2003, 44, 2177-2186.	3.8	16
28	Computer simulations of the early stages of crystal nucleation of linear and short chain branched polyethylene on carbon nanotubes. European Polymer Journal, 2014, 56, 194-204.	5.4	15
29	Diosgenone Synthesis, Anti-Malarial Activity and QSAR of Analogues of This Natural Product. Molecules, 2013, 18, 3356-3378.	3.8	14
30	Computational studies of the Brookhart's type catalysts for ethylene polymerization. 1. Effect of the active site conformations on the catalyst activities. Polymer, 2001, 42, 8019-8023.	3.8	12
31	Synthesis, characterization and catalytic behaviour of ansa-zirconocene complexes containing tetraphenylcyclopentadienyl rings: X-ray crystal structures of [Zr{Me2Si(Î·5-C5Ph4)(Î·5-C5H3R)}Cl2] (R=H,) Tj ETQq1 1 0.784314 rgBT /(	3.8	12
32	Assessment of the Intrinsic Conformational Preferences of Dipeptide Amino Acids in Aqueous Solution by Combined Umbrella Sampling/MBAR Statistics. A Comparison with Experimental Results. Journal of Physical Chemistry B, 2012, 116, 469-475.	2.6	11
33	Isomeric effect of the Et(H4Ind)2Zr(CH3)2 catalyst on the copolymerization of ethylene and styrene: A computational study. Journal of Polymer Science Part A, 2006, 44, 4752-4761.	2.3	10
34	A QM/MM study of the ethylene and styrene insertion process into the ion pair [Me2Si(C5Me4)(NtBu)Ti(CH2CH2CH3)]+[Î¼-Meâ€“Al(Me)2â€“(AlOMe)6Me]â^'. Polymer, 2006, 47, 883-896.	3.8	10
35	Leishmanicidal activity of withajardins and acnistins. An experimental and computational study. Tetrahedron, 2006, 62, 6822-6829.	1.9	9
36	Density functional study for the polymerization of ethylene monomer using a new nickel catalyst. Journal of Polymer Science Part A, 2010, 48, 1160-1165.	2.3	8

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37	Conformational flexibility of the ErbB2 ectodomain and trastuzumab antibody complex as revealed by molecular dynamics and principal component analysis. Journal of Molecular Modeling, 2013, 19, 1227-1236.	1.8	8
38	Simulation of homology models for the extracellular domains (ECD) of ErbB3, ErbB4 and the ErbB2â€“ErbB3 complex in their active conformations. Journal of Molecular Modeling, 2013, 19, 931-941.	1.8	8
39	Ab initio study of ethylene insertion into Mâ€“C bonds of alkylamidinates complexes of group IV ({Râ€²NCRNRâ€²} 2 MCH 3 + , M=Zr, Ti, R=H, Ph and Râ€²=H, SiMe 3). Polymer, 2001, 42, 7275-7284.	3.8	7
40	Exploring the dynamics and interaction of a full ErbB2 receptor and Trastuzumab-Fab antibody in a lipid bilayer model using Martini coarse-grained force field. Journal of Computer-Aided Molecular Design, 2014, 28, 1093-1107.	2.9	7
41	Dissimilar interaction of CB1/CB2 with lipid bilayers as revealed by molecular dynamics simulation. Physical Chemistry Chemical Physics, 2011, 13, 3660-3668.	2.8	6
42	Hydrodynamic and Electrophoretic Properties of Trastuzumab/HER2 Extracellular Domain Complexes as Revealed by Experimental Techniques and Computational Simulations. International Journal of Molecular Sciences, 2019, 20, 1076.	4.1	5
43	Proposed Polymerization Termination Mechanism for 3-R-Indenyl ansa-Zirconocenes (R =) Tj ETQq1 1 0.784314 rgBT /Overlock 7413-7415.	4.8	4
44	A Curtinâ€“Hammett mechanism for the copolymerization of ethylene and methyl acrylate monomer using a PymNox nickel catalyst as revealed by DFT computational studies. Journal of Molecular Modeling, 2012, 18, 515-523.	1.8	4
45	The Role of Key Amino Acids in the Antimicrobial Mechanism of a Bacteriocin Model Revealed by Molecular Simulations. Journal of Chemical Information and Modeling, 2021, 61, 6066-6078.	5.4	4
46	Conformational analysis of short polar side-chain amino-acids through umbrella sampling and DFT calculations. Journal of Molecular Modeling, 2016, 22, 273.	1.8	2
47	Protein-Protein and Protein-Membrane Interactions Regarding the Erbb2/Trastuzumab-Fab Complexes. A Coarse-Grained Molecular Dynamics Description. Biophysical Journal, 2014, 106, 666a-667a.	0.5	1