Victor L Cruz

List of Publications by Year
in descending order

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47 papers	1,077 citations	331538 21 h-index	434063 31 g-index
49 all docs	49 docs citations	49 times ranked	1173 citing authors

#	Article	IF	Citations
1	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.	2.5	4
2	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.	1.8	5
3	Conformational analysis of short polar side-chain amino-acids through umbrella sampling and DFT calculations. Journal of Molecular Modeling, 2016, 22, 273.	0.8	2
4	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.	2.6	15
5	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.	1.3	7
6	3D-QSAR as a Tool for Understanding and Improving Single-Site Polymerization Catalysts. A Review. Organometallics, 2014, 33, 2944-2959.	1.1	56
7	Protein-Protein and Protein-Membrane Interactions Regarding the Erbb2/Trastuzumab-Fab Complexes. A Coarse-Grained Molecular Dynamics Description. Biophysical Journal, 2014, 106, 666a-667a.	0.2	1
8	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.	0.8	8
9	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.	0.8	8
10	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.	1.4	37
11	Diosgenone Synthesis, Anti-Malarial Activity and QSAR of Analogues of This Natural Product. Molecules, 2013, 18, 3356-3378.	1.7	14
12	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.	1.2	11
13	Polymerization Activity Prediction of Zirconocene Single-Site Catalysts Using 3D Quantitative Structureâ€“Activity Relationship Modeling. Organometallics, 2012, 31, 1673-1679.	1.1	26
14	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.	0.8	4
15	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.	1.2	33
16	Dissimilar interaction of CB1/CB2 with lipid bilayers as revealed by molecular dynamics simulation. Physical Chemistry Chemical Physics, 2011, 13, 3660-3668.	1.3	6
17	Surfaceâ€enhanced Raman spectra of dimethoate and omethoate. Journal of Raman Spectroscopy, 2011, 42, 980-985.	1.2	35
18	Density functional study for the polymerization of ethylene monomer using a new nickel catalyst. Journal of Polymer Science Part A, 2010, 48, 1160-1165.	2.5	8

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19	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.	1.1	43
20	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 ETQq0 0 0 rgBT /Overlock	1.1	12
21	[1,2,3]Triazolo[1,5-a]pyridines. A theoretical (DFT) study of the ringâ€“chain isomerization. Tetrahedron, 2008, 64, 11150-11158.	1.0	17
22	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.	1.5	34
23	Nickel 2-Iminopyridine N-Oxide (PymNox) Complexes: Cationic Counterparts of Salicylaldiminate-Based Neutral Ethylene Polymerization Catalysts. Organometallics, 2008, 27, 4711-4723.	1.1	64
24	Proposed Polymerization Termination Mechanism for 3-R-Indenyl ansa-Zirconocenes (R =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 5 7413-7415.	2.2	4
25	QSAR model for ethylene polymerisation catalysed by supported bis(imino)pyridine iron complexes. Polymer, 2007, 48, 7672-7678.	1.8	30
26	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.	1.7	23
27	3D-QSAR study of ansa-metallocene catalytic behavior in ethylene polymerization. Polymer, 2007, 48, 4663-4674.	1.8	30
28	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.	2.5	10
29	Leishmanicidal activity of withajardins and acnistins. An experimental and computational study. Tetrahedron, 2006, 62, 6822-6829.	1.0	9
30	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.	1.8	10
31	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.	2.5	28
32	Ethylene-styrene copolymerization with constrained geometry catalysts: A density functional study. Journal of Chemical Physics, 2005, 122, 074901.	1.2	17
33	Structureâ^'Activity Relationship Study of the Metallocene Catalyst Activity in Ethylene Polymerization. Organometallics, 2005, 24, 5095-5102.	1.1	58
34	3D-QSAR analysis of metallocene-based catalysts used in ethylene polymerisation. Polymer, 2004, 45, 2061-2072.	1.8	55
35	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.	1.8	21
36	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.	1.8	21

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37	DFT study of hydrogenolysis as a chain transfer mechanism in olefin polymerisation catalysed by nickel-diimine-type catalysts. Polymer, 2003, 44, 2177-2186.	1.8	16
38	Computational studies of the Brookhart's type catalysts for ethylene polymerisation. Part 2: ethylene insertion and chain transfer mechanisms. Polymer, 2003, 44, 2169-2176.	1.8	20
39	Structure of Bacteriocin AS-48: From Soluble State to Membrane Bound State. Journal of Molecular Biology, 2003, 334, 541-549.	2.0	92
40	A computational study of iron-based Gibsonâ€“Brookhart catalysts for the copolymerisation of ethylene and 1-hexene. Polymer, 2002, 43, 3635-3645.	1.8	28
41	A theoretical study of ethyleneâ€“styrene copolymerization by using half-sandwich Cp-based titanium catalysts. Polymer, 2002, 43, 7017-7026.	1.8	27
42	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.	1.8	7
43	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.	1.8	12
44	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.	2.5	23
45	Ab initio study of hydrogenolysis as a chain transfer mechanism in olefin polymerization catalyzed by metallocenes. Polymer, 2000, 41, 6161-6169.	1.8	22
46	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.	2.5	36
47	Ab initio calculation of ethylene insertion in zirconocene catalyst systems: A comparative study between bridged and unbridged complexes. Polymer, 1996, 37, 1663-1667.	1.8	27