Javier Ramos

List of Publications by Year in descending order

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67 papers	1,468 citations	318942 23 h-index	406436 35 g-index
70 all docs	70 docs citations	70 times ranked	1790 citing authors

#	Article	IF	Citations
1	Melting Temperature Depression of Polymer Single Crystals: Application to the Eco-Design of Tie-Layers in Polyolefinic-Based Multilayered Films. Polymers, 2022, 14, 1622.	2.0	2
2	Revisiting Polymerâ€“Particle Interaction in PEO Solutions. Langmuir, 2021, 37, 3808-3816.	1.6	6
3	A computer simulation of the effect of temperature on melt chain dimensions of random short chain branched polyethylene. Polymer, 2021, 225, 123772.	1.8	1
4	Stereospecific Synthesis of Chiral Titanium Complexes Bearing a Bifunctionalized Cyclopentadienyl-Terpenoid Ligand Derived from Î±-Pinene. Organometallics, 2021, 40, 3076-3086.	1.1	1
5	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
6	Halogen bonding (HaB) in Eâ€“Iâ‹¯Xâ€“M systems: influence of the halogen donor on the HaB nature. CrystEngComm, 2020, 22, 870-877.	1.3	9
7	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
8	Predicting experimental results for polyethylene by computer simulation. European Polymer Journal, 2018, 99, 298-331.	2.6	47
9	Chiral Titanium(IV) Complexes Containing Polydentate Ligands Based on Î±-Pinene. Catalytic Activity in Sulfoxidation with Hydrogen Peroxide. Organometallics, 2018, 37, 3437-3449.	1.1	9
10	Thermophysical Properties of Homologous Tetracyanoborate-Based Ionic Liquids Using Experiments and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2017, 121, 4145-4157.	1.2	16
11	Molecular and hydrodynamic properties of human epidermal growth factor receptor HER2 extracellular domain and its homodimer: Experiments and multi-scale simulations. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 2406-2416.	1.1	7
12	Coarse-grained simulations on the crystallization, melting and annealing processes of short chain branched polyolefins. European Polymer Journal, 2016, 85, 478-488.	2.6	14
13	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
14	A new insight into the conformation and melt dynamics of hydrogenated polybutadiene as revealed by computer simulations. Soft Matter, 2016, 12, 3929-3936.	1.2	8
15	Molecular Dynamics Simulations for the Description of Experimental Molecular Conformation, Melt Dynamics, and Phase Transitions in Polyethylene. Macromolecules, 2015, 48, 5016-5027.	2.2	76
16	Monte Carlo simulations of structure and entanglements in polymer melts. Molecular Simulation, 2015, 41, 993-995.	0.9	2
17	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
18	Strong influence of branching on the early stage of nucleation and crystal formation of fast cooled ultralong n-alkanes as revealed by computer simulation. European Polymer Journal, 2014, 50, 190-199.	2.6	22

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19	Effect of short chain branching in molecular dimensions and Newtonian viscosity of ethylene/1-hexene copolymers: matching conformational and rheological experimental properties and atomistic simulations. Rheologica Acta, 2014, 53, 1-13.	1.1	17
20	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
21	3D-QSAR as a Tool for Understanding and Improving Single-Site Polymerization Catalysts. A Review. Organometallics, 2014, 33, 2944-2959.	1.1	56
22	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
23	Effect of high molar mass species on linear viscoelastic properties of polyethylene melts. European Polymer Journal, 2013, 49, 2748-2758.	2.6	8
24	Thermophysical Properties of the Ionic Liquids [EMIM][B(CN)₄] and [HMIM][B(CN)₄]. Journal of Physical Chemistry B, 2013, 117, 8512-8523.	1.2	39
25	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
26	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
27	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
28	Structure and entanglements in short chain branched polyolefin melts. AIP Conference Proceedings, 2013, , .	0.3	2
29	Monte Carlo Simulation of Short Chain Branched Polyolefins: Structure and Properties. Macromolecules, 2012, 45, 8453-8466.	2.2	25
30	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
31	Following the Crystallization Process of Polyethylene Single Chain by Molecular Dynamics: The Role of Lateral Chain Defects. Macromolecular Symposia, 2012, 312, 97-107.	0.4	17
32	Polymerization Activity Prediction of Zirconocene Single-Site Catalysts Using 3D Quantitative Structureâ€“Activity Relationship Modeling. Organometallics, 2012, 31, 1673-1679.	1.1	26
33	Structure, thermodynamic and transport properties of imidazolium-based bis(trifluoromethylsulfonyl)imide ionic liquids from molecular dynamics simulations. Molecular Physics, 2012, 110, 1139-1152.	0.8	23
34	Assessment of entanglement features and dynamics from atomistic simulations and experiments in linear and short chain branched polyolefins. Soft Matter, 2012, 8, 6256.	1.2	17
35	Development of a united-atom force field for 1-ethyl-3-methylimidazolium tetracyanoborate ionic liquid. Molecular Physics, 2012, 110, 1115-1126.	0.8	28
36	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

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37	Effect of molecular weight distribution on Newtonian viscosity of linear polyethylene. Rheologica Acta, 2012, 51, 81-87.	1.1	23
38	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
39	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
40	Computer modeling of the crystallization process of singleâ€chain ethylene/1â€hexene copolymers from dilute solutions. Journal of Polymer Science, Part B: Polymer Physics, 2011, 49, 421-430.	2.4	21
41	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
42	Molecular Modeling of Imidazolium-Based [Tf₂N^{â^'}] Ionic Liquids: Microscopic Structure, Thermodynamic and Dynamic Properties, and Segmental Dynamics. Journal of Physical Chemistry B, 2009, 113, 7211-7224.	1.2	92
43	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
44	Highly active ethylene/hydroxyl comonomers copolymerization using metallocene catalysts. Journal of Applied Polymer Science, 2008, 109, 1529-1534.	1.3	10
45	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 /O	1.8	32
46	Entanglement Relaxation Time in Polyethylene: Simulation versus Experimental Data. Macromolecules, 2008, 41, 2959-2962.	2.2	46
47	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
48	Isolobal Zwitterionic Niobium and Tantalum Imido and Zirconium Monocyclopentadienyl Complexes: Theoretical and Methyl Methacrylate Polymerization Studies. Organometallics, 2008, 27, 1417-1426.	1.1	22
49	Nickel 2-Iminopyridine N-Oxide (PymNox) Complexes: Cationic Counterparts of Salicylaldiminate-Based Neutral Ethylene Polymerization Catalysts. Organometallics, 2008, 27, 4711-4723.	1.1	64
50	Multi-scale Modeling of Structure, Dynamic and Thermodynamic Properties of Imidazolium-based Ionic Liquids: Ab initio DFT Calculations, Molecular Simulation and Equation of State Predictions. Oil and Gas Science and Technology, 2008, 63, 283-293.	1.4	20
51	Monte Carlo Simulation of Short Chain Branched Polyolefins in the Molten State. Macromolecules, 2007, 40, 9640-9650.	2.2	86
52	QSAR model for ethylene polymerisation catalysed by supported bis(imino)pyridine iron complexes. Polymer, 2007, 48, 7672-7678.	1.8	30
53	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
54	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

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55	Synthesis and properties of ethylene/styrene copolymers produced by metallocene catalysts. Journal of Applied Polymer Science, 2006, 102, 3420-3429.	1.3	10
56	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
57	Ethylene-styrene copolymerization with constrained geometry catalysts: A density functional study. Journal of Chemical Physics, 2005, 122, 074901.	1.2	17
58	Structureâ^'Activity Relationship Study of the Metallocene Catalyst Activity in Ethylene Polymerization. Organometallics, 2005, 24, 5095-5102.	1.1	58
59	3D-QSAR analysis of metallocene-based catalysts used in ethylene polymerisation. Polymer, 2004, 45, 2061-2072.	1.8	55
60	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
61	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
62	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
63	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
64	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
65	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
66	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
67	Ab initio study of hydrogenolysis as a chain transfer mechanism in olefin polymerization catalyzed by metallocenes. Polymer, 2000, 41, 6161-6169.	1.8	22