

Fernando Ruiperez

List of Publications by Year in descending order

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87
papers

3,011
citations

172457

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docs citations

89
times ranked

3470
citing authors

#	ARTICLE	IF	CITATIONS
1	Supramolecular-Enhanced Charge Transfer within Entangled Polyamide Chains as the Origin of the Universal Blue Fluorescence of Polymer Carbon Dots. <i>Journal of the American Chemical Society</i> , 2018, 140, 12862-12869.	13.7	242
2	Organocatalysed depolymerisation of PET in a fully sustainable cycle using thermally stable protic ionic salt. <i>Green Chemistry</i> , 2018, 20, 1205-1212.	9.0	182
3	Design of new disulfide-based organic compounds for the improvement of self-healing materials. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 1758-1770.	2.8	139
4	Transient mechanochromism in epoxy vitrimer composites containing aromatic disulfide crosslinks. <i>Journal of Materials Chemistry C</i> , 2016, 4, 6220-6223.	5.5	125
5	Selective Chemical Upcycling of Mixed Plastics Guided by a Thermally Stable Organocatalyst. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 6710-6717.	13.8	118
6	A natural orbital functional for multiconfigurational states. <i>Journal of Chemical Physics</i> , 2011, 134, 164102.	3.0	114
7	Pro-oxidant activity of aluminum: Promoting the Fenton reaction by reducing Fe(III) to Fe(II). <i>Journal of Inorganic Biochemistry</i> , 2012, 117, 118-123.	3.5	106
8	Aromatic diselenide crosslinkers to enhance the reprocessability and self-healing of polyurethane thermosets. <i>Polymer Chemistry</i> , 2017, 8, 3641-3646.	3.9	102
9	Reprocessable and recyclable crosslinked poly(urea-urethane)s based on dynamic amine/urea exchange. <i>Polymer</i> , 2018, 145, 127-136.	3.8	77
10	Room temperature synthesis of non-isocyanate polyurethanes (NIPUs) using highly reactive N-substituted 8-membered cyclic carbonates. <i>Polymer Chemistry</i> , 2016, 7, 2105-2111.	3.9	71
11	Synthesis of Functionalized Cyclic Carbonates through Commodity Polymer Upcycling. <i>ACS Macro Letters</i> , 2020, 9, 443-447.	4.8	69
12	Sustainable Poly(Ionic Liquids) for CO ₂ Capture Based on Deep Eutectic Monomers. <i>ACS Sustainable Chemistry and Engineering</i> , 2016, 4, 7200-7208.	6.7	68
13	Rational Study of DBU Salts for the CO ₂ Insertion into Epoxides for the Synthesis of Cyclic Carbonates. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 10633-10640.	6.7	68
14	Organocatalyzed Synthesis of Aliphatic Polyesters from Ethylene Brassylate: A Cheap and Renewable Macrolactone. <i>ACS Macro Letters</i> , 2014, 3, 849-853.	4.8	67
15	Pro-oxidant Activity of Aluminum: Stabilization of the Aluminum Superoxide Radical Ion. <i>Journal of Physical Chemistry A</i> , 2011, 115, 6717-6723.	2.5	60
16	Complete vs Restricted Active Space Perturbation Theory Calculation of the Cr ₂ Potential Energy Surface. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1640-1646.	5.3	53
17	Nanoporous amide networks based on tetraphenyladamantane for selective CO ₂ capture. <i>Journal of Materials Chemistry A</i> , 2016, 4, 8190-8197.	10.3	51
18	Innovative Poly(Ionic Liquid)s by the Polymerization of Deep Eutectic Monomers. <i>Macromolecular Rapid Communications</i> , 2016, 37, 1135-1142.	3.9	45

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19	An ab Initio Theoretical Study of the Electronic Structure of UO_2^{2+} and $[\text{UO}_2(\text{CO}_3)_3]^{5-}$. Journal of Physical Chemistry A, 2009, 113, 1420-1428.	2.5	42
20	Experimental and computational studies of ring-opening polymerization of ethylene brassylate macrolactone and copolymerization with ϵ -caprolactone and TBD-guanidine organic catalyst. Journal of Polymer Science Part A, 2015, 53, 552-561.	2.3	42
21	ALUMINIUM IN BIOLOGICAL ENVIRONMENTS: A COMPUTATIONAL APPROACH. Computational and Structural Biotechnology Journal, 2014, 9, e201403002.	4.1	41
22	Bond lengths of and states of hexahalides. Journal of Solid State Chemistry, 2005, 178, 464-469.	2.9	40
23	The natural orbital functional theory of the bonding in Cr_2 , Mo_2 and W_2 . Physical Chemistry Chemical Physics, 2013, 15, 2055-2062.	2.8	38
24	Communication: Chemical bonding in carbon dimer isovalent series from the natural orbital functional theory perspective. Journal of Chemical Physics, 2013, 138, 151102.	3.0	38
25	The role of non-covalent interactions in the self-healing mechanism of disulfide-based polymers. Physical Chemistry Chemical Physics, 2017, 19, 18461-18470.	2.8	37
26	Homolytic molecular dissociation in natural orbital functional theory. Physical Chemistry Chemical Physics, 2011, 13, 20129.	2.8	35
27	On the Termination Mechanism in the Radical Polymerization of Acrylates. Macromolecular Rapid Communications, 2016, 37, 1364-1368.	3.9	35
28	Diselenide Bonds as an Alternative to Outperform the Efficiency of Disulfides in Self-Healing Materials. Journal of Organic Chemistry, 2019, 84, 4200-4210.	3.2	32
29	Selective Organocatalytic Preparation of Trimethylene Carbonate from Oxetane and Carbon Dioxide. ACS Catalysis, 2020, 10, 5399-5404.	11.2	31
30	Quantum chemical study of $4f^1 5d$ excitations of trivalent lanthanide ions doped in the cubic elpasolite $\text{Cs}_2\text{NaYCl}_6$. Ce^{3+} to Tb^{3+} . Journal of Chemical Physics, 2005, 123, 244703.	3.0	30
31	Determining the effect of side reactions on product distributions in RAFT polymerization by MALDI-TOF MS. Polymer Chemistry, 2015, 6, 5437-5450.	3.9	29
32	Theoretical design of conjugated diradicaloids as singlet fission sensitizers: quinones and methylene derivatives. Physical Chemistry Chemical Physics, 2017, 19, 30227-30238.	2.8	29
33	Experimental Evidence Shedding Light on the Origin of the Reduction of Branching of Acrylates in ATRP. Macromolecules, 2014, 47, 964-972.	4.8	27
34	Dihydrogen bond interactions as a result of H_2 cleavage at Cu, Ag and Au centres. Physical Chemistry Chemical Physics, 2016, 18, 12810-12818.	2.8	26
35	Diradicals and Diradicaloids in Natural Orbital Functional Theory. ChemPhysChem, 2011, 12, 1061-1065.	2.1	25
36	Fullerene-Based Materials as Hole-Transporting/Electron-Blocking Layers: Applications in Perovskite Solar Cells. Chemistry - A European Journal, 2018, 24, 8524-8529.	3.3	25

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37	Effect of Regioisomerism on Processability and Mechanical Properties of Amine/Urea Exchange Based Poly(urea-urethane) Vitrimers. <i>ACS Applied Polymer Materials</i> , 2019, 1, 2472-2481.	4.4	25
38	Performance of PNOF5 Natural Orbital Functional for Radical Formation Reactions: Hydrogen Atom Abstraction and C-C and O-O Homolytic Bond Cleavage in Selected Molecules. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2646-2652.	5.3	24
39	Thioxanthone-Based Photobase Generators for the Synthesis of Polyurethanes via the Photopolymerization of Polyols and Polyisocyanates. <i>Macromolecules</i> , 2020, 53, 2069-2076.	4.8	24
40	The Electronic Structure of the Al ₃ ⁺ Anion: Is it Aromatic?. <i>Chemistry - A European Journal</i> , 2015, 21, 9610-9614.	3.3	23
41	Natural Orbital Functional Theory and Reactivity Studies of Diradical Rearrangements: Ethylene Torsion as a Case Study. <i>ChemPhysChem</i> , 2011, 12, 1673-1676.	2.1	22
42	An interpretation of the absorption and emission spectra of the gold dimer using modern theoretical tools. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 8732.	2.8	22
43	Application of quantum chemical methods in polymer chemistry. <i>International Reviews in Physical Chemistry</i> , 2019, 38, 343-403.	2.3	22
44	Benzoic Acid as an Efficient Organocatalyst for the Statistical Ring-Opening Copolymerization of ϵ -Caprolactone and L-Lactide: A Computational Investigation. <i>Macromolecules</i> , 2019, 52, 9238-9247.	4.8	22
45	Charge Transfer in Uranyl(VI) Halides [UO ₂ X ₄] ²⁻ (X = F, Cl, Br). <i>J. Phys. Chem. B</i> 107, 3615-3621.	0.784314 2.5	21
46	Pyridinium Containing Amide Based Polymeric Ionic Liquids for CO ₂ /CH ₄ Separation. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 10241-10247.	6.7	21
47	Selective Chemical Upcycling of Mixed Plastics Guided by a Thermally Stable Organocatalyst. <i>Angewandte Chemie</i> , 2021, 133, 6784-6791.	2.0	20
48	Prediction of pressure-induced redshift of f _{1d} excitations in Cs ₂ NaYCl ₆ :Ce ³⁺ and its connection with bond-length shortening. <i>Journal of Chemical Physics</i> , 2005, 122, 234507.	3.0	19
49	Probing the electronic structure and Au-C chemical bonding in AuCn ⁺ and AuCnH ⁺ (n = 2, 4, and 6) using high-resolution photoelectron spectroscopy. <i>Journal of Chemical Physics</i> , 2016, 145, 064304.	3.0	18
50	Why can Dispolreg 007 control the nitroxide mediated polymerization of methacrylates?. <i>Polymer Chemistry</i> , 2019, 10, 106-113.	3.9	18
51	Ionic Inter-Particle Complexation Effect on the Performance of Waterborne Coatings. <i>Polymers</i> , 2021, 13, 3098.	4.5	17
52	Quantum chemical study of the catalytic activation of methane by copper oxide and copper hydroxide cations. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 1148-1153.	2.8	16
53	Sulfenamides as Building Blocks for Efficient Disulfide-Based Self-Healing Materials. A Quantum Chemical Study. <i>ChemistryOpen</i> , 2018, 7, 248-255.	1.9	16
54	Effect of Molecular Structure in the Chain Mobility of Dichalcogenide-Based Polymers with Self-Healing Capacity. <i>Polymers</i> , 2019, 11, 1960.	4.5	16

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55	Proton trap effect on catechol-pyridine redox polymer nanoparticles as organic electrodes for lithium batteries. <i>Sustainable Energy and Fuels</i> , 2020, 4, 3934-3942.	4.9	16
56	In situ Investigations of a Proton Trap Material: A PEDOT-Based Copolymer with Hydroquinone and Pyridine Side Groups Having Robust Cyclability in Organic Electrolytes and Ionic Liquids. <i>ACS Applied Energy Materials</i> , 2019, 2, 4486-4495.	5.1	15
57	Hydrogen Bonds and Their Lithium and Gold Analogues: MP2 and CASPT2 Calculations. <i>ChemPhysChem</i> , 2017, 18, 2409-2417.	2.1	14
58	The 5f ³ manifold of the free-ion U ³⁺ : Ab initio calculations. <i>Chemical Physics Letters</i> , 2007, 434, 1-5.	2.6	13
59	Probing the structures and bonding of auropolynes, Au _n (C) _n Au (n = 1-3), using high-resolution photoelectron imaging. <i>Journal of Chemical Physics</i> , 2018, 149, 144307.	3.0	13
60	Electronic Structure and Bonding in Heteronuclear Dimers of V, Cr, Mo, and W: a CASSCF/CASPT2 Study. <i>Inorganic Chemistry</i> , 2011, 50, 9219-9229.	4.0	12
61	Molecules with High Bond Orders and Ultrashort Bond Lengths: CrU, MoU, and WU. <i>Inorganic Chemistry</i> , 2013, 52, 2838-2843.	4.0	12
62	Electronic spectroscopy and electronic structure of diatomic IrSi. <i>Journal of Chemical Physics</i> , 2013, 138, 154306.	3.0	12
63	Toward an Understanding of the Hydrogenation Reaction of MO ₂ Gas-Phase Clusters (M = Ti, Zr, Hf, Th, U). <i>Journal of Chemical Physics</i> , 2013, 138, 154306.	2.5	12
64	Evaluation of modern DFT functionals and G3n-RAD composite methods in the modelization of organic singlet diradicals. <i>Journal of Molecular Modeling</i> , 2016, 22, 76.	1.8	12
65	Perovskite Solar Cells Based on Oligotriarylamine Hexaarylbenzene as Hole-Transporting Materials. <i>Organic Letters</i> , 2019, 21, 3261-3264.	4.6	12
66	Mild Open-Shell Character of BODIPY and Its Impact on Singlet and Triplet Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5825-5838.	5.3	12
67	Matrix Infrared Spectroscopy and a Theoretical Investigation of SUO and US ₂ . <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 4457-4463.	2.0	11
68	Detailed interpretation of the 5f-6d absorption spectrum of U ³⁺ in Cs ₂ NaYCl ₆ and high pressure effects based on an ab initio simulation. <i>Journal of Chemical Physics</i> , 2007, 127, 144712.	3.0	10
69	A computational study on the intriguing mechanisms of the gas-phase thermal activation of methane by bare [Ni(H)(OH)] ⁺ . <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 9306.	2.8	10
70	Potential Use of Squarates and Croconates as Singlet Fission Sensitizers. <i>ChemPhysChem</i> , 2018, 19, 2224-2233.	2.1	10
71	Novel imino- and aryl-sulfonate based photoacid generators for the cationic ring-opening polymerization of ϵ -caprolactone. <i>Polymer Chemistry</i> , 2021, 12, 4035-4042.	3.9	10
72	Assessment of the second-order perturbative corrections to PNOF5. <i>Molecular Physics</i> , 2014, 112, 1-8.	1.7	9

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73	Performance of PNOF6 for Hydrogen Abstraction Reactions. <i>Journal of Physical Chemistry A</i> , 2015, 119, 6981-6988.	2.5	9
74	How cyclic chain topology can reduce the crystallization rate of poly(3-hexylthiophene) and promote the formation of liquid crystalline phases in comparison with linear analogue chains. <i>Journal of Materials Chemistry C</i> , 2019, 7, 6548-6558.	5.5	9
75	Improvement of the electrochemical and singlet fission properties of anthraquinones by modification of the diradical character. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7941-7952.	2.8	8
76	Copolymerization of (meth)acrylates with vinyl aromatic macromonomers: understanding the mechanism of retardation on the kinetics with acrylates. <i>Polymer Chemistry</i> , 2019, 10, 1769-1779.	3.9	8
77	Nearly Perfect 3D Structures Obtained by Assembly of Printed Parts of Polyamide Ionene Self-Healing Elastomer. <i>ACS Applied Polymer Materials</i> , 2020, 2, 4352-4359.	4.4	7
78	Singlet open-shell diradical nature and redox properties of conjugated carbonyls: a quantum chemical study. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	1.4	6
79	Computational study of the transamination reaction in vinylogous acyls: Paving the way to design vitrimers with controlled exchange kinetics. <i>Journal of Polymer Science</i> , 2022, 60, 1988-1999.	3.8	6
80	Computational study of Be ₂ using Piris natural orbital functionals. <i>Journal of Molecular Modeling</i> , 2013, 19, 1967-1972.	1.8	5
81	Fundamental Insights into Free-Radical Polymerization in the Presence of Catechols and Catechol-Functionalized Monomers. <i>Macromolecules</i> , 2022, 55, 49-64.	4.8	4
82	Quantum Chemical Study of the Reactions between Pd ⁺ /Pt ⁺ and H ₂ O/H ₂ S. <i>Chemistry - A European Journal</i> , 2013, 19, 8832-8838.	3.3	3
83	Understanding the emulsion copolymerization kinetics of vinyl acetate and vinyl silanes. <i>Polymer Chemistry</i> , 2020, 11, 2390-2398.	3.9	3
84	Theoretical Characterization of New Frustrated Lewis Pairs for Responsive Materials. <i>Polymers</i> , 2021, 13, 1573.	4.5	1
85	Combined DFT and MD Simulation Protocol to Characterize Self-Healing Properties in Disulfide-Containing Materials: Polyurethanes and Polymethacrylates as Case Studies. <i>Frontiers in Materials</i> , 2022, 9, .	2.4	1
86	Aging effect of Catechol Redox Polymer Nanoparticles for Hybrid Supercapacitors. <i>Batteries and Supercaps</i> , 0, , .	4.7	1
87	Frontispiece: The Electronic Structure of the Al ³⁺ Anion: Is it Aromatic?. <i>Chemistry - A European Journal</i> , 2015, 21, n/a-n/a.	3.3	0