Fernando Ruiperez

List of Publications by Year
in descending order

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87 papers	3,011 citations	172457 29 h-index	182427 51 g-index
89 all docs	89 docs citations	89 times ranked	3470 citing authors

#	Article	IF	Citations
1	Combined DFT and MD Simulation Protocol to Characterize Self-Healing Properties in Disulfide-Containing Materials: Polyurethanes and Polymethacrylates as Case Studies. Frontiers in Materials, 2022, 9, .	2.4	1
2	Computational study of the transamination reaction in vinylogous acyls: Paving the way to design vitrimers with controlled exchange kinetics. Journal of Polymer Science, 2022, 60, 1988-1999.	3.8	6
3	Fundamental Insights into Free-Radical Polymerization in the Presence of Catechols and Catechol-Functionalized Monomers. Macromolecules, 2022, 55, 49-64.	4.8	4
4	Selective Chemical Upcycling of Mixed Plastics Guided by a Thermally Stable Organocatalyst. Angewandte Chemie, 2021, 133, 6784-6791.	2.0	20
5	Selective Chemical Upcycling of Mixed Plastics Guided by a Thermally Stable Organocatalyst. Angewandte Chemie - International Edition, 2021, 60, 6710-6717.	13.8	118
6	Theoretical Characterization of New Frustrated Lewis Pairs for Responsive Materials. Polymers, 2021, 13, 1573.	4.5	1
7	Mild Open-Shell Character of BODIPY and Its Impact on Singlet and Triplet Excitation Energies. Journal of Chemical Theory and Computation, 2021, 17, 5825-5838.	5.3	12
8	Ionic Inter-Particle Complexation Effect on the Performance of Waterborne Coatings. Polymers, 2021, 13, 3098.	4.5	17
9	Novel imino- and aryl-sulfonate based photoacid generators for the cationic ring-opening polymerization of Îµ-caprolactone. Polymer Chemistry, 2021, 12, 4035-4042.	3.9	10
10	Proton trap effect on catecholâ€“pyridine redox polymer nanoparticles as organic electrodes for lithium batteries. Sustainable Energy and Fuels, 2020, 4, 3934-3942.	4.9	16
11	Thioxanthone-Based Photobase Generators for the Synthesis of Polyurethanes via the Photopolymerization of Polyols and Polyisocyanates. Macromolecules, 2020, 53, 2069-2076.	4.8	24
12	Synthesis of Functionalized Cyclic Carbonates through Commodity Polymer Upcycling. ACS Macro Letters, 2020, 9, 443-447.	4.8	69
13	Understanding the emulsion copolymerization kinetics of vinyl acetate and vinyl silanes. Polymer Chemistry, 2020, 11, 2390-2398.	3.9	3
14	Selective Organocatalytic Preparation of Trimethylene Carbonate from Oxetane and Carbon Dioxide. ACS Catalysis, 2020, 10, 5399-5404.	11.2	31
15	Nearly Perfect 3D Structures Obtained by Assembly of Printed Parts of Polyamide Ionene Self-Healing Elastomer. ACS Applied Polymer Materials, 2020, 2, 4352-4359.	4.4	7
16	Application of quantum chemical methods in polymer chemistry. International Reviews in Physical Chemistry, 2019, 38, 343-403.	2.3	22
17	Effect of Regioisomerism on Processability and Mechanical Properties of Amine/Urea Exchange Based Poly(urea-urethane) Vitrimers. ACS Applied Polymer Materials, 2019, 1, 2472-2481.	4.4	25
18	Why can Dispolreg 007 control the nitroxide mediated polymerization of methacrylates?. Polymer Chemistry, 2019, 10, 106-113.	3.9	18

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19	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. ACS Applied Energy Materials, 2019, 2, 4486-4495.	5.1	15
20	Pyridinium Containing Amide Based Polymeric Ionic Liquids for CO₂/CH₄ Separation. ACS Sustainable Chemistry and Engineering, 2019, 7, 10241-10247.	6.7	21
21	Rational Study of DBU Salts for the CO₂ Insertion into Epoxides for the Synthesis of Cyclic Carbonates. ACS Sustainable Chemistry and Engineering, 2019, 7, 10633-10640.	6.7	68
22	Perovskite Solar Cells Based on Oligotriarylamine Hexaarylbenzene as Hole-Transporting Materials. Organic Letters, 2019, 21, 3261-3264.	4.6	12
23	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. Journal of Materials Chemistry C, 2019, 7, 6548-6558.	5.5	9
24	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
25	Improvement of the electrochemical and singlet fission properties of anthraquinones by modification of the diradical character. Physical Chemistry Chemical Physics, 2019, 21, 7941-7952.	2.8	8
26	Copolymerization of (meth)acrylates with vinyl aromatic macromonomers: understanding the mechanism of retardation on the kinetics with acrylates. Polymer Chemistry, 2019, 10, 1769-1779.	3.9	8
27	Benzoic Acid as an Efficient Organocatalyst for the Statistical Ring-Opening Copolymerization of Îµ-Caprolactone and <scp>L</scp>-Lactide: A Computational Investigation. Macromolecules, 2019, 52, 9238-9247.	4.8	22
28	Effect of Molecular Structure in the Chain Mobility of Dichalcogenide-Based Polymers with Self-Healing Capacity. Polymers, 2019, 11, 1960.	4.5	16
29	Organocatalysed depolymerisation of PET in a fully sustainable cycle using thermally stable protic ionic salt. Green Chemistry, 2018, 20, 1205-1212.	9.0	182
30	Sulfenamides as Building Blocks for Efficient Disulfideâ€Based Selfâ€Healing Materials. A Quantum Chemical Study. ChemistryOpen, 2018, 7, 248-255.	1.9	16
31	Reprocessable and recyclable crosslinked poly(urea-urethane)s based on dynamic amine/urea exchange. Polymer, 2018, 145, 127-136.	3.8	77
32	Fullereneâ€Based Materials as Holeâ€Transporting/Electronâ€Blocking Layers: Applications in Perovskite Solar Cells. Chemistry - A European Journal, 2018, 24, 8524-8529.	3.3	25
33	Probing the structures and bonding of auropolyynes, Auâ€”(Câ‰¡C)nâ€”Auâ¯ (n = 1â€“3), using high-resolution photoelectron imaging. Journal of Chemical Physics, 2018, 149, 144307.	3.0	13
34	Supramolecular-Enhanced Charge Transfer within Entangled Polyamide Chains as the Origin of the Universal Blue Fluorescence of Polymer Carbon Dots. Journal of the American Chemical Society, 2018, 140, 12862-12869.	13.7	242
35	Potential Use of Squarates and Croconates as Singlet Fission Sensitizers. ChemPhysChem, 2018, 19, 2224-2233.	2.1	10
36	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

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37	Aromatic diselenide crosslinkers to enhance the reprocessability and self-healing of polyurethane thermosets. Polymer Chemistry, 2017, 8, 3641-3646.	3.9	102
38	Singlet open-shell diradical nature and redox properties of conjugated carbonyls: a quantum chemical study. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	6
39	Ï€â‹…â‹…â‹…H⁺â‹…â‹…â‹…Ï€ Hydrogen Bonds and Their Lithium and Gold Analogues: MP2 and CASPT2 Calculations. ChemPhysChem, 2017, 18, 2409-2417.	2.1	14
40	Theoretical design of conjugated diradicaloids as singlet fission sensitizers: quinones and methylene derivatives. Physical Chemistry Chemical Physics, 2017, 19, 30227-30238.	2.8	29
41	Innovative Poly(Ionic Liquid)s by the Polymerization of Deep Eutectic Monomers. Macromolecular Rapid Communications, 2016, 37, 1135-1142.	3.9	45
42	On the Termination Mechanism in the Radical Polymerization of Acrylates. Macromolecular Rapid Communications, 2016, 37, 1364-1368.	3.9	35
43	Probing the electronic structure and Auâ€”C chemical bonding in AuCnâ¯ and AuCnHâ¯ (n = 2, 4, and 6) using high-resolution photoelectron spectroscopy. Journal of Chemical Physics, 2016, 145, 064304.	3.0	18
44	Evaluation of modern DFT functionals and G3n-RAD composite methods in the modelization of organic singlet diradicals. Journal of Molecular Modeling, 2016, 22, 76.	1.8	12
45	Nanoporous amide networks based on tetraphenyladamantane for selective CO₂ capture. Journal of Materials Chemistry A, 2016, 4, 8190-8197.	10.3	51
46	Dihydrogen bond interactions as a result of H₂cleavage at Cu, Ag and Au centres. Physical Chemistry Chemical Physics, 2016, 18, 12810-12818.	2.8	26
47	Sustainable Poly(Ionic Liquids) for CO₂ Capture Based on Deep Eutectic Monomers. ACS Sustainable Chemistry and Engineering, 2016, 4, 7200-7208.	6.7	68
48	Transient mechanochromism in epoxy vitrimer composites containing aromatic disulfide crosslinks. Journal of Materials Chemistry C, 2016, 4, 6220-6223.	5.5	125
49	Design of new disulfide-based organic compounds for the improvement of self-healing materials. Physical Chemistry Chemical Physics, 2016, 18, 1758-1770.	2.8	139
50	Room temperature synthesis of non-isocyanate polyurethanes (NIPUs) using highly reactive N-substituted 8-membered cyclic carbonates. Polymer Chemistry, 2016, 7, 2105-2111.	3.9	71
51	Frontispiece: The Electronic Structure of the Al3â¯Anion: Is it Aromatic?. Chemistry - A European Journal, 2015, 21, n/a-n/a.	3.3	0
52	The Electronic Structure of the Al₃^{â¯} Anion: Is it Aromatic?. Chemistry - A European Journal, 2015, 21, 9610-9614.	3.3	23
53	Performance of PNOF6 for Hydrogen Abstraction Reactions. Journal of Physical Chemistry A, 2015, 119, 6981-6988.	2.5	9
54	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

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55	Experimental and computational studies of ring-opening polymerization of ethylene brassylate macrolactone and copolymerization with Îµ-caprolactone and TBD-guanidine organic catalyst. Journal of Polymer Science Part A, 2015, 53, 552-561.	2.3	42
56	Assessment of the second-order perturbative corrections to PNOF5. Molecular Physics, 2014, 112, 1-8.	1.7	9
57	ALUMINIUM IN BIOLOGICAL ENVIRONMENTS: A COMPUTATIONAL APPROACH. Computational and Structural Biotechnology Journal, 2014, 9, e201403002.	4.1	41
58	Organocatalyzed Synthesis of Aliphatic Polyesters from Ethylene Brassylate: A Cheap and Renewable Macrolactone. ACS Macro Letters, 2014, 3, 849-853.	4.8	67
59	Experimental Evidence Shedding Light on the Origin of the Reduction of Branching of Acrylates in ATRP. Macromolecules, 2014, 47, 964-972.	4.8	27
60	Computational study of Be2 using Piris natural orbital functionals. Journal of Molecular Modeling, 2013, 19, 1967-1972.	1.8	5
61	Quantum chemical study of the catalytic activation of methane by copper oxide and copper hydroxide cations. Physical Chemistry Chemical Physics, 2013, 15, 1148-1153.	2.8	16
62	The natural orbital functional theory of the bonding in Cr₂, Mo₂and W₂. Physical Chemistry Chemical Physics, 2013, 15, 2055-2062.	2.8	38
63	Molecules with High Bond Orders and Ultrashort Bond Lengths: CrU, MoU, and WU. Inorganic Chemistry, 2013, 52, 2838-2843.	4.0	12
64	Electronic spectroscopy and electronic structure of diatomic IrSi. Journal of Chemical Physics, 2013, 138, 154306.	3.0	12
65	Quantum Chemical Study of the Reactions between Pd⁺/Pt⁺ and H₂O/H₂S. Chemistry - A European Journal, 2013, 19, 8832-8838.	3.3	3
66	Toward an Understanding of the Hydrogenation Reaction of MO₂ Gas-Phase Clusters (M =) Tj ETQq0 0 0 rgBT /Overlock 10	2.5	12
67	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
68	A computational study on the intriguing mechanisms of the gas-phase thermal activation of methane by bare [Ni(H)(OH)]+. Physical Chemistry Chemical Physics, 2012, 14, 9306.	2.8	10
69	An interpretation of the absorption and emission spectra of the gold dimer using modern theoretical tools. Physical Chemistry Chemical Physics, 2012, 14, 8732.	2.8	22
70	Pro-oxidant activity of aluminum: Promoting the Fenton reaction by reducing Fe(III) to Fe(II). Journal of Inorganic Biochemistry, 2012, 117, 118-123.	3.5	106
71	Performance of PNOF5 Natural Orbital Functional for Radical Formation Reactions: Hydrogen Atom Abstraction and Câ€“C and Oâ€“O Homolytic Bond Cleavage in Selected Molecules. Journal of Chemical Theory and Computation, 2012, 8, 2646-2652.	5.3	24
72	Homolytic molecular dissociation in natural orbital functional theory. Physical Chemistry Chemical Physics, 2011, 13, 20129.	2.8	35

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73	Pro-oxidant Activity of Aluminum: Stabilization of the Aluminum Superoxide Radical Ion. Journal of Physical Chemistry A, 2011, 115, 6717-6723.	2.5	60
74	Complete vs Restricted Active Space Perturbation Theory Calculation of the Cr₂ Potential Energy Surface. Journal of Chemical Theory and Computation, 2011, 7, 1640-1646.	5.3	53
75	Electronic Structure and Bonding in Heteronuclear Dimers of V, Cr, Mo, and W: a CASSCF/CASPT2 Study. Inorganic Chemistry, 2011, 50, 9219-9229.	4.0	12
76	Matrix Infrared Spectroscopy and a Theoretical Investigation of SUO and US2. European Journal of Inorganic Chemistry, 2011, 2011, 4457-4463.	2.0	11
77	Diradicals and Diradicaloids in Natural Orbital Functional Theory. ChemPhysChem, 2011, 12, 1061-1065.	2.1	25
78	Natural Orbital Functional Theory and Reactivity Studies of Diradical Rearrangements: Ethylene Torsion as a Case Study. ChemPhysChem, 2011, 12, 1673-1676.	2.1	22
79	A natural orbital functional for multiconfigurational states. Journal of Chemical Physics, 2011, 134, 164102.	3.0	114
80	Charge Transfer in Uranyl(VI) Halides [UO₂X₄]^{2â^'} (X = F, Cl, Br,) Tj ETQq0 0 0 rgBT /Overlock 10 3615-3621.	2.5	21
81	An ab Initio Theoretical Study of the Electronic Structure of UO₂⁺ and [UO₂(CO₃)₃]^{5â^'}. Journal of Physical Chemistry A, 2009, 113, 1420-1428.	2.5	42
82	Detailed interpretation of the 5f-6d absorption spectrum of U3+ in Cs2NaYCl6 and high pressure effects based on an ab initio simulation. Journal of Chemical Physics, 2007, 127, 144712.	3.0	10
83	The 5f3 manifold of the free-ion U3+: Ab initio calculations. Chemical Physics Letters, 2007, 434, 1-5.	2.6	13
84	Bond lengths of and states of hexahalides. Journal of Solid State Chemistry, 2005, 178, 464-469.	2.9	40
85	Quantum chemical study of 4fâ†'5d excitations of trivalent lanthanide ions doped in the cubic elpasolite Cs2NaYCl6. Ce3+ to Tb3+. Journal of Chemical Physics, 2005, 123, 244703.	3.0	30
86	Prediction of pressure-induced redshift of f1â†'d(t2g)1 excitations in Cs2NaYCl6:Ce3+ and its connection with bond-length shortening. Journal of Chemical Physics, 2005, 122, 234507.	3.0	19
87	Aging effect of Catechol Redox Polymer Nanoparticles for Hybrid Supercapacitors. Batteries and Supercaps, 0, , .	4.7	1