Jon M Matxain

List of Publications by Year
in descending order

107 papers	3,442 citations	109311 35 h-index	161844 54 g-index
110 all docs	110 docs citations	110 times ranked	3279 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. Journal of the American Chemical Society, 2018, 140, 12862-12869.	13.7	242
2	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
3	Transient mechanochromism in epoxy vitrimer composites containing aromatic disulfide crosslinks. Journal of Materials Chemistry C, 2016, 4, 6220-6223.	5.5	125
4	A natural orbital functional for multiconfigurational states. Journal of Chemical Physics, 2011, 134, 164102.	3.0	114
5	Theoretical methods that help understanding the structure and reactivity of gas phase ions. International Journal of Mass Spectrometry, 2005, 240, 37-99.	1.5	104
6	Structure and Properties of ZnS Nanoclusters. Journal of Physical Chemistry B, 2005, 109, 2703-2709.	2.6	102
7	Aromatic diselenide crosslinkers to enhance the reprocessability and self-healing of polyurethane thermosets. Polymer Chemistry, 2017, 8, 3641-3646.	3.9	102
8	Electronic Excitation Energies of ZniOiClusters. Journal of the American Chemical Society, 2003, 125, 9494-9499.	13.7	98
9	Small clusters of II-VI materials:ZniOi,i=1â€“9. Physical Review A, 2000, 62, .	2.5	88
10	Small clusters of II-VI materials:â€ƒZniSi,i=1â€“9. Physical Review A, 2000, 61, .	2.5	85
11	Theoretical Study of the Antioxidant Properties of Pyridoxine. Journal of Physical Chemistry A, 2006, 110, 13068-13072.	2.5	77
12	Reprocessable and recyclable crosslinked poly(urea-urethane)s based on dynamic amine/urea exchange. Polymer, 2018, 145, 127-136.	3.8	77
13	Evidence of High â€¢OH Radical Quenching Efficiency by Vitamin B₆. Journal of Physical Chemistry B, 2009, 113, 9629-9632.	2.6	73
14	New Solids Based on B₁₂N₁₂ Fullerenes. Journal of Physical Chemistry C, 2007, 111, 13354-13360.	3.1	72
15	Mechanism of Photoinduced Decomposition of Ketoprofen. Journal of Medicinal Chemistry, 2007, 50, 1735-1743.	6.4	69
16	Resonance Structures of the Amide Bond: The Advantages of Planarity. Chemistry - A European Journal, 2006, 12, 7215-7224.	3.3	68
17	Communications: Accurate description of atoms and molecules by natural orbital functional theory. Journal of Chemical Physics, 2010, 132, 031103.	3.0	68
18	Communication: The role of the positivity N-representability conditions in natural orbital functional theory. Journal of Chemical Physics, 2010, 133, 111101.	3.0	60

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19	A DFT/TDDFT study on the optoelectronic properties of the amine-capped magic (CdSe)13 nanocluster. Physical Chemistry Chemical Physics, 2013, 15, 10996.	2.8	57
20	Clusters of IIâˆ’VI Materials:Â CdiXi, X = S, Se, Te,iâ‰ 16. Journal of Physical Chemistry A, 2004, 108, 10502-10508.	2.5	56
21	The intrapair electron correlation in natural orbital functional theory. Journal of Chemical Physics, 2013, 139, 234109.	3.0	55
22	Spin conserving natural orbital functional theory. Journal of Chemical Physics, 2009, 131, 021102.	3.0	52
23	Mono- and Multidecker Sandwich-Like Complexes of the Tetraazacyclobutadiene Aromatic Ring. Angewandte Chemie - International Edition, 2004, 43, 5485-5488.	13.8	42
24	Theoretical Study of the Reaction of Vitamin B6 with1O2. Chemistry - A European Journal, 2007, 13, 4636-4642.	3.3	41
25	Sandwich Complexes Based on the â€œAll-Metalâ€•Al42âˆ’ Aromatic Ring. Chemistry - A European Journal, 2006, 12, 4495-4502.	3.3	40
26	The extended Koopmansâ€™ theorem: Vertical ionization potentials from natural orbital functional theory. Journal of Chemical Physics, 2012, 136, 174116.	3.0	39
27	The natural orbital functional theory of the bonding in Cr₂, Mo₂and W₂. Physical Chemistry Chemical Physics, 2013, 15, 2055-2062.	2.8	38
28	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
29	Stability and Aromaticity of BiNi Rings and Fullerenes. Journal of Physical Chemistry A, 2003, 107, 10004-10010.	2.5	37
30	pH-Dependent Electronic and Spectroscopic Properties of Pyridoxine (Vitamin B6). Journal of Physical Chemistry B, 2006, 110, 16774-16780.	2.6	37
31	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
32	Small clusters of group-(IIâ€“VI) materials:ZniXi,X=Se,Te,i=1â€“9. Physical Review A, 2001, 64, .	2.5	36
33	Quantum chemical assessment of the binding energy of CuO+. Journal of Chemical Physics, 2011, 134, 064304.	3.0	36
34	Computational Study on the Attack of [.]OH Radicals on Aromatic Amino Acids. Chemistry - A European Journal, 2013, 19, 6862-6873.	3.3	36
35	Homolytic molecular dissociation in natural orbital functional theory. Physical Chemistry Chemical Physics, 2011, 13, 20129.	2.8	35
36	Electronic excitation energies ofZniSiclusters. Physical Review A, 2001, 64, .	2.5	34

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37	The one-electron picture in the Piris natural orbital functional 5 (PNOF5). Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	33
38	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
39	Plasmonic Resonances in the Al₁₃^{â€“} Cluster: Quantification and Origin of Exciton Collectivity. Journal of Physical Chemistry C, 2016, 120, 12742-12750.	3.1	30
40	Endohedral (X@ZniSi)i=4-160,Â± Nanoclusters, X = Li, Na, K, Cl, Br. Journal of Physical Chemistry C, 2007, 111, 3560-3565.	3.1	27
41	Electronic excitation energies of smallZniSiclusters. Physical Review A, 2000, 63, .	2.5	26
42	Breaking Bonds and Forming Nanographene Diradicals with Pressure. Angewandte Chemie - International Edition, 2017, 56, 16212-16217.	13.8	26
43	Molecular Dynamics Simulation of Bovine Pancreatic Ribonuclease Aâ^'CpA and Transition State-like Complexes. Journal of Physical Chemistry B, 2010, 114, 7371-7382.	2.6	25
44	Diradicals and Diradicaloids in Natural Orbital Functional Theory. ChemPhysChem, 2011, 12, 1061-1065.	2.1	25
45	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
46	Endohedral Stannaspherenes Mn@Sn₁₂ and its Dimer: Ferromagnetic or Antiferromagnetic?. ChemPhysChem, 2007, 8, 2096-2099.	2.1	24
47	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
48	Clusters of Group IIâ^'VI Materials:â€‰ CdiOi (i â‰¤ 15). Journal of Physical Chemistry A, 2003, 107, 9918-9923.	2.5	22
49	Performance of PNOF3 for reactivity studies: X[BO] and X[CN] isomerization reactions (X = H, Li) as a case study. Physical Chemistry Chemical Physics, 2010, 12, 12931.	2.8	22
50	Natural Orbital Functional Theory and Reactivity Studies of Diradical Rearrangements: Ethylene Torsion as a Case Study. ChemPhysChem, 2011, 12, 1673-1676.	2.1	22
51	Chirality-Induced Electron Spin Polarization and Enantiospecific Response in Solid-State Cross-Polarization Nuclear Magnetic Resonance. ACS Nano, 2018, 12, 11426-11433.	14.6	21
52	The first solvation shell of aluminum (III) and magnesium (II) cations in a protein model environment. International Journal of Quantum Chemistry, 2004, 98, 409-424.	2.0	19
53	Thermally Stable Solids Based on Endohedrally Doped ZnS Clusters. Chemistry - A European Journal, 2009, 15, 5138-5144.	3.3	19
54	Â·OH Oxidation Toward S- and OH-Containing Amino Acids. Journal of Physical Chemistry B, 2015, 119, 15430-15442.	2.6	19

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55	Piris natural orbital functional study of the dissociation of the radical helium dimer. Journal of Chemical Physics, 2008, 129, 014108.	3.0	18
56	Quantum Monte Carlo study of the ground state and low-lying excited states of the scandium dimer. Journal of Chemical Physics, 2008, 128, 194315.	3.0	18
57	The Nature of Chemical Bonds from PNOF5 Calculations. ChemPhysChem, 2012, 13, 2297-2303.	2.1	18
58	Aluminum (III) interactions with the side chains of aromatic aminoacids. International Journal of Quantum Chemistry, 2002, 90, 859-881.	2.0	17
59	Discordant results on the FeO+â€‰+â€‰H2reaction reconciled by quantum Monte Carlo theory. Molecular Physics, 2004, 102, 2635-2637.	1.7	17
60	On the Mechanism of Cross-Dehydrogenative Couplings between N-aryl Glycinates and Indoles: A Computational Study. Journal of Organic Chemistry, 2020, 85, 13133-13140.	3.2	17
61	Proton-responsive Ruthenium(II) Catalysts for the Solvolysis of Ammonia-Borane. Organometallics, 2020, 39, 1238-1248.	2.3	17
62	Combined ab Initio Computational and Statistical Investigation of a Model Câ^'HÂ·Â·Â·O Hydrogen Bonded Dimer as Occurring in 1,4-Benzoquinone. Journal of Physical Chemistry A, 1999, 103, 2784-2792.	2.5	16
63	Electronic excitation energies of ZniSinanoparticles. Nanotechnology, 2006, 17, 4100-4105.	2.6	16
64	Sandwich Complexes of the Metalloaromatic Î·³-Al₃R₃ Ligand. Journal of the American Chemical Society, 2009, 131, 6949-6951.	13.7	16
65	Sulfenamides as Building Blocks for Efficient Disulfideâ€Based Selfâ€Healing Materials. A Quantum Chemical Study. ChemistryOpen, 2018, 7, 248-255.	1.9	16
66	Effect of Molecular Structure in the Chain Mobility of Dichalcogenide-Based Polymers with Self-Healing Capacity. Polymers, 2019, 11, 1960.	4.5	16
67	Methoxyphenols?antioxidant principles in food plants and spices: Pulse radiolysis, EPR spectroscopy, and density functional theory calculations. International Journal of Quantum Chemistry, 2002, 90, 969-979.	2.0	14
68	sp3 Hybrid orbitals and ionization energies of methane from PNOF5. Chemical Physics Letters, 2012, 531, 272-274.	2.6	14
69	Doped Aluminum Cluster Anions: Size Matters. Journal of Physical Chemistry A, 2014, 118, 4309-4314.	2.5	14
70	MALDI-ToF MS Study of Macrocyclic Polyethers Generated by Electrophilic Zwitterionic Ring Expansion Polymerization of Monosubstituted Epoxides with B(C₆F₅)₃. Macromolecules, 2019, 52, 6369-6381.	4.8	14
71	The role of CT excitations in PDI aggregates. Physical Chemistry Chemical Physics, 2020, 22, 15908-15918.	2.8	14
72	Structure and Stability of the Endohedrally Doped (X@CdiSi)i=4,9,12,15,16q=0,Â±1, X = Na, K, Cl, Br, Nanoclusters. Journal of Physical Chemistry C, 2010, 114, 2476-2483.	3.1	13

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73	Pdâ€Catalyzed C(sp²)â”H Alkoxycarbonylation of Phenethylâ€•and Benzylamines with Chloroformates as CO Surrogates. Chemistry - A European Journal, 2021, 27, 5782-5789.	3.3	13
74	Complete basis set limit extrapolation calculations with PNOF3. Chemical Physics Letters, 2010, 499, 164-167.	2.6	12
75	Self-assembling endohedrally doped CdS nanoclusters: new porous solid phases of CdS. Physical Chemistry Chemical Physics, 2012, 14, 9676.	2.8	12
76	Incremental binding free energies of aluminum (III) vs. magnesium (II) complexes. Chemical Physics, 2003, 295, 175-184.	1.9	11
77	A computational study of radical initiated protein backbone homolytic dissociation on all natural amino acids. Physical Chemistry Chemical Physics, 2016, 18, 30972-30981.	2.8	11
78	Breaking Bonds and Forming Nanographene Diradicals with Pressure. Angewandte Chemie, 2017, 129, 16430-16435.	2.0	11
79	Magnetic Endohedral Transitionâ€Metalâ€Doped Semiconductingâ€Nanoclusters. Chemistry - A European Journal, 2008, 14, 8547-8554.	3.3	10
80	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
81	Theoretical study of the pH-dependent antioxidant properties of vitamin C. Journal of Molecular Modeling, 2013, 19, 1945-1952.	1.8	10
82	Enantiospecific Response in Cross-Polarization Solid-State Nuclear Magnetic Resonance of Optically Active Metal Organic Frameworks. Journal of the American Chemical Society, 2020, 142, 17989-17996.	13.7	10
83	Assessment of the second-order perturbative corrections to PNOF5. Molecular Physics, 2014, 112, 1-8.	1.7	9
84	Photosensitization mechanism of Cu(<scp>ii</scp>) porphyrins. Physical Chemistry Chemical Physics, 2017, 19, 20533-20540.	2.8	9
85	Oxidation of Acid, Base, and Amide Side-Chain Amino Acid Derivatives via Hydroxyl Radical. Journal of Physical Chemistry B, 2018, 122, 4956-4971.	2.6	9
86	Ruâ€Catalyzed Câ”H Hydroxylation of Tyrosineâ€Containing Diâ€•and Tripeptides toward the Assembly of Lâ€DOPA Derivatives. Advanced Synthesis and Catalysis, 2022, 364, 2072-2079.	4.3	9
87	Thermal Stability of Endohedral First-Row Transition-Metal TM@ZniSi Structures, i = 12, 16. Journal of Physical Chemistry C, 2011, 115, 7829-7835.	3.1	7
88	Electronic metastable bound states of Mn22+ and Co22+. Chemical Physics Letters, 2003, 372, 82-89.	2.6	6
89	Structural and optical properties of the naked and passivated Al5Au5 bimetallic nanoclusters. Journal of Chemical Physics, 2016, 144, 114302.	3.0	6
90	Quantum Chemical Study of the Reaction between Ni⁺ and H₂S. ChemPhysChem, 2010, 11, 3172-3178.	2.1	5

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91	Computational study of Be2 using Piris natural orbital functionals. Journal of Molecular Modeling, 2013, 19, 1967-1972.	1.8	5
92	Second-Row Transition-Metal Doping of (ZniSi), i = 12, 16 Nanoclusters: Structural and Magnetic Properties. Computation, 2013, 1, 31-45.	2.0	5
93	Quantum Chemical Study of the Reactions between Pd⁺/Pt⁺ and H₂O/H₂S. Chemistry - A European Journal, 2013, 19, 8832-8838.	3.3	3
94	CdS nanoclusters doped with divalent atoms. Journal of Molecular Modeling, 2014, 20, 2227.	1.8	2
95	Reply to â€œComment on â€˜Chirality-Induced Electron Spin Polarization and Enantiospecific Response in Solid-State Cross-Polarization Nuclear Magnetic Resonanceâ€™â€. ACS Nano, 2019, 13, 6133-6136.	14.6	2
96	Metalâ€“Polymer Heterojunction in Colloidal-Phase Plasmonic Catalysis. Journal of Physical Chemistry Letters, 2022, 13, 2264-2272.	4.6	2
97	Metal Ion Dependent Adhesion Sites in Integrins:â€‰ A Combined DFT and QMC Study on Mn2+. Journal of Physical Chemistry B, 2007, 111, 9099-9103.	2.6	1
98	Theoretical Characterization of New Frustrated Lewis Pairs for Responsive Materials. Polymers, 2021, 13, 1573.	4.5	1
99	Computational approach to (ZnS)i nanoclusters in ionic liquids. Physical Review E, 2021, 104, 024604.	2.1	1
100	The one-electron picture in the Piris natural orbital functional 5 (PNOF5). Highlights in Theoretical Chemistry, 2014, , 5-15.	0.0	1
101	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
102	Stability and Aromaticity of BiNi Rings and Fullerenes. ChemInform, 2004, 35, no.	0.0	0
103	Mono- and Multidecker Sandwich-Like Complexes of the Tetraazacyclobutadiene Aromatic Ring.. ChemInform, 2004, 35, no.	0.0	0
104	Clusters of II?VI Materials: CdiXi, X: S, Se, Te, i ? 16.. ChemInform, 2005, 36, no.	0.0	0
105	Structure and Properties of ZnS Nanoclusters. ChemInform, 2005, 36, no.	0.0	0
106	Role of Dispersion Interactions in Endohedral TM@(ZnS)12 Structures. ACS Omega, 2021, 6, 16612-16622.	3.5	0
107	Building machine learning assisted phase diagrams: Three chemically relevant examples. AIP Advances, 2022, 12, 075206.	1.3	0