Jesus M Ugalde

List of Publications by Year
in descending order

246 papers	7,419 citations	53794 45 h-index	79698 73 g-index
257 all docs	257 docs citations	257 times ranked	5240 citing authors

#	Article	IF	Citations
1	Water Clusters: Towards an Understanding Based on First Principles of Their Static and Dynamic Properties. Angewandte Chemie - International Edition, 2000, 39, 717-721.	13.8	229
2	High Impact of Antiphospholipid Syndrome on Irreversible Organ Damage and Survival of Patients With Systemic Lupus Erythematosus. Archives of Internal Medicine, 2004, 164, 77.	3.8	195
3	A semiempirical theoretical study on the formation of .beta.-lactams from ketenes and imines. Journal of the American Chemical Society, 1993, 115, 995-1004.	13.7	152
4	The Curiously Stable Cluster and its Neutral and Anionic Counterparts:Â The Advantages of Planarityâ€. Journal of Physical Chemistry A, 2000, 104, 397-403.	2.5	149
5	Measuring the Spinâ€Polarization Power of a Single Chiral Molecule. Small, 2017, 13, 1602519.	10.0	143
6	Unexpected trends in halogen-bond based noncovalent adducts. Chemical Communications, 2012, 48, 7708.	4.1	136
7	On the directionality of halogen bonding. Physical Chemistry Chemical Physics, 2013, 15, 10350.	2.8	136
8	Recent developments and future prospects of all-metal aromatic compounds. Chemical Society Reviews, 2015, 44, 6519-6534.	38.1	128
9	Unravelling phenomenon of internal rotation in B13+ through chemical bonding analysis. Chemical Communications, 2011, 47, 6242.	4.1	120
10	Reactivity of Cr+(6S,4D), Mn+(7S,5S), and Fe+(6D,4F): Reaction of Cr+, Mn+, and Fe+with Water. Journal of the American Chemical Society, 1999, 121, 8549-8558.	13.7	116
11	Reactivity of Co+(3F,5F), Ni+(2D,4F), and Cu+(1S,3D): Reaction of Co+, Ni+, and Cu+with Water. Journal of the American Chemical Society, 2000, 122, 114-122.	13.7	114
12	A natural orbital functional for multiconfigurational states. Journal of Chemical Physics, 2011, 134, 164102.	3.0	114
13	Catalytic and Solvent Effects on the Cycloaddition Reaction between Ketenes and Carbonyl Compounds To Form 2-Oxetanones. Journal of the American Chemical Society, 1994, 116, 9613-9619.	13.7	113
14	Theoretical Study of Two-State Reactivity of Transition Metal Cations:Â The â€œDifficultâ€•Case of Iron Ion Interacting with Water, Ammonia, and Methane. Journal of Physical Chemistry A, 2004, 108, 1069-1081.	2.5	112
15	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
16	Chiral Control in the Staudinger Reaction between Ketenes and Imines. A Theoretical SCF-MO Study on Asymmetric Torquoselectivity. Journal of the American Chemical Society, 1994, 116, 2085-2093.	13.7	104
17	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
18	Reactivity of Sc+(3D,1D) and V+(5D,3F):Â Reaction of Sc+and V+with Water. Journal of the American Chemical Society, 1999, 121, 574-580.	13.7	102

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19	Sandwich-Like Complexes Based on â€œAll-Metalâ€•(Al42-) Aromatic Compounds. Journal of the American Chemical Society, 2004, 126, 3380-3381.	13.7	102
20	Structure and Properties of ZnS Nanoclusters. Journal of Physical Chemistry B, 2005, 109, 2703-2709.	2.6	102
21	Bond Paths Show Preferable Interactions: Ab Initio and QTAIM Studies on the Xâ˜HÂ·Â·Â·Ï€ Hydrogen Bond. Journal of Physical Chemistry A, 2010, 114, 7223-7229.	2.5	101
22	Electronic Excitation Energies of ZniOiClusters. Journal of the American Chemical Society, 2003, 125, 9494-9499.	13.7	98
23	Small clusters of II-VI materials:ZniOi,i=1â€“9. Physical Review A, 2000, 62, .	2.5	88
24	Small clusters of II-VI materials:â€ƒZniSi,i=1â€“9. Physical Review A, 2000, 61, .	2.5	85
25	A Joint Experimental and Theoretical Study of Cationâ˜Ï€ Interactions:Â Multiple-Decker Sandwich Complexes of Ferrocene with Alkali Metal Ions (Li+, Na+, K+, Rb+, Cs+). Journal of the American Chemical Society, 2005, 127, 10656-10666.	13.7	81
26	Designing 3-D Molecular Stars. Journal of the American Chemical Society, 2009, 131, 9426-9431.	13.7	78
27	A Chirality-Based Quantum Leap. ACS Nano, 2022, 16, 4989-5035.	14.6	74
28	Iterative diagonalization for orbital optimization in natural orbital functional theory. Journal of Computational Chemistry, 2009, 30, 2078-2086.	3.3	73
29	Perspective on natural orbital functional theory. International Journal of Quantum Chemistry, 2014, 114, 1169-1175.	2.0	69
30	Benchmark Assessment of Density Functional Methods on Group IIâ€“VI MX (M = Zn, Cd; X = S, Se, Te) Quantum Dots. Journal of Chemical Theory and Computation, 2014, 10, 76-89.	5.3	69
31	On the Stereochemical Outcome of the Catalyzed and Uncatalyzed Cycloaddition Reaction between Activated Ketenes and Aldehydes to form cis- and trans-2-Oxetanones. An ab Initio Study. Journal of the American Chemical Society, 1995, 117, 12314-12321.	13.7	68
32	Communications: Accurate description of atoms and molecules by natural orbital functional theory. Journal of Chemical Physics, 2010, 132, 031103.	3.0	68
33	On the Reactivity of Ti+(4F,2F). Reaction of Ti+ with OH2. Journal of Physical Chemistry A, 1998, 102, 293-300.	2.5	67
34	Antiphospholipid antibodies predict early damage in patients with systemic lupus erythematosus. Lupus, 2004, 13, 900-905.	1.6	60
35	Communication: The role of the positivity N-representability conditions in natural orbital functional theory. Journal of Chemical Physics, 2010, 133, 111101.	3.0	60
36	Pro-oxidant Activity of Aluminum: Stabilization of the Aluminum Superoxide Radical Ion. Journal of Physical Chemistry A, 2011, 115, 6717-6723.	2.5	60

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37	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
38	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
39	Planar tetracoordinate carbon in CE42âˆ’ (E=Alâ€“Tl) clusters. Chemical Physics Letters, 2012, 519-520, 29-33.	2.6	56
40	CBe5Eâˆ’ (E = Al, Ga, In, Tl): planar pentacoordinate carbon in heptaatomic clusters. Physical Chemistry Chemical Physics, 2012, 14, 14764.	2.8	55
41	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
42	Spin conserving natural orbital functional theory. Journal of Chemical Physics, 2009, 131, 021102.	3.0	52
43	Al12and theAl@Al12clusters. Physical Review A, 1998, 58, 383-388.	2.5	51
44	The Ferroceneâˆ’Lithium Cation Complex in the Gas Phase. Journal of the American Chemical Society, 2001, 123, 5040-5043.	13.7	51
45	An Ideal Spin Filter: Long-Range, High-Spin Selectivity in Chiral Helicoidal 3-Dimensional Metal Organic Frameworks. Nano Letters, 2020, 20, 8476-8482.	9.1	47
46	Solvent and Substituent Effects in the Periselectivity of the Staudinger Reaction between Ketenes and Î±,Î²-Unsaturated Imines. A Theoretical and Experimental Study. Journal of Organic Chemistry, 1996, 61, 3070-3079.	3.2	46
47	Dispersion interactions within the Piris natural orbital functional theory: The helium dimer. Journal of Chemical Physics, 2007, 126, 214103.	3.0	46
48	A first-principles study of IIâ€“VI (II = Zn; VI = O, S, Se, Te) semiconductor nanostructures. Journal of Materials Chemistry, 2012, 22, 21453.	6.7	45
49	Mono- and Multidecker Sandwich-Like Complexes of the Tetraazacyclobutadiene Aromatic Ring. Angewandte Chemie - International Edition, 2004, 43, 5485-5488.	13.8	42
50	The Bond Order of C₂ from a Strictly Nâ€Representable Natural Orbital Energy Functional Perspective. Chemistry - A European Journal, 2016, 22, 4109-4115.	3.3	42
51	Hydrogen-Bonding Interactions between Formic Acid and Pyridine. Journal of Physical Chemistry A, 2002, 106, 4187-4191.	2.5	41
52	Molecular Dynamics Simulations of Iron- and Aluminum-Loaded Serum Transferrin: Protonation of Tyr188 Is Necessary To Prompt Metal Release. Biochemistry, 2012, 51, 7017-7027.	2.5	41
53	ALUMINIUM IN BIOLOGICAL ENVIRONMENTS: A COMPUTATIONAL APPROACH. Computational and Structural Biotechnology Journal, 2014, 9, e201403002.	4.1	41
54	Theoretical Study of the C2P Radical and (C2P)+ Species. The Journal of Physical Chemistry, 1994, 98, 3985-3988.	2.9	40

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55	A study of the coordination shell of aluminum(III) and magnesium(II) in model protein environments: Thermodynamics of the complex formation and metal exchange reactions. Journal of Inorganic Biochemistry, 2006, 100, 374-384.	3.5	40
56	Sandwich Complexes Based on the â€œAll-Metalâ€•Al42â^' Aromatic Ring. Chemistry - A European Journal, 2006, 12, 4495-4502.	3.3	40
57	Intracule densities and electron correlation in the hydrogen molecule. Journal of Physics B: Atomic, Molecular and Optical Physics, 1988, 21, 2555-2561.	1.5	39
58	Substituent and Solvent Effects in the [2 + 2] Cycloaddition Reaction between Olefins and Isocyanates. Journal of the American Chemical Society, 1995, 117, 12306-12313.	13.7	39
59	The extended Koopmansâ€™ theorem: Vertical ionization potentials from natural orbital functional theory. Journal of Chemical Physics, 2012, 136, 174116.	3.0	39
60	The natural orbital functional theory of the bonding in Cr₂, Mo₂and W₂. Physical Chemistry Chemical Physics, 2013, 15, 2055-2062.	2.8	38
61	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
62	Quantum mechanical calculations on phosphate hydrolysis reactions. Journal of Computational Chemistry, 2000, 21, 43-51.	3.3	37
63	Stability and Aromaticity of BiNi Rings and Fullerenes. Journal of Physical Chemistry A, 2003, 107, 10004-10010.	2.5	37
64	Small clusters of group-(IIâ€“VI) materials:ZniXi,X=Se,Te,i=1â€“9. Physical Review A, 2001, 64, .	2.5	36
65	The Spin Dependence of the Spatial Size of Fe(II) and of the Structure of Fe(II)-Porphyrins. Journal of Physical Chemistry A, 2004, 108, 4653-4657.	2.5	36
66	Homolytic molecular dissociation in natural orbital functional theory. Physical Chemistry Chemical Physics, 2011, 13, 20129.	2.8	35
67	Electronic excitation energies ofZniSiclusters. Physical Review A, 2001, 64, .	2.5	34
68	The one-electron picture in the Piris natural orbital functional 5 (PNOF5). Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	33
69	The aromaticity of dicupra[10]annulenes. Physical Chemistry Chemical Physics, 2017, 19, 9669-9675.	2.8	33
70	The evaluation of electronic extracule and intracule densities and related probability functions in terms of Gaussian basis functions. Journal of Mathematical Chemistry, 1991, 6, 51-61.	1.5	32
71	Role of the isomerization pathways in the Staudinger reaction. A theoretical study on the interaction between activated ketenes and imidates. Tetrahedron Letters, 1994, 35, 4465-4468.	1.4	31
72	A theoretical study of the principles regulating the specificity for Al(III) against Mg(II) in protein cavities. Journal of Inorganic Biochemistry, 2007, 101, 1192-1200.	3.5	31

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73	New Approximation to the Third-Order Density. Application to the Calculation of Correlated Multicenter Indices. Journal of Chemical Theory and Computation, 2014, 10, 3055-3065.	5.3	31
74	Upper bounds to the electron-electron coalescence density in terms of the one-electron density function. Physical Review A, 1994, 49, 3081-3082.	2.5	30
75	Can correlation bring electrons closer together?. Molecular Physics, 2009, 107, 1089-1093.	1.7	30
76	A QM/MM study of the complexes formed by aluminum and iron with serum transferrin at neutral and acidic pH. Journal of Inorganic Biochemistry, 2011, 105, 1446-1456.	3.5	30
77	Plasmonic Resonances in the Al‹sub›13‹/sub›‹sup›â€“‹/sup› Cluster: Quantification and Origin of Exciton Collectivity. Journal of Physical Chemistry C, 2016, 120, 12742-12750.	3.1	30
78	Many low-lying isomers of the cationic and neutral niobium trimer and tetramer. Physical Review A, 1999, 60, 3058-3070.	2.5	27
79	Comparative Study of Various Mechanisms for Metallocene-Catalyzed Î±-Olefin Polymerization. Organometallics, 2005, 24, 3233-3246.	2.3	27
80	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
81	Modeling Surface Passivation of ZnS Quantum Dots. Journal of Physical Chemistry C, 2012, 116, 2740-2750.	3.1	27
82	The Laplacian of the intracule and extracule densities and their relationship to the shell structure of atoms. Journal of Chemical Physics, 1992, 96, 6778-6783.	3.0	26
83	Electronic excitation energies of smallZniSiclusters. Physical Review A, 2000, 63, .	2.5	26
84	Comparison of Ti, Zr, and Hf as Cations for Metallocene-Catalyzed Olefin Polymerization. Organometallics, 2006, 25, 4483-4490.	2.3	26
85	Aluminum speciation in biological environments. The deprotonation of free and aluminum bound citrate in aqueous solution. Physical Chemistry Chemical Physics, 2012, 14, 12465.	2.8	26
86	An ab initio study on the mechanism of the alkeneâ€“isocyanate cycloaddition reaction to form Î²-lactams. Journal of the Chemical Society Chemical Communications, 1993, , 1450-1452.	2.0	25
87	Aluminum(III) Interactions with the Acidic Amino Acid Chains. Journal of Physical Chemistry A, 1998, 102, 7006-7012.	2.5	25
88	Diradicals and Diradicaloids in Natural Orbital Functional Theory. ChemPhysChem, 2011, 12, 1061-1065.	2.1	25
89	Theoretical studies of possible processes for the interstellar production of phosphorus compounds: reaction of phosphorus(1+) with ammonia. The Journal of Physical Chemistry, 1991, 95, 170-175.	2.9	24
90	Activation of Methane by the Iron Dimer Cation. A Theoretical Study. Journal of Physical Chemistry A, 2006, 110, 12501-12511.	2.5	24

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91	Endohedral Stannaspherenes Mn@Sn‹sub›12‹/sub› and its Dimer: Ferromagnetic or Antiferromagnetic?. ChemPhysChem, 2007, 8, 2096-2099.	2.1	24
92	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
93	Experimental and Theoretical Study of a Cadmium Coordination Polymer Based on Aminonicotinate with Second-Timescale Blue/Green Photoluminescent Emission. Inorganic Chemistry, 2017, 56, 3149-3152.	4.0	24
94	The evaluation of extracule and intracule densities in the first-row hydrides, LiH, BeH, BH, CH, NH, OH and FH, from self-consistent field molecular orbital wavefunctions. Journal of Physics B: Atomic, Molecular and Optical Physics, 1990, 23, 1095-1105.	1.5	23
95	High-level ab initio calculations on low barrier hydrogen bonds and proton bound homodimers. Chemical Physics Letters, 2010, 493, 37-44.	2.6	23
96	The Electronic Structure of the Al‹sub›3‹/sub›‹sup›â^'‹/sup› Anion: Is it Aromatic?. Chemistry - A European Journal, 2015, 21, 9610-9614.	3.3	23
97	Atomic configuration-interaction electron-electron counterbalance densities. Physical Review A, 1999, 59, 4255-4258.	2.5	22
98	Aluminum(III) Interactions with the Acid Derivative Amino Acid Chains. Journal of Physical Chemistry A, 2000, 104, 7053-7060.	2.5	22
99	Clusters of Group IIâ^'VI Materials:â€‰ CdiOi (i â‰ 15). Journal of Physical Chemistry A, 2003, 107, 9918-9923.	2.5	22
100	Protein Side Chains Facilitate Mg/Al Exchange in Model Protein Binding Sites. ChemPhysChem, 2007, 8, 2119-2124.	2.1	22
101	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
102	Natural Orbital Functional Theory and Reactivity Studies of Diradical Rearrangements: Ethylene Torsion as a Case Study. ChemPhysChem, 2011, 12, 1673-1676.	2.1	22
103	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
104	Correlation holes for the helium dimer. Journal of Chemical Physics, 2008, 128, 134102.	3.0	21
105	Elucidating the 3D structures of Al(‹scp›iii‹/scp›)â€“Aî² complexes: a template free strategy based on the pre-organization hypothesis. Chemical Science, 2017, 8, 5041-5049.	7.4	21
106	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
107	Conformations and charge distributions in 1,2-dinitrosoethylene and furoxan. 1. An ab initio molecular orbital study. The Journal of Physical Chemistry, 1988, 92, 5094-5096.	2.9	20
108	Theoretical studies of possible processes for the interstellar production of phosphorus compounds: reaction of phosphorus(1+) with water. The Journal of Physical Chemistry, 1991, 95, 5443-5445.	2.9	20

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109	Computational evaluation of pK a for oxygenated side chain containing amino acids interacting with Aluminum. Theoretical Chemistry Accounts, 2011, 128, 477-484.	1.4	20
110	Quantum Dot Photoactivation of Pt(IV) Anticancer Agents: Evidence of an Electron Transfer Mechanism Driven by Electronic Coupling. Journal of Physical Chemistry C, 2014, 118, 8712-8721.	3.1	20
111	The effect of TiO₂ surface on the electron injection efficiency in PbS quantum dot solar cells: a first-principles study. Physical Chemistry Chemical Physics, 2015, 17, 6076-6086.	2.8	20
112	The electronic states of Fe2+. Chemical Physics Letters, 2003, 376, 310-317.	2.6	19
113	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
114	Non-Bornâ€“Oppenheimer treatment of the H2 Hookean molecule. Journal of Chemical Physics, 2005, 123, 024102.	3.0	19
115	Thermally Stable Solids Based on Endohedrally Doped ZnS Clusters. Chemistry - A European Journal, 2009, 15, 5138-5144.	3.3	19
116	A theoretical study of the structures and stabilities of (H2PO)+ species and the proton affinities of HPO and POH. The Journal of Physical Chemistry, 1991, 95, 4318-4323.	2.9	18
117	Density Functional Studies of the bï€.aïƒ Charge-Transfer Complex Formed between Ethyne and Chlorine Monofluoride. Journal of Physical Chemistry A, 1997, 101, 3021-3024.	2.5	18
118	Ab-InitioStudies of Alternant X2Y2Rings (X = N, P, As, and Sb and Y = O, S, Se, and Te). PlanarversusButterfly Structures. Journal of Physical Chemistry A, 1997, 101, 5574-5579.	2.5	18
119	Piris natural orbital functional study of the dissociation of the radical helium dimer. Journal of Chemical Physics, 2008, 129, 014108.	3.0	18
120	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
121	The Nature of Chemical Bonds from PNOF5 Calculations. ChemPhysChem, 2012, 13, 2297-2303.	2.1	18
122	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
123	Theoretical studies of possible processes for interstellar production of phosphorus compounds: reaction of phosphorus(1+) with methane. The Journal of Physical Chemistry, 1991, 95, 6553-6557.	2.9	17
124	Aluminum (III) interactions with the side chains of aromatic aminoacids. International Journal of Quantum Chemistry, 2002, 90, 859-881.	2.0	17
125	Discordant results on the FeO+â€‰+â€‰H2reaction reconciled by quantum Monte Carlo theory. Molecular Physics, 2004, 102, 2635-2637.	1.7	17
126	Bound excited states ofHâ^’andHeâ^’in the statically screened Coulomb potential. Physical Review A, 1998, 57, 2550-2555.	2.5	16

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127	Critical conditions for stable dipole-bound dianions. Journal of Chemical Physics, 1999, 110, 11717-11719.	3.0	16
128	Electronic excitation energies of ZniSinanoparticles. Nanotechnology, 2006, 17, 4100-4105.	2.6	16
129	Exact non-Born-Oppenheimer wave functions for three-particle Hookean systems with arbitrary masses. Physical Review A, 2006, 74, .	2.5	16
130	Sandwich Complexes of the Metalloaromatic Î·³-Al₃R₃ Ligand. Journal of the American Chemical Society, 2009, 131, 6949-6951.	13.7	16
131	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
132	Mapping the affinity of aluminum(<scp>iii</scp>) for biophosphates: interaction mode and binding affinity in 1â€‰:â€‰1 complexes. Physical Chemistry Chemical Physics, 2014, 16, 20107.	2.8	16
133	Theoretical study of possible processes for the interstellar production of phosphorus compounds. Reaction of phosphorus(1+) with hydrogen sulfide. The Journal of Physical Chemistry, 1993, 97, 1521-1525.	2.9	15
134	Field-Mediated Chirality Information Transfer in Moleculeâ€“Nanoparticle Hybrids. Journal of Physical Chemistry C, 2020, 124, 1560-1565.	3.1	15
135	Intracule and Extracule Densities: Historical Perspectives and Future Prospects. Mathematical and Computational Chemistry, 2000, , 231-248.	0.3	15
136	An ab initio SCF-MO study of the decomposition reaction of nitrosoethylene to formaldehyde and hydrogen cyanide. Computational and Theoretical Chemistry, 1992, 258, 167-174.	1.5	14
137	Natural orbital functional description of van der Waals interactions: A case study of the effect of the basis set for the helium dimer. International Journal of Quantum Chemistry, 2008, 108, 1660-1663.	2.0	14
138	Ab Initio Study of Microsolvated Al³⁺â^'Aromatic Amino Acid Complexes. Journal of Physical Chemistry B, 2010, 114, 9017-9022.	2.6	14
139	sp3 Hybrid orbitals and ionization energies of methane from PNOF5. Chemical Physics Letters, 2012, 531, 272-274.	2.6	14
140	Doped Aluminum Cluster Anions: Size Matters. Journal of Physical Chemistry A, 2014, 118, 4309-4314.	2.5	14
141	Exchange-correlation effects in momentum space for atoms: an analysis of the isoelectronic series of Li2S and Be1S. Journal of Physics B: Atomic and Molecular Physics, 1987, 20, 2153-2163.	1.6	13
142	Theoretical Studies of Possible Processes for the Interstellar Production of Phosphorus Compounds. The Reaction of P+ with Acetylene. The Journal of Physical Chemistry, 1995, 99, 6432-6440.	2.9	13
143	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
144	Carbo-Cages: A Computational Study. Journal of Organic Chemistry, 2014, 79, 5463-5470.	3.2	13

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145	The trans Effect in Palladium Phosphine Sulfonate Complexes. Journal of Physical Chemistry A, 2017, 121, 7709-7716.	2.5	13
146	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
147	Dynamic screening of swift hydrogenlike ions moving in condensed matter. Nuclear Instruments & Methods in Physics Research B, 1990, 48, 21-24.	1.4	12
148	Transition structures for the reformatsky reaction. A theoretical (MNDO-PM3) study.. Tetrahedron Letters, 1993, 34, 6111-6114.	1.4	12
149	Aluminum (III) Interactions with Sulfur-Containing Amino Acid Chains. Journal of Physical Chemistry A, 2001, 105, 7446-7453.	2.5	12
150	A reinterpretation of the nature of the Fermi hole. Journal of Chemical Physics, 2004, 120, 540-547.	3.0	12
151	Exact non-Born-Oppenheimer wave function for the Hooke-Calogero model of the H2 molecule. European Physical Journal D, 2006, 37, 351-359.	1.3	12
152	Complete basis set limit extrapolation calculations with PNOF3. Chemical Physics Letters, 2010, 499, 164-167.	2.6	12
153	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
154	Non-Born-Oppenheimer electronic and nuclear densities for a Hooke-Calogero three-particle model: Non-uniqueness of density-derived molecular structure. Journal of Chemical Physics, 2012, 136, 084103.	3.0	12
155	Self-assembling endohedrally doped CdS nanoclusters: new porous solid phases of CdS. Physical Chemistry Chemical Physics, 2012, 14, 9676.	2.8	12
156	Molecules with High Bond Orders and Ultrashort Bond Lengths: CrU, MoU, and WU. Inorganic Chemistry, 2013, 52, 2838-2843.	4.0	12
157	Effect of Structural Dynamics on the Opto-Electronic Properties of Bare and Hydrated ZnS QDs. Journal of Physical Chemistry C, 2014, 118, 3274-3284.	3.1	12
158	Ceramide increases free volume voids in DPPC membranes. RSC Advances, 2015, 5, 44282-44290.	3.6	12
159	Theoretical and experimental studies on the periselectivity of the cycloaddition reaction between activated ketenes and conjugated imines. Tetrahedron Letters, 1994, 35, 7825-7828.	1.4	12
160	Ab initio characterization of gaseous phosphorus oxide (P2O2). The Journal of Physical Chemistry, 1993, 97, 4078-4079.	2.9	11
161	Electronâ€"electron counterbalance density for molecules: Exchange and correlation effects. Journal of Chemical Physics, 2001, 115, 1987-1994.	3.0	11
162	Incremental binding free energies of aluminum (III) vs. magnesium (II) complexes. Chemical Physics, 2003, 295, 175-184.	1.9	11

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163	Complexation of Al^{III} by Aromatic Amino Acids in the Gas Phase. Inorganic Chemistry, 2007, 46, 6413-6419.	4.0	11
164	The stability of biradicaloid versus closed-shell [E(Î¼-XR)]₂ (E = P, As; X = N, P, As) rings. Does aromaticity play a role?. Physical Chemistry Chemical Physics, 2016, 18, 11879-11884.	2.8	11
165	Advances in approximate natural orbital functional theory. Advances in Quantum Chemistry, 2019, 79, 155-177.	0.8	11
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