

Jesus M Ugalde

List of Publications by Year in descending order

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246
papers

7,419
citations

53660

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79541

73
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257
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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. <i>Angewandte Chemie - International Edition</i> , 2000, 39, 717-721.	7.2	229
2	High Impact of Antiphospholipid Syndrome on Irreversible Organ Damage and Survival of Patients With Systemic Lupus Erythematosus. <i>Archives of Internal Medicine</i> , 2004, 164, 77.	4.3	195
3	A semiempirical theoretical study on the formation of .beta.-lactams from ketenes and imines. <i>Journal of the American Chemical Society</i> , 1993, 115, 995-1004.	6.6	152
4	The Curiously Stable Cluster and its Neutral and Anionic Counterparts:Â The Advantages of PlanarityÂ€. <i>Journal of Physical Chemistry A</i> , 2000, 104, 397-403.	1.1	149
5	Measuring the Spinâ€Polarization Power of a Single Chiral Molecule. <i>Small</i> , 2017, 13, 1602519.	5.2	143
6	Unexpected trends in halogen-bond based noncovalent adducts. <i>Chemical Communications</i> , 2012, 48, 7708.	2.2	136
7	On the directionality of halogen bonding. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 10350.	1.3	136
8	Recent developments and future prospects of all-metal aromatic compounds. <i>Chemical Society Reviews</i> , 2015, 44, 6519-6534.	18.7	128
9	Unravelling phenomenon of internal rotation in B13+ through chemical bonding analysis. <i>Chemical Communications</i> , 2011, 47, 6242.	2.2	120
10	Reactivity of Cr+(6S,4D), Mn+(7S,5S), and Fe+(6D,4F): Reaction of Cr+, Mn+, and Fe+with Water. <i>Journal of the American Chemical Society</i> , 1999, 121, 8549-8558.	6.6	116
11	Reactivity of Co+(3F,5F), Ni+(2D,4F), and Cu+(1S,3D): Reaction of Co+, Ni+, and Cu+with Water. <i>Journal of the American Chemical Society</i> , 2000, 122, 114-122.	6.6	114
12	A natural orbital functional for multiconfigurational states. <i>Journal of Chemical Physics</i> , 2011, 134, 164102.	1.2	114
13	Catalytic and Solvent Effects on the Cycloaddition Reaction between Ketenes and Carbonyl Compounds To Form 2-Oxetanones. <i>Journal of the American Chemical Society</i> , 1994, 116, 9613-9619.	6.6	113
14	Theoretical Study of Two-State Reactivity of Transition Metal Cations:Â The â€œDifficultyâ€-Case of Iron Ion Interacting with Water, Ammonia, and Methane. <i>Journal of Physical Chemistry A</i> , 2004, 108, 1069-1081.	1.1	112
15	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.	1.5	106
16	Chiral Control in the Staudinger Reaction between Ketenes and Imines. A Theoretical SCF-MO Study on Asymmetric Torquoselectivity. <i>Journal of the American Chemical Society</i> , 1994, 116, 2085-2093.	6.6	104
17	Theoretical methods that help understanding the structure and reactivity of gas phase ions. <i>International Journal of Mass Spectrometry</i> , 2005, 240, 37-99.	0.7	104
18	Reactivity of Sc+(3D,1D) and V+(5D,3F):Â Reaction of Sc+and V+with Water. <i>Journal of the American Chemical Society</i> , 1999, 121, 574-580.	6.6	102

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19	Sandwich-Like Complexes Based on σ -All-Metal-(Al ₄ 2-) Aromatic Compounds. Journal of the American Chemical Society, 2004, 126, 3380-3381.	6.6	102
20	Structure and Properties of ZnS Nanoclusters. Journal of Physical Chemistry B, 2005, 109, 2703-2709.	1.2	102
21	Bond Paths Show Preferable Interactions: Ab Initio and QTAIM Studies on the $X \cdots H \cdots A \cdots B$ Hydrogen Bond. Journal of Physical Chemistry A, 2010, 114, 7223-7229.	1.1	101
22	Electronic Excitation Energies of ZnO Clusters. Journal of the American Chemical Society, 2003, 125, 9494-9499.	6.6	98
23	Small clusters of II-VI materials: ZnO _i , i=1-9. Physical Review A, 2000, 62, .	1.0	88
24	Small clusters of II-VI materials: ZnSi _i , i=1-9. Physical Review A, 2000, 61, .	1.0	85
25	A Joint Experimental and Theoretical Study of Cation- π Interactions: A 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.	6.6	81
26	Designing 3-D Molecular Stars. Journal of the American Chemical Society, 2009, 131, 9426-9431.	6.6	78
27	A Chirality-Based Quantum Leap. ACS Nano, 2022, 16, 4989-5035.	7.3	74
28	Iterative diagonalization for orbital optimization in natural orbital functional theory. Journal of Computational Chemistry, 2009, 30, 2078-2086.	1.5	73
29	Perspective on natural orbital functional theory. International Journal of Quantum Chemistry, 2014, 114, 1169-1175.	1.0	69
30	Benchmark Assessment of Density Functional Methods on Group II-VI MX (M = Zn, Cd; X = S, Se, Te) Quantum Dots. Journal of Chemical Theory and Computation, 2014, 10, 76-89.	2.3	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.	6.6	68
32	Communications: Accurate description of atoms and molecules by natural orbital functional theory. Journal of Chemical Physics, 2010, 132, 031103.	1.2	68
33	On the Reactivity of Ti ⁺ (4F,2F). Reaction of Ti ⁺ with OH ₂ . Journal of Physical Chemistry A, 1998, 102, 293-300.	1.1	67
34	Antiphospholipid antibodies predict early damage in patients with systemic lupus erythematosus. Lupus, 2004, 13, 900-905.	0.8	60
35	Communication: The role of the positivity N-representability conditions in natural orbital functional theory. Journal of Chemical Physics, 2010, 133, 111101.	1.2	60
36	Pro-oxidant Activity of Aluminum: Stabilization of the Aluminum Superoxide Radical Ion. Journal of Physical Chemistry A, 2011, 115, 6717-6723.	1.1	60

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37	A DFT/TDDFT study on the optoelectronic properties of the amine-capped magic (CdSe) ₁₃ nanocluster. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 10996.	1.3	57
38	Clusters of II ^{VI} Materials: Cd_iX_i , X = S, Se, Te, $i \leq 16$. <i>Journal of Physical Chemistry A</i> , 2004, 108, 10502-10508.	1.1	56
39	Planar tetracoordinate carbon in CE_4 (E=Al, Ga, In, Tl) clusters. <i>Chemical Physics Letters</i> , 2012, 519-520, 29-33.	1.2	56
40	CBe_5E (E = Al, Ga, In, Tl): planar pentacoordinate carbon in heptaatomic clusters. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14764.	1.3	55
41	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.	2.3	53
42	Spin conserving natural orbital functional theory. <i>Journal of Chemical Physics</i> , 2009, 131, 021102.	1.2	52
43	Al_{12} and the $\text{Al}@_{12}$ clusters. <i>Physical Review A</i> , 1998, 58, 383-388.	1.0	51
44	The Ferrocene ⁺ Lithium Cation Complex in the Gas Phase. <i>Journal of the American Chemical Society</i> , 2001, 123, 5040-5043.	6.6	51
45	An Ideal Spin Filter: Long-Range, High-Spin Selectivity in Chiral Helicoidal 3-Dimensional Metal Organic Frameworks. <i>Nano Letters</i> , 2020, 20, 8476-8482.	4.5	47
46	Solvent and Substituent Effects in the Periselectivity of the Staudinger Reaction between Ketenes and $\hat{1}, \hat{2}$ -Unsaturated Imines. A Theoretical and Experimental Study. <i>Journal of Organic Chemistry</i> , 1996, 61, 3070-3079.	1.7	46
47	Dispersion interactions within the Piris natural orbital functional theory: The helium dimer. <i>Journal of Chemical Physics</i> , 2007, 126, 214103.	1.2	46
48	A first-principles study of II ^{VI} (II = Zn; VI = O, S, Se, Te) semiconductor nanostructures. <i>Journal of Materials Chemistry</i> , 2012, 22, 21453.	6.7	45
49	Mono- and Multidecker Sandwich-Like Complexes of the Tetraazacyclobutadiene Aromatic Ring. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 5485-5488.	7.2	42
50	The Bond Order of C_2 from a Strictly N -Representable Natural Orbital Energy Functional Perspective. <i>Chemistry - A European Journal</i> , 2016, 22, 4109-4115.	1.7	42
51	Hydrogen-Bonding Interactions between Formic Acid and Pyridine. <i>Journal of Physical Chemistry A</i> , 2002, 106, 4187-4191.	1.1	41
52	Molecular Dynamics Simulations of Iron- and Aluminum-Loaded Serum Transferrin: Protonation of Tyr188 Is Necessary To Prompt Metal Release. <i>Biochemistry</i> , 2012, 51, 7017-7027.	1.2	41
53	ALUMINIUM IN BIOLOGICAL ENVIRONMENTS: A COMPUTATIONAL APPROACH. <i>Computational and Structural Biotechnology Journal</i> , 2014, 9, e201403002.	1.9	41
54	Theoretical Study of the C_2P Radical and $(\text{C}_2\text{P})^+$ Species. <i>The Journal of Physical Chemistry</i> , 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. <i>Journal of Inorganic Biochemistry</i> , 2006, 100, 374-384.	1.5	40
56	Sandwich Complexes Based on the π -All-Metal- π -Al ₄ Aromatic Ring. <i>Chemistry - A European Journal</i> , 2006, 12, 4495-4502.	1.7	40
57	Intracule densities and electron correlation in the hydrogen molecule. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 1988, 21, 2555-2561.	0.6	39
58	Substituent and Solvent Effects in the [2 + 2] Cycloaddition Reaction between Olefins and Isocyanates. <i>Journal of the American Chemical Society</i> , 1995, 117, 12306-12313.	6.6	39
59	The extended Koopmans's theorem: Vertical ionization potentials from natural orbital functional theory. <i>Journal of Chemical Physics</i> , 2012, 136, 174116.	1.2	39
60	The natural orbital functional theory of the bonding in Cr ₂ , Mo ₂ and W ₂ . <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 2055-2062.	1.3	38
61	Communication: Chemical bonding in carbon dimer isovalent series from the natural orbital functional theory perspective. <i>Journal of Chemical Physics</i> , 2013, 138, 151102.	1.2	38
62	Quantum mechanical calculations on phosphate hydrolysis reactions. <i>Journal of Computational Chemistry</i> , 2000, 21, 43-51.	1.5	37
63	Stability and Aromaticity of BiNi Rings and Fullerenes. <i>Journal of Physical Chemistry A</i> , 2003, 107, 10004-10010.	1.1	37
64	Small clusters of group-(II-VI) materials: Zn _i X _i , X=Se, Te, i=1-9. <i>Physical Review A</i> , 2001, 64, .	1.0	36
65	The Spin Dependence of the Spatial Size of Fe(II) and of the Structure of Fe(II)-Porphyrins. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4653-4657.	1.1	36
66	Homolytic molecular dissociation in natural orbital functional theory. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20129.	1.3	35
67	Electronic excitation energies of ZnSi clusters. <i>Physical Review A</i> , 2001, 64, .	1.0	34
68	The one-electron picture in the Piris natural orbital functional 5 (PNOF5). <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	33
69	The aromaticity of dicupra[10]annulenes. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 9669-9675.	1.3	33
70	The evaluation of electronic extracule and intracule densities and related probability functions in terms of Gaussian basis functions. <i>Journal of Mathematical Chemistry</i> , 1991, 6, 51-61.	0.7	32
71	Role of the isomerization pathways in the Staudinger reaction. A theoretical study on the interaction between activated ketenes and imidates. <i>Tetrahedron Letters</i> , 1994, 35, 4465-4468.	0.7	31
72	A theoretical study of the principles regulating the specificity for Al(III) against Mg(II) in protein cavities. <i>Journal of Inorganic Biochemistry</i> , 2007, 101, 1192-1200.	1.5	31

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73	New Approximation to the Third-Order Density. Application to the Calculation of Correlated Multicenter Indices. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3055-3065.	2.3	31
74	Upper bounds to the electron-electron coalescence density in terms of the one-electron density function. <i>Physical Review A</i> , 1994, 49, 3081-3082.	1.0	30
75	Can correlation bring electrons closer together?. <i>Molecular Physics</i> , 2009, 107, 1089-1093.	0.8	30
76	A QM/MM study of the complexes formed by aluminum and iron with serum transferrin at neutral and acidic pH. <i>Journal of Inorganic Biochemistry</i> , 2011, 105, 1446-1456.	1.5	30
77	Plasmonic Resonances in the Al ₁₃ ⁺ Cluster: Quantification and Origin of Exciton Collectivity. <i>Journal of Physical Chemistry C</i> , 2016, 120, 12742-12750.	1.5	30
78	Many low-lying isomers of the cationic and neutral niobium trimer and tetramer. <i>Physical Review A</i> , 1999, 60, 3058-3070.	1.0	27
79	Comparative Study of Various Mechanisms for Metallocene-Catalyzed $\hat{\pm}$ -Olefin Polymerization. <i>Organometallics</i> , 2005, 24, 3233-3246.	1.1	27
80	Endohedral (X@ZnSi) _{i=4-160} [±] Nanoclusters, X = Li, Na, K, Cl, Br. <i>Journal of Physical Chemistry C</i> , 2007, 111, 3560-3565.	1.5	27
81	Modeling Surface Passivation of ZnS Quantum Dots. <i>Journal of Physical Chemistry C</i> , 2012, 116, 2740-2750.	1.5	27
82	The Laplacian of the intracule and extracule densities and their relationship to the shell structure of atoms. <i>Journal of Chemical Physics</i> , 1992, 96, 6778-6783.	1.2	26
83	Electronic excitation energies of small ZnSi clusters. <i>Physical Review A</i> , 2000, 63, .	1.0	26
84	Comparison of Ti, Zr, and Hf as Cations for Metallocene-Catalyzed Olefin Polymerization. <i>Organometallics</i> , 2006, 25, 4483-4490.	1.1	26
85	Aluminum speciation in biological environments. The deprotonation of free and aluminum bound citrate in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 12465.	1.3	26
86	An ab initio study on the mechanism of the alkene-isocyanate cycloaddition reaction to form $\hat{2}$ -lactams. <i>Journal of the Chemical Society Chemical Communications</i> , 1993, , 1450-1452.	2.0	25
87	Aluminum(III) Interactions with the Acidic Amino Acid Chains. <i>Journal of Physical Chemistry A</i> , 1998, 102, 7006-7012.	1.1	25
88	Diradicals and Diradicaloids in Natural Orbital Functional Theory. <i>ChemPhysChem</i> , 2011, 12, 1061-1065.	1.0	25
89	Theoretical studies of possible processes for the interstellar production of phosphorus compounds: reaction of phosphorus(1+) with ammonia. <i>The Journal of Physical Chemistry</i> , 1991, 95, 170-175.	2.9	24
90	Activation of Methane by the Iron Dimer Cation. A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12501-12511.	1.1	24

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91	Endohedral Stannaspherenes Mn@Sn ₁₂ and its Dimer: Ferromagnetic or Antiferromagnetic?. ChemPhysChem, 2007, 8, 2096-2099.	1.0	24
92	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. Journal of Chemical Theory and Computation, 2012, 8, 2646-2652.	2.3	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.	1.9	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.	0.6	23
95	High-level ab initio calculations on low barrier hydrogen bonds and proton bound homodimers. Chemical Physics Letters, 2010, 493, 37-44.	1.2	23
96	The Electronic Structure of the Al ₃ ⁻ Anion: Is it Aromatic?. Chemistry - A European Journal, 2015, 21, 9610-9614.	1.7	23
97	Atomic configuration-interaction electron-electron counterbalance densities. Physical Review A, 1999, 59, 4255-4258.	1.0	22
98	Aluminum(III) Interactions with the Acid Derivative Amino Acid Chains. Journal of Physical Chemistry A, 2000, 104, 7053-7060.	1.1	22
99	Clusters of Group II-VI Materials: CdO (i = 15). Journal of Physical Chemistry A, 2003, 107, 9918-9923.	1.1	22
100	Protein Side Chains Facilitate Mg/Al Exchange in Model Protein Binding Sites. ChemPhysChem, 2007, 8, 2119-2124.	1.0	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.	1.3	22
102	Natural Orbital Functional Theory and Reactivity Studies of Diradical Rearrangements: Ethylene Torsion as a Case Study. ChemPhysChem, 2011, 12, 1673-1676.	1.0	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.	1.3	22
104	Correlation holes for the helium dimer. Journal of Chemical Physics, 2008, 128, 134102.	1.2	21
105	Elucidating the 3D structures of Al(ⁱⁱⁱ)-Al ²⁺ complexes: a template free strategy based on the pre-organization hypothesis. Chemical Science, 2017, 8, 5041-5049.	3.7	21
106	Chirality-Induced Electron Spin Polarization and Enantiospecific Response in Solid-State Cross-Polarization Nuclear Magnetic Resonance. ACS Nano, 2018, 12, 11426-11433.	7.3	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. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 477-484.	0.5	20
110	Quantum Dot Photoactivation of Pt(IV) Anticancer Agents: Evidence of an Electron Transfer Mechanism Driven by Electronic Coupling. <i>Journal of Physical Chemistry C</i> , 2014, 118, 8712-8721.	1.5	20
111	The effect of TiO ₂ surface on the electron injection efficiency in PbS quantum dot solar cells: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 6076-6086.	1.3	20
112	The electronic states of Fe ²⁺ . <i>Chemical Physics Letters</i> , 2003, 376, 310-317.	1.2	19
113	The first solvation shell of aluminum (III) and magnesium (II) cations in a protein model environment. <i>International Journal of Quantum Chemistry</i> , 2004, 98, 409-424.	1.0	19
114	Non-Born-Oppenheimer treatment of the H ₂ Hookean molecule. <i>Journal of Chemical Physics</i> , 2005, 123, 024102.	1.2	19
115	Thermally Stable Solids Based on Endohedrally Doped ZnS Clusters. <i>Chemistry - A European Journal</i> , 2009, 15, 5138-5144.	1.7	19
116	A theoretical study of the structures and stabilities of (H ₂ PO) ⁺ species and the proton affinities of HPO and POH. <i>The Journal of Physical Chemistry</i> , 1991, 95, 4318-4323.	2.9	18
117	Density Functional Studies of the σ -Charge-Transfer Complex Formed between Ethyne and Chlorine Monofluoride. <i>Journal of Physical Chemistry A</i> , 1997, 101, 3021-3024.	1.1	18
118	Ab-Initio Studies of Alternant X ₂ Y ₂ Rings (X = N, P, As, and Sb and Y = O, S, Se, and Te). Planar versus Butterfly Structures. <i>Journal of Physical Chemistry A</i> , 1997, 101, 5574-5579.	1.1	18
119	Piriz natural orbital functional study of the dissociation of the radical helium dimer. <i>Journal of Chemical Physics</i> , 2008, 129, 014108.	1.2	18
120	Quantum Monte Carlo study of the ground state and low-lying excited states of the scandium dimer. <i>Journal of Chemical Physics</i> , 2008, 128, 194315.	1.2	18
121	The Nature of Chemical Bonds from PNOF5 Calculations. <i>ChemPhysChem</i> , 2012, 13, 2297-2303.	1.0	18
122	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.	1.2	18
123	Theoretical studies of possible processes for interstellar production of phosphorus compounds: reaction of phosphorus(1+) with methane. <i>The Journal of Physical Chemistry</i> , 1991, 95, 6553-6557.	2.9	17
124	Aluminum (III) interactions with the side chains of aromatic amino acids. <i>International Journal of Quantum Chemistry</i> , 2002, 90, 859-881.	1.0	17
125	Discordant results on the FeO + H ₂ reaction reconciled by quantum Monte Carlo theory. <i>Molecular Physics</i> , 2004, 102, 2635-2637.	0.8	17
126	Bound excited states of H ⁺ and He ⁺ in the statically screened Coulomb potential. <i>Physical Review A</i> , 1998, 57, 2550-2555.	1.0	16

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127	Critical conditions for stable dipole-bound dianions. <i>Journal of Chemical Physics</i> , 1999, 110, 11717-11719.	1.2	16
128	Electronic excitation energies of ZnSinanoparticles. <i>Nanotechnology</i> , 2006, 17, 4100-4105.	1.3	16
129	Exact non-Born-Oppenheimer wave functions for three-particle Hookean systems with arbitrary masses. <i>Physical Review A</i> , 2006, 74, .	1.0	16
130	Sandwich Complexes of the Metalloaromatic $\text{I}^{3-}\text{Al}_3\text{R}_3$ Ligand. <i>Journal of the American Chemical Society</i> , 2009, 131, 6949-6951.	6.6	16
131	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.	1.3	16
132	Mapping the affinity of aluminum(III) for biophosphates: interaction mode and binding affinity in $1\text{-}\alpha\text{-D-Glc-1-P}$ complexes. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 20107.	1.3	16
133	Theoretical study of possible processes for the interstellar production of phosphorus compounds. Reaction of phosphorus(1+) with hydrogen sulfide. <i>The Journal of Physical Chemistry</i> , 1993, 97, 1521-1525.	2.9	15
134	Field-Mediated Chirality Information Transfer in Molecule-Nanoparticle Hybrids. <i>Journal of Physical Chemistry C</i> , 2020, 124, 1560-1565.	1.5	15
135	Intracule and Extracule Densities: Historical Perspectives and Future Prospects. <i>Mathematical and Computational Chemistry</i> , 2000, , 231-248.	0.3	15
136	An ab initio SCF-MO study of the decomposition reaction of nitrosoethylene to formaldehyde and hydrogen cyanide. <i>Computational and Theoretical Chemistry</i> , 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. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1660-1663.	1.0	14
138	Ab Initio Study of Microsolvated Al^{3+} -Aromatic Amino Acid Complexes. <i>Journal of Physical Chemistry B</i> , 2010, 114, 9017-9022.	1.2	14
139	sp^3 Hybrid orbitals and ionization energies of methane from PNOF5. <i>Chemical Physics Letters</i> , 2012, 531, 272-274.	1.2	14
140	Doped Aluminum Cluster Anions: Size Matters. <i>Journal of Physical Chemistry A</i> , 2014, 118, 4309-4314.	1.1	14
141	Exchange-correlation effects in momentum space for atoms: an analysis of the isoelectronic series of Li_2S and Be_1S . <i>Journal of Physics B: Atomic and Molecular Physics</i> , 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. <i>The Journal of Physical Chemistry</i> , 1995, 99, 6432-6440.	2.9	13
143	Structure and Stability of the Endohedrally Doped $(\text{X}@C_d\text{Si})_{i=4,9,12,15,16}q=0,\pm 1$, $\text{X} = \text{Na, K, Cl, Br}$, Nanoclusters. <i>Journal of Physical Chemistry C</i> , 2010, 114, 2476-2483.	1.5	13
144	Carbo-Cages: A Computational Study. <i>Journal of Organic Chemistry</i> , 2014, 79, 5463-5470.	1.7	13

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145	The trans Effect in Palladium Phosphine Sulfonate Complexes. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7709-7716.	1.1	13
146	Probing the structures and bonding of auropolyynes, Au ⁿ⁺ (C _n) ⁿ⁻ Au ⁿ⁺ (n = 1-3), using high-resolution photoelectron imaging. <i>Journal of Chemical Physics</i> , 2018, 149, 144307.	1.2	13
147	Dynamic screening of swift hydrogenlike ions moving in condensed matter. <i>Nuclear Instruments & Methods in Physics Research B</i> , 1990, 48, 21-24.	0.6	12
148	Transition structures for the reformatsky reaction. A theoretical (MNDO-PM3) study.. <i>Tetrahedron Letters</i> , 1993, 34, 6111-6114.	0.7	12
149	Aluminum (III) Interactions with Sulfur-Containing Amino Acid Chains. <i>Journal of Physical Chemistry A</i> , 2001, 105, 7446-7453.	1.1	12
150	A reinterpretation of the nature of the Fermi hole. <i>Journal of Chemical Physics</i> , 2004, 120, 540-547.	1.2	12
151	Exact non-Born-Oppenheimer wave function for the Hooke-Calogero model of the H2 molecule. <i>European Physical Journal D</i> , 2006, 37, 351-359.	0.6	12
152	Complete basis set limit extrapolation calculations with PNOF3. <i>Chemical Physics Letters</i> , 2010, 499, 164-167.	1.2	12
153	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.	1.9	12
154	Non-Born-Oppenheimer electronic and nuclear densities for a Hooke-Calogero three-particle model: Non-uniqueness of density-derived molecular structure. <i>Journal of Chemical Physics</i> , 2012, 136, 084103.	1.2	12
155	Self-assembling endohedrally doped CdS nanoclusters: new porous solid phases of CdS. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 9676.	1.3	12
156	Molecules with High Bond Orders and Ultrashort Bond Lengths: CrU, MoU, and WU. <i>Inorganic Chemistry</i> , 2013, 52, 2838-2843.	1.9	12
157	Effect of Structural Dynamics on the Opto-Electronic Properties of Bare and Hydrated ZnS QDs. <i>Journal of Physical Chemistry C</i> , 2014, 118, 3274-3284.	1.5	12
158	Ceramide increases free volume voids in DPPC membranes. <i>RSC Advances</i> , 2015, 5, 44282-44290.	1.7	12
159	Theoretical and experimental studies on the periselectivity of the cycloaddition reaction between activated ketenes and conjugated imines. <i>Tetrahedron Letters</i> , 1994, 35, 7825-7828.	0.7	12
160	Ab initio characterization of gaseous phosphorus oxide (P2O2). <i>The Journal of Physical Chemistry</i> , 1993, 97, 4078-4079.	2.9	11
161	Electron ⁺ electron counterbalance density for molecules: Exchange and correlation effects. <i>Journal of Chemical Physics</i> , 2001, 115, 1987-1994.	1.2	11
162	Incremental binding free energies of aluminum (III) vs. magnesium (II) complexes. <i>Chemical Physics</i> , 2003, 295, 175-184.	0.9	11

#	ARTICLE	IF	CITATIONS
163	Complexation of Al ^{III} by Aromatic Amino Acids in the Gas Phase. <i>Inorganic Chemistry</i> , 2007, 46, 6413-6419.	1.9	11
164	The stability of biradicaloid <i>versus</i> closed-shell [E(¼-XR)] ₂ (E = P, As; X = N, P, As) rings. Does aromaticity play a role?. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 11879-11884.	1.3	11
165	Advances in approximate natural orbital functional theory. <i>Advances in Quantum Chemistry</i> , 2019, 79, 155-177.	0.4	11
166	Magnetic Endohedral Transition-Metal-Doped Semiconducting Nanoclusters. <i>Chemistry - A European Journal</i> , 2008, 14, 8547-8554.	1.7	10
167	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.	1.3	10
168	Aluminum Interaction with Glutamate and α -Ketoglutarate: A Computational Study. <i>Journal of Physical Chemistry B</i> , 2014, 118, 6680-6686.	1.2	10
169	Enantiospecific Response in Cross-Polarization Solid-State Nuclear Magnetic Resonance of Optically Active Metal Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2020, 142, 17989-17996.	6.6	10
170	Density Functional Studies of the Charge-Transfer Complex between Sulfur Dioxide and Chlorine Monofluoride. <i>Journal of Physical Chemistry A</i> , 1998, 102, 8974-8978.	1.1	9
171	Atomic charge states in a weakly coupled plasma environment. <i>Physical Review E</i> , 2002, 66, 026408.	0.8	9
172	Electron correlation studies by means of local-scaling transformations and electron-pair density functions. <i>Journal of Mathematical Chemistry</i> , 2005, 37, 211-231.	0.7	9
173	Performance of PNOF6 for Hydrogen Abstraction Reactions. <i>Journal of Physical Chemistry A</i> , 2015, 119, 6981-6988.	1.1	9
174	Photosensitization mechanism of Cu(II) porphyrins. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 20533-20540.	1.3	9
175	Conformations and charge distributions in fluoronitrosoethylenes and nitrosoethylene. <i>Canadian Journal of Chemistry</i> , 1990, 68, 762-769.	0.6	8
176	Theoretical and experimental studies on the regioselectivity of the cycloaddition reaction between activated ketenes and conjugated imines. <i>Tetrahedron Letters</i> , 1994, 35, 7825-7828.	0.7	8
177	G2 Study of the Triplet and Singlet [H ₃ , P ₂] ⁺ Potential Energy Surfaces. Mechanisms for the Reaction of P ⁺ (1D,3P) with PH ₃ . <i>Journal of Physical Chemistry A</i> , 1997, 101, 2166-2172.	1.1	8
178	Extracuclear densities of the non-Born-Oppenheimer H ₂ molecule. <i>Chemical Physics Letters</i> , 2005, 412, 381-385.	1.2	8
179	Assessment of Approximate Density Functional Methods for the Study of the Interactions of Al(III) with Aromatic Amino Acids. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1830-1836.	2.3	8
180	Synthesis of Cationic Polyelectrolytes by Inverse Microemulsion Polymerization. <i>Macromolecular Rapid Communications</i> , 2009, 30, 2036-2041.	2.0	8

#	ARTICLE	IF	CITATIONS
181	Ab initio calculations on C_6H_6 - $(HF)_n$ clusters. <i>Canadian Journal of Chemistry</i> , 2010, 88, 769-778.		8
182	Homopolymerization of Ethylene by Palladium Phosphine Sulfonate Catalysts: The Role of Structural and Environmental Factors. <i>Organometallics</i> , 2015, 34, 373-380.	1.1	8
183	Topological evidence for an N-N bond in 1,2-dinitrosoethene: The remarkable structure of the di-N-oxide of 1,2-diazacyclobutadiene. <i>Journal of Physical Organic Chemistry</i> , 1990, 3, 143-146.	0.9	7
184	Analysis of the electron pair density for the ground state of carbon dioxide. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 1992, 25, 1137-1145.	0.6	7
185	Electronic structures of the bound excited quartet states of the helium anion. <i>Physical Review A</i> , 1999, 60, 4375-4378.	1.0	7
186	Charge-density concentration and electron-electron coalescence density in atoms and molecules. <i>Physical Review A</i> , 2000, 62, .	1.0	7
187	Determination of the integrated x-ray scattering intensities through the electron-pair relative-motion density at the origin. <i>Physical Review A</i> , 2001, 64, .	1.0	7
188	Role of electron-electron coalescence density in density functional theory. <i>International Journal of Quantum Chemistry</i> , 2002, 86, 40-45.	1.0	7
189	Thermal Stability of Endohedral First-Row Transition-Metal $TM@ZnSi$ Structures, $i = 12, 16$. <i>Journal of Physical Chemistry C</i> , 2011, 115, 7829-7835.	1.5	7
190	Ion energetics in electron-rich nanoplasmas. <i>New Journal of Physics</i> , 2012, 14, 075017.	1.2	7
191	Selective Transmission of Phonons in Molecular Junctions with Nanoscopic Thermal Baths. <i>Journal of Physical Chemistry C</i> , 2019, 123, 9680-9687.	1.5	7
192	Chemical reactivity studies by the natural orbital functional second-order Møller-Plesset (NOF-MP2) method: water dehydrogenation by the scandium cation. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	7
193	Exchange energy from Gaussian-type basis sets. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 1994, 27, 423-427.	0.6	6
194	Characterization of the $P+Ln$ Ion Molecule Clusters of the First- and Second-Row Hydrides. <i>Journal of the American Chemical Society</i> , 1994, 116, 10670-10678.	6.6	6
195	Mechanisms for the Reaction of Triplet P^+ with XH ($X = Cl, F$). Formation of the $P-X$ Bond. <i>The Journal of Physical Chemistry</i> , 1995, 99, 6812-6818.	2.9	6
196	G1 and G2 Study of the Triplet $[H_4, C, O, P]^+$ Potential Energy Surface. Mechanisms for the Reaction of P^+ (3P) with Methanol. <i>The Journal of Physical Chemistry</i> , 1995, 99, 12170-12178.	2.9	6
197	Characterization of $(P+Lx)$ Lylon Molecule Clusters of First-Row Hydrides. <i>Journal of the American Chemical Society</i> , 1996, 118, 2718-2725.	6.6	6
198	Electronic metastable bound states of Mn^{22+} and Co^{22+} . <i>Chemical Physics Letters</i> , 2003, 372, 82-89.	1.2	6

#	ARTICLE	IF	CITATIONS
199	Electron correlation in the GK state of the hydrogen molecule. <i>Journal of Chemical Physics</i> , 2007, 127, 074307.	1.2	6
200	Structural and optical properties of the naked and passivated Al ₅ Au ₅ bimetallic nanoclusters. <i>Journal of Chemical Physics</i> , 2016, 144, 114302.	1.2	6
201	Phosphorylation promotes Al(III) binding to proteins: GE ₂ EGSGG as a case study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 7197-7207.	1.3	6
202	Electron-Pair Distribution in Chemical Bond Formation. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1916-1923.	1.1	6
203	The Coulomb Hole of the Ne Atom. <i>ChemistryOpen</i> , 2019, 8, 411-417.	0.9	6
204	Conformations and charges distributions in 1,2-dinitrosoethylene and furoxan: 2-ab initio electrostatic potentials and relative bond strengths. <i>Tetrahedron</i> , 1989, 45, 6537-6544.	1.0	5
205	Ab-initio study of phosphorus ion complexes of ammonia and water. <i>The Journal of Physical Chemistry</i> , 1993, 97, 9337-9340.	2.9	5
206	Ab Initio Studies on the Structure of Silyl Isocyanate in the Gas Phase, in Solution, and in the Crystalline State. <i>The Journal of Physical Chemistry</i> , 1996, 100, 9619-9623.	2.9	5
207	Properties of some weakly bound complexes obtained with various density functionals. <i>Computational and Theoretical Chemistry</i> , 1997, 397, 191-197.	1.5	5
208	G2 study of triplet [H ₄ , Si, P] ⁺ potential energy surface: Mechanism for reaction of P ⁺ (3P) with silane. <i>Journal of Computational Chemistry</i> , 1997, 18, 9-19.	1.5	5
209	Quantum Chemical Study of the Reaction between Ni ⁺ and H ₂ S. <i>ChemPhysChem</i> , 2010, 11, 3172-3178.	1.0	5
210	Second-Row Transition-Metal Doping of (ZnSi) _i , i = 12, 16 Nanoclusters: Structural and Magnetic Properties. <i>Computation</i> , 2013, 1, 31-45.	1.0	5
211	Dynamic screening of He-like ions. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 1988, 21, L415-L417.	0.6	4
212	Ab initio characterization of novel gaseous phosphorus oxide ((PO) ₂) ⁺ species. <i>The Journal of Physical Chemistry</i> , 1993, 97, 5860-5863.	2.9	4
213	On the accuracy of density functional theory for ion-molecule clusters. A case study of PL _n ⁺ clusters of the first and second row hydrides. <i>Canadian Journal of Chemistry</i> , 1996, 74, 1032-1048.	0.6	4
214	Molecular and Electronic Structures of TiXH ₆ ⁺ (X = B, Al, Ga) Compounds. <i>Journal of Physical Chemistry A</i> , 1997, 101, 5953-5957.	1.1	4
215	A spin-density polarization index. <i>Journal of Chemical Physics</i> , 1998, 108, 2824-2830.	1.2	4
216	Radial moments of the electron density: Gas phase results and the effects of solvation. <i>Journal of Chemical Physics</i> , 2000, 112, 1113-1121.	1.2	4

#	ARTICLE	IF	CITATIONS
217	Electron-pair density relaxation holes. <i>Journal of Chemical Physics</i> , 2008, 128, 214105.	1.2	4
218	Theoretical study of the PSI ₂ radical. <i>Canadian Journal of Chemistry</i> , 1996, 74, 2476-2480.	0.6	3
219	On the Molecular and Electronic Structures of the H ₃ TiH ₃ Species. <i>The Journal of Physical Chemistry</i> , 1996, 100, 12277-12279.	2.9	3
220	Binding of Carbon Rings to a Graphite Plane. <i>Journal of Physical Chemistry B</i> , 2002, 106, 6871-6874.	1.2	3
221	Minimal dipole charge for a dipole-bound dianion. <i>Molecular Physics</i> , 2003, 101, 2529-2532.	0.8	3
222	Electron-pair density decomposition for core-valence separable systems. <i>Journal of Computational Chemistry</i> , 2012, 33, 2243-2249.	1.5	3
223	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.	1.7	3
224	Nanocluster-Assembled Materials. <i>Series in Materials Science and Engineering</i> , 2016, , 113-148.	0.1	3
225	Ab Initio Characterization of Gaseous (CO ₂) ⁺ Species. <i>The Journal of Physical Chemistry</i> , 1994, 98, 2294-2297.	2.9	2
226	Topological Analysis of the Charge Density for Phosphorus Ion Molecule Complexes Bound to Water and Ammonia Molecules. <i>The Journal of Physical Chemistry</i> , 1994, 98, 3148-3153.	2.9	2
227	Reaction of P ⁺ (3P) with Methylamine: A Detailed Study of the Potential Energy Surface and Reaction Mechanisms. <i>Journal of Physical Chemistry A</i> , 1997, 101, 4807-4813.	1.1	2
228	Molecular and Electronic Structures of (TiXH ₆) ^{0/-} , X = B, Al, Ga, Compounds. <i>Journal of Physical Chemistry A</i> , 1998, 102, 2055-2064.	1.1	2
229	Primary Reaction of the Titanium-Catalyzed Oligomerization of Phosphorus in the Gas Phase. <i>Journal of the American Chemical Society</i> , 2000, 122, 1411-1413.	6.6	2
230	Electron correlation in the 3 ¹ Σ ⁺ g+1 and 2 ¹ Σ ⁺ u+1 excited state lithium molecule. <i>Journal of Chemical Physics</i> , 2006, 125, 234102.	1.2	2
231	Heavy periodane. <i>Journal of Molecular Modeling</i> , 2013, 19, 1953-1958.	0.8	2
232	CdS nanoclusters doped with divalent atoms. <i>Journal of Molecular Modeling</i> , 2014, 20, 2227.	0.8	2
233	Reply to "Comment on "Chirality-Induced Electron Spin Polarization and Enantiospecific Response in Solid-State Cross-Polarization Nuclear Magnetic Resonance". <i>ACS Nano</i> , 2019, 13, 6133-6136.	7.3	2
234	Experiment and Theory Clarify: Sc ⁺ Receives One Oxygen Atom from SO ₂ to Form ScO ⁺ , which Proves to be a Catalyst for the Hidden Oxygen-Exchange with SO ₂ . <i>ChemPhysChem</i> , 2021, , .	1.0	2

#	ARTICLE	IF	CITATIONS
235	Vicinage effect in inner-shell ionization. Physical Review B, 1988, 38, 735-736.	1.1	1
236	KINETIC ENERGY FUNCTIONALS: EXACT ONES FROM ANALYTIC MODEL WAVE FUNCTIONS AND APPROXIMATE ONES IN ORBITAL-FREE MOLECULAR DYNAMICS. International Journal of Modern Physics B, 2010, 24, 5139-5151.	1.0	1
237	The one-electron picture in the Piris natural orbital functional 5 (PNOF5). Highlights in Theoretical Chemistry, 2014, , 5-15.	0.0	1
238	Stability and Aromaticity of BiNi Rings and Fullerenes. ChemInform, 2004, 35, no.	0.1	0
239	Mono- and Multidecker Sandwich-Like Complexes of the Tetraazacyclobutadiene Aromatic Ring.. ChemInform, 2004, 35, no.	0.1	0
240	Clusters of II?VI Materials: CdiXi, X: S, Se, Te, i ? 16.. ChemInform, 2005, 36, no.	0.1	0
241	Structure and Properties of ZnS Nanoclusters. ChemInform, 2005, 36, no.	0.1	0
242	Second International Theoretical Biophysics Symposium, Å–rebro University, Sweden, June 28â€“July 1, 2005. International Journal of Quantum Chemistry, 2007, 107, 259-260.	1.0	0
243	Model for a biexciton in a lateral quantum dot based on exact solutions for the Hookean H₂ molecule. I. Theoretical aspects. International Journal of Quantum Chemistry, 2011, 111, 1808-1818.	1.0	0
244	Methane activation by alternant [N2O2]+ and [N2S2]+ cluster radical cations. International Journal of Mass Spectrometry, 2019, 438, 72-77.	0.7	0
245	Electronic Structure and Electron Delocalization in Bare and Dressed Boron Pentamer Clusters. Journal of Physical Chemistry A, 2021, 125, 5246-5255.	1.1	0
246	THE ELECTRON-PAIR DENSITY AND THE MODELING OF THE SPHERICALLY AVERAGED EXCHANGE-CORRELATION HOLE. , 2003, , .		0