Jesus M Ugalde

List of Publications by Year
in descending order

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246 papers	7,419 citations	53660 45 h-index	79541 73 g-index
257 all docs	257 docs citations	257 times ranked	5240 citing authors

#	Article	IF	Citations
1	A Chirality-Based Quantum Leap. ACS Nano, 2022, 16, 4989-5035.	7.3	74
2	Chemical reactivity studies by the natural orbital functional second-order MÃ¸llerâ€“Plesset (NOF-MP2) method: water dehydrogenation by the scandium cation. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	7
3	Electronic Structure and Electron Delocalization in Bare and Dressed Boron Pentamer Clusters. Journal of Physical Chemistry A, 2021, 125, 5246-5255.	1.1	0
4	Experiment and Theory Clarify: Sc + Receives One Oxygen Atom from SO 2 to Form ScO + , which Proves to be a Catalyst for the Hidden Oxygenâ€Exchange with SO 2. ChemPhysChem, 2021, , .	1.0	2
5	Field-Mediated Chirality Information Transfer in Moleculeâ€“Nanoparticle Hybrids. Journal of Physical Chemistry C, 2020, 124, 1560-1565.	1.5	15
6	An Ideal Spin Filter: Long-Range, High-Spin Selectivity in Chiral Helicoidal 3-Dimensional Metal Organic Frameworks. Nano Letters, 2020, 20, 8476-8482.	4.5	47
7	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.	6.6	10
8	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.	7.3	2
9	Advances in approximate natural orbital functional theory. Advances in Quantum Chemistry, 2019, 79, 155-177.	0.4	11
10	Methane activation by alternant [N2O2]+ and [N2S2]+ cluster radical cations. International Journal of Mass Spectrometry, 2019, 438, 72-77.	0.7	0
11	Selective Transmission of Phonons in Molecular Junctions with Nanoscopic Thermal Baths. Journal of Physical Chemistry C, 2019, 123, 9680-9687.	1.5	7
12	The Coulomb Hole of the Ne Atom. ChemistryOpen, 2019, 8, 411-417.	0.9	6
13	Electron-Pair Distribution in Chemical Bond Formation. Journal of Physical Chemistry A, 2018, 122, 1916-1923.	1.1	6
14	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
15	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.	1.2	13
16	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
17	Elucidating the 3D structures of Al(<scp>iii</scp>)â€“Alî2 complexes: a template free strategy based on the pre-organization hypothesis. Chemical Science, 2017, 8, 5041-5049.	3.7	21
18	The aromaticity of dicupra[10]annulenes. Physical Chemistry Chemical Physics, 2017, 19, 9669-9675.	1.3	33

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19	The trans Effect in Palladium Phosphine Sulfonate Complexes. Journal of Physical Chemistry A, 2017, 121, 7709-7716.	1.1	13
20	Photosensitization mechanism of Cu(<scp>ii</scp>) porphyrins. Physical Chemistry Chemical Physics, 2017, 19, 20533-20540.	1.3	9
21	Measuring the Spinâ€Polarization Power of a Single Chiral Molecule. Small, 2017, 13, 1602519.	5.2	143
22	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.	1.2	18
23	Structural and optical properties of the naked and passivated Al5Au5 bimetallic nanoclusters. Journal of Chemical Physics, 2016, 144, 114302.	1.2	6
24	Plasmonic Resonances in the Al₁₃^{â€“} Cluster: Quantification and Origin of Exciton Collectivity. Journal of Physical Chemistry C, 2016, 120, 12742-12750.	1.5	30
25	Nanocluster-Assembled Materials. Series in Materials Science and Engineering, 2016, , 113-148.	0.1	3
26	The Bond Order of C₂ from a Strictly Nâ€Representable Natural Orbital Energy Functional Perspective. Chemistry - A European Journal, 2016, 22, 4109-4115.	1.7	42
27	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.	1.3	11
28	Phosphorylation promotes Al(<scp>iii</scp>) binding to proteins: GEGEGSGG as a case study. Physical Chemistry Chemical Physics, 2016, 18, 7197-7207.	1.3	6
29	The Electronic Structure of the Al₃^{â¯} Anion: Is it Aromatic?. Chemistry - A European Journal, 2015, 21, 9610-9614.	1.7	23
30	Recent developments and future prospects of all-metal aromatic compounds. Chemical Society Reviews, 2015, 44, 6519-6534.	18.7	128
31	Homopolymerization of Ethylene by Palladium Phosphine Sulfonate Catalysts: The Role of Structural and Environmental Factors. Organometallics, 2015, 34, 373-380.	1.1	8
32	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.	1.3	20
33	Performance of PNOF6 for Hydrogen Abstraction Reactions. Journal of Physical Chemistry A, 2015, 119, 6981-6988.	1.1	9
34	Ceramide increases free volume voids in DPPC membranes. RSC Advances, 2015, 5, 44282-44290.	1.7	12
35	Effect of Structural Dynamics on the Opto-Electronic Properties of Bare and Hydrated ZnS QDs. Journal of Physical Chemistry C, 2014, 118, 3274-3284.	1.5	12
36	Perspective on natural orbital functional theory. International Journal of Quantum Chemistry, 2014, 114, 1169-1175.	1.0	69

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37	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.	2.3	69
38	Doped Aluminum Cluster Anions: Size Matters. Journal of Physical Chemistry A, 2014, 118, 4309-4314.	1.1	14
39	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.	1.5	20
40	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.	1.3	16
41	ALUMINIUM IN BIOLOGICAL ENVIRONMENTS: A COMPUTATIONAL APPROACH. Computational and Structural Biotechnology Journal, 2014, 9, e201403002.	1.9	41
42	CdS nanoclusters doped with divalent atoms. Journal of Molecular Modeling, 2014, 20, 2227.	0.8	2
43	Carbo-Cages: A Computational Study. Journal of Organic Chemistry, 2014, 79, 5463-5470.	1.7	13
44	Aluminum Interaction with Glutamate and Î±-Ketoglutarate: A Computational Study. Journal of Physical Chemistry B, 2014, 118, 6680-6686.	1.2	10
45	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.	2.3	31
46	The one-electron picture in the Piris natural orbital functional 5 (PNOF5). Highlights in Theoretical Chemistry, 2014, , 5-15.	0.0	1
47	Quantum chemical study of the catalytic activation of methane by copper oxide and copper hydroxide cations. Physical Chemistry Chemical Physics, 2013, 15, 1148-1153.	1.3	16
48	The natural orbital functional theory of the bonding in Cr₂, Mo₂and W₂. Physical Chemistry Chemical Physics, 2013, 15, 2055-2062.	1.3	38
49	Heavy periodane. Journal of Molecular Modeling, 2013, 19, 1953-1958.	0.8	2
50	Molecules with High Bond Orders and Ultrashort Bond Lengths: CrU, MoU, and WU. Inorganic Chemistry, 2013, 52, 2838-2843.	1.9	12
51	The one-electron picture in the Piris natural orbital functional 5 (PNOF5). Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	33
52	On the directionality of halogen bonding. Physical Chemistry Chemical Physics, 2013, 15, 10350.	1.3	136
53	Quantum Chemical Study of the Reactions between Pd⁺/Pt⁺ and H₂O/H₂S. Chemistry - A European Journal, 2013, 19, 8832-8838.	1.7	3
54	A DFT/TDDFT study on the optoelectronic properties of the amine-capped magic (CdSe)13 nanocluster. Physical Chemistry Chemical Physics, 2013, 15, 10996.	1.3	57

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55	Communication: Chemical bonding in carbon dimer isovalent series from the natural orbital functional theory perspective. Journal of Chemical Physics, 2013, 138, 151102.	1.2	38
56	Second-Row Transition-Metal Doping of (ZniSi), i = 12, 16 Nanoclusters: Structural and Magnetic Properties. Computation, 2013, 1, 31-45.	1.0	5
57	Ion energetics in electron-rich nanoplasmas. New Journal of Physics, 2012, 14, 075017.	1.2	7
58	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.	1.2	12
59	Aluminum speciation in biological environments. The deprotonation of free and aluminum bound citrate in aqueous solution. Physical Chemistry Chemical Physics, 2012, 14, 12465.	1.3	26
60	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.	1.3	10
61	Molecular Dynamics Simulations of Iron- and Aluminum-Loaded Serum Transferrin: Protonation of Tyr188 Is Necessary To Prompt Metal Release. Biochemistry, 2012, 51, 7017-7027.	1.2	41
62	Modeling Surface Passivation of ZnS Quantum Dots. Journal of Physical Chemistry C, 2012, 116, 2740-2750.	1.5	27
63	CBe5Eâ^' (E = Al, Ga, In, Tl): planar pentacoordinate carbon in heptaatomic clusters. Physical Chemistry Chemical Physics, 2012, 14, 14764.	1.3	55
64	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
65	Self-assembling endohedrally doped CdS nanoclusters: new porous solid phases of CdS. Physical Chemistry Chemical Physics, 2012, 14, 9676.	1.3	12
66	Pro-oxidant activity of aluminum: Promoting the Fenton reaction by reducing Fe(III) to Fe(II). Journal of Inorganic Biochemistry, 2012, 117, 118-123.	1.5	106
67	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
68	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.	2.3	24
69	The extended Koopmansâ€™ theorem: Vertical ionization potentials from natural orbital functional theory. Journal of Chemical Physics, 2012, 136, 174116.	1.2	39
70	Electronâ€pair density decomposition for coreâ€“valence separable systems. Journal of Computational Chemistry, 2012, 33, 2243-2249.	1.5	3
71	The Nature of Chemical Bonds from PNOF5 Calculations. ChemPhysChem, 2012, 13, 2297-2303.	1.0	18
72	Unexpected trends in halogen-bond based noncovalent adducts. Chemical Communications, 2012, 48, 7708.	2.2	136

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73	Planar tetracoordinate carbon in CE42â˜ (E=Alâ€“Tl) clusters. Chemical Physics Letters, 2012, 519-520, 29-33.	1.2	56
74	sp3 Hybrid orbitals and ionization energies of methane from PNOF5. Chemical Physics Letters, 2012, 531, 272-274.	1.2	14
75	Homolytic molecular dissociation in natural orbital functional theory. Physical Chemistry Chemical Physics, 2011, 13, 20129.	1.3	35
76	Thermal Stability of Endohedral First-Row Transition-Metal TM@ZniSi Structures, i = 12, 16. Journal of Physical Chemistry C, 2011, 115, 7829-7835.	1.5	7
77	Pro-oxidant Activity of Aluminum: Stabilization of the Aluminum Superoxide Radical Ion. Journal of Physical Chemistry A, 2011, 115, 6717-6723.	1.1	60
78	Complete vs Restricted Active Space Perturbation Theory Calculation of the Cr₂ Potential Energy Surface. Journal of Chemical Theory and Computation, 2011, 7, 1640-1646.	2.3	53
79	Unravelling phenomenon of internal rotation in B13+ through chemical bonding analysis. Chemical Communications, 2011, 47, 6242.	2.2	120
80	Electronic Structure and Bonding in Heteronuclear Dimers of V, Cr, Mo, and W: a CASSCF/CASPT2 Study. Inorganic Chemistry, 2011, 50, 9219-9229.	1.9	12
81	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.	1.5	30
82	Computational evaluation of pK a for oxygenated side chain containing amino acids interacting with Aluminum. Theoretical Chemistry Accounts, 2011, 128, 477-484.	0.5	20
83	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
84	Diradicals and Diradicaloids in Natural Orbital Functional Theory. ChemPhysChem, 2011, 12, 1061-1065.	1.0	25
85	Natural Orbital Functional Theory and Reactivity Studies of Diradical Rearrangements: Ethylene Torsion as a Case Study. ChemPhysChem, 2011, 12, 1673-1676.	1.0	22
86	A natural orbital functional for multiconfigurational states. Journal of Chemical Physics, 2011, 134, 164102.	1.2	114
87	Quantum Chemical Study of the Reaction between Ni⁺ and H₂S. ChemPhysChem, 2010, 11, 3172-3178.	1.0	5
88	High-level ab initio calculations on low barrier hydrogen bonds and proton bound homodimers. Chemical Physics Letters, 2010, 493, 37-44.	1.2	23
89	Complete basis set limit extrapolation calculations with PNOF3. Chemical Physics Letters, 2010, 499, 164-167.	1.2	12
90	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

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91	Communications: Accurate description of atoms and molecules by natural orbital functional theory. Journal of Chemical Physics, 2010, 132, 031103.	1.2	68
92	Communication: The role of the positivity N-representability conditions in natural orbital functional theory. Journal of Chemical Physics, 2010, 133, 111101.	1.2	60
93	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.	1.1	101
94	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.	1.5	13
95	Ab Initio Study of Microsolvated Al³⁺â˜Aromatic Amino Acid Complexes. Journal of Physical Chemistry B, 2010, 114, 9017-9022.	1.2	14
96	Ab initio calculations onÂC₆H₆Â·Â·Â·(HF)_nclustersÂâ€”ÂXâ€“HÂ·Â·Â·Ï€ÂhydrogenÂbond. Canadian Journal of Chemistry, 2010, 88, 769-778.	1.3	8
97	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
98	Can correlation bring electrons closer together?. Molecular Physics, 2009, 107, 1089-1093.	0.8	30
99	Spin conserving natural orbital functional theory. Journal of Chemical Physics, 2009, 131, 021102.	1.2	52
100	Thermally Stable Solids Based on Endohedrally Doped ZnS Clusters. Chemistry - A European Journal, 2009, 15, 5138-5144.	1.7	19
101	Iterative diagonalization for orbital optimization in natural orbital functional theory. Journal of Computational Chemistry, 2009, 30, 2078-2086.	1.5	73
102	Synthesis of Cationic Polyelectrolytes by Inverse Microemulsion Polymerization. Macromolecular Rapid Communications, 2009, 30, 2036-2041.	2.0	8
103	Designing 3-D Molecular Stars. Journal of the American Chemical Society, 2009, 131, 9426-9431.	6.6	78
104	Sandwich Complexes of the Metalloaromatic Î·³-Al₃R₃ Ligand. Journal of the American Chemical Society, 2009, 131, 6949-6951.	6.6	16
105	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.	1.0	14
106	Magnetic Endohedral Transitionâ€Metalâ€Doped Semiconductingâ€Nanoclusters. Chemistry - A European Journal, 2008, 14, 8547-8554.	1.7	10
107	Electron-pair density relaxation holes. Journal of Chemical Physics, 2008, 128, 214105.	1.2	4
108	Correlation holes for the helium dimer. Journal of Chemical Physics, 2008, 128, 134102.	1.2	21

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109	Piris natural orbital functional study of the dissociation of the radical helium dimer. Journal of Chemical Physics, 2008, 129, 014108.	1.2	18
110	Quantum Monte Carlo study of the ground state and low-lying excited states of the scandium dimer. Journal of Chemical Physics, 2008, 128, 194315.	1.2	18
111	Dispersion interactions within the Piris natural orbital functional theory: The helium dimer. Journal of Chemical Physics, 2007, 126, 214103.	1.2	46
112	Electron correlation in the GK state of the hydrogen molecule. Journal of Chemical Physics, 2007, 127, 074307.	1.2	6
113	Endohedral (X@ZniSi)i=4-160,Â± Nanoclusters, X = Li, Na, K, Cl, Br. Journal of Physical Chemistry C, 2007, 111, 3560-3565.	1.5	27
114	Complexation of Al^{III} by Aromatic Amino Acids in the Gas Phase. Inorganic Chemistry, 2007, 46, 6413-6419.	1.9	11
115	Assessment of Approximate Density Functional Methods for the Study of the Interactions of Al(III) with Aromatic Amino Acids. Journal of Chemical Theory and Computation, 2007, 3, 1830-1836.	2.3	8
116	Protein Side Chains Facilitate Mg/Al Exchange in Model Protein Binding Sites. ChemPhysChem, 2007, 8, 2119-2124.	1.0	22
117	Endohedral Stannaspherenes Mn@Sn₁₂ and its Dimer: Ferromagnetic or Antiferromagnetic?. ChemPhysChem, 2007, 8, 2096-2099.	1.0	24
118	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.	1.5	31
119	Second International Theoretical Biophysics Symposium, Ã–rebro University, Sweden, June 28â€“July 1, 2005. International Journal of Quantum Chemistry, 2007, 107, 259-260.	1.0	0
120	Activation of Methane by the Iron Dimer Cation. A Theoretical Study. Journal of Physical Chemistry A, 2006, 110, 12501-12511.	1.1	24
121	Electron correlation in the 3Î£g+1 and 2Î£u+1 excited state lithium molecule. Journal of Chemical Physics, 2006, 125, 234102.	1.2	2
122	Comparison of Ti, Zr, and Hf as Cations for Metallocene-Catalyzed Olefin Polymerization. Organometallics, 2006, 25, 4483-4490.	1.1	26
123	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.	1.5	40
124	Exact non-Born-Oppenheimer wave function for the Hooke-Calogero model of the H2 molecule. European Physical Journal D, 2006, 37, 351-359.	0.6	12
125	Sandwich Complexes Based on the â€œAll-Metalâ€•Al42â^' Aromatic Ring. Chemistry - A European Journal, 2006, 12, 4495-4502.	1.7	40
126	Electronic excitation energies of ZniSinanoparticles. Nanotechnology, 2006, 17, 4100-4105.	1.3	16

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127	Exact non-Born-Oppenheimer wave functions for three-particle Hookean systems with arbitrary masses. Physical Review A, 2006, 74, .	1.0	16
128	Theoretical methods that help understanding the structure and reactivity of gas phase ions. International Journal of Mass Spectrometry, 2005, 240, 37-99.	0.7	104
129	Extracular densities of the non-Bornâ€“Oppenheimer Hookean H2 molecule. Chemical Physics Letters, 2005, 412, 381-385.	1.2	8
130	Clusters of II?VI Materials: CdiXi, X: S, Se, Te, i ? 16.. ChemInform, 2005, 36, no.	0.1	0
131	Structure and Properties of ZnS Nanoclusters. ChemInform, 2005, 36, no.	0.1	0
132	Electron correlation studies by means of local-scaling transformations and electron-pair density functions. Journal of Mathematical Chemistry, 2005, 37, 211-231.	0.7	9
133	Non-Bornâ€“Oppenheimer treatment of the H2 Hookean molecule. Journal of Chemical Physics, 2005, 123, 024102.	1.2	19
134	Comparative Study of Various Mechanisms for Metallocene-Catalyzed Î±-Olefin Polymerization. Organometallics, 2005, 24, 3233-3246.	1.1	27
135	A Joint Experimental and Theoretical Study of Cationâˆ'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.	6.6	81
136	Structure and Properties of ZnS Nanoclusters. Journal of Physical Chemistry B, 2005, 109, 2703-2709.	1.2	102
137	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.	1.0	19
138	Mono- and Multidecker Sandwich-Like Complexes of the Tetraazacyclobutadiene Aromatic Ring. Angewandte Chemie - International Edition, 2004, 43, 5485-5488.	7.2	42
139	Stability and Aromaticity of BiNi Rings and Fullerenes. ChemInform, 2004, 35, no.	0.1	0
140	Mono- and Multidecker Sandwich-Like Complexes of the Tetraazacyclobutadiene Aromatic Ring.. ChemInform, 2004, 35, no.	0.1	0
141	A reinterpretation of the nature of the Fermi hole. Journal of Chemical Physics, 2004, 120, 540-547.	1.2	12
142	Discordant results on the FeO+â€‰+â€‰H2reaction reconciled by quantum Monte Carlo theory. Molecular Physics, 2004, 102, 2635-2637.	0.8	17
143	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.	1.1	112
144	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.	1.1	36

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145	Sandwich-Like Complexes Based on â€œAll-Metalâ€•(Al42-) Aromatic Compounds. Journal of the American Chemical Society, 2004, 126, 3380-3381.	6.6	102
146	Clusters of IIâˆ’VI Materials:Â CdiXi, X = S, Se, Te,iâ‰ 16. Journal of Physical Chemistry A, 2004, 108, 10502-10508.	1.1	56
147	High Impact of Antiphospholipid Syndrome on Irreversible Organ Damage and Survival of Patients With Systemic Lupus Erythematosus. Archives of Internal Medicine, 2004, 164, 77.	4.3	195
148	Antiphospholipid antibodies predict early damage in patients with systemic lupus erythematosus. Lupus, 2004, 13, 900-905.	0.8	60
149	Incremental binding free energies of aluminum (III) vs. magnesium (II) complexes. Chemical Physics, 2003, 295, 175-184.	0.9	11
150	Electronic metastable bound states of Mn22+ and Co22+. Chemical Physics Letters, 2003, 372, 82-89.	1.2	6
151	The electronic states of Fe2+. Chemical Physics Letters, 2003, 376, 310-317.	1.2	19
152	Electronic Excitation Energies of ZniOiClusters. Journal of the American Chemical Society, 2003, 125, 9494-9499.	6.6	98
153	Clusters of Group IIâˆ’VI Materials:â€‰ CdiOi (i â‰ 15). Journal of Physical Chemistry A, 2003, 107, 9918-9923.	1.1	22
154	Stability and Aromaticity of BiNi Rings and Fullerenes. Journal of Physical Chemistry A, 2003, 107, 10004-10010.	1.1	37
155	Minimal dipole charge for a dipole-bound dianion. Molecular Physics, 2003, 101, 2529-2532.	0.8	3
156	THE ELECTRON-PAIR DENSITY AND THE MODELING OF THE SPHERICALLY AVERAGED EXCHANGE-CORRELATION HOLE. , 2003, , .		0
157	Atomic charge states in a weakly coupled plasma environment. Physical Review E, 2002, 66, 026408.	0.8	9
158	Binding of Carbon Rings to a Graphite Plane. Journal of Physical Chemistry B, 2002, 106, 6871-6874.	1.2	3
159	Hydrogen-Bonding Interactions between Formic Acid and Pyridine. Journal of Physical Chemistry A, 2002, 106, 4187-4191.	1.1	41
160	Aluminum (III) interactions with the side chains of aromatic aminoacids. International Journal of Quantum Chemistry, 2002, 90, 859-881.	1.0	17
161	Role of electron-electron coalescence density in density functional theory. International Journal of Quantum Chemistry, 2002, 86, 40-45.	1.0	7
162	The Ferroceneâˆ’Lithium Cation Complex in the Gas Phase. Journal of the American Chemical Society, 2001, 123, 5040-5043.	6.6	51

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163	Aluminum (III) Interactions with Sulfur-Containing Amino Acid Chains. Journal of Physical Chemistry A, 2001, 105, 7446-7453.	1.1	12
164	Electronâ€“electron counterbalance density for molecules: Exchange and correlation effects. Journal of Chemical Physics, 2001, 115, 1987-1994.	1.2	11
165	Small clusters of group-(IIâ€“VI) materials:ZniXi,X=Se,Te,i=1â€“9. Physical Review A, 2001, 64, .	1.0	36
166	Determination of the integrated x-ray scattering intensities through the electron-pair relative-motion density at the origin. Physical Review A, 2001, 64, .	1.0	7
167	Electronic excitation energies ofZniSiclusters. Physical Review A, 2001, 64, .	1.0	34
168	Water Clusters: Towards an Understanding Based on First Principles of Their Static and Dynamic Properties. Angewandte Chemie - International Edition, 2000, 39, 717-721.	7.2	229
169	Quantum mechanical calculations on phosphate hydrolysis reactions. Journal of Computational Chemistry, 2000, 21, 43-51.	1.5	37
170	Charge-density concentration and electron-electron coalescence density in atoms and molecules. Physical Review A, 2000, 62, .	1.0	7
171	Electronic excitation energies of smallZniSiclusters. Physical Review A, 2000, 63, .	1.0	26
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