

Josep Maria Poblet

List of Publications by Year in descending order

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298
papers

13,400
citations

19608

61
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34900

98
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326
all docs

326
docs citations

326
times ranked

7548
citing authors

#	ARTICLE	IF	CITATIONS
1	Managing the Computational Chemistry Big Data Problem: The ioChem-BD Platform. Journal of Chemical Information and Modeling, 2015, 55, 95-103.	2.5	403
2	Structure, properties and reactivity of polyoxometalates: a theoretical perspective. Chemical Society Reviews, 2012, 41, 7537.	18.7	392
3	Polyoxometalate electrocatalysts based on earth-abundant metals for efficient water oxidation in acidic media. Nature Chemistry, 2018, 10, 24-30.	6.6	375
4	Endohedral metallofullerenes: a unique host-guest association. Chemical Society Reviews, 2011, 40, 3551.	18.7	359
5	Design and fabrication of memory devices based on nanoscale polyoxometalate clusters. Nature, 2014, 515, 545-549.	13.7	301
6	Electronic Properties of Polyoxometalates: Electron and Proton Affinity of Mixed-Addenda Keggin and Wells Dawson Anions. Journal of the American Chemical Society, 2002, 124, 12574-12582.	6.6	281
7	Ab initio and DFT modelling of complex materials: towards the understanding of electronic and magnetic properties of polyoxometalates. Chemical Society Reviews, 2003, 32, 297-308.	18.7	275
8	Electronic and Magnetic Properties of Keggin Anions: A DFT Study of $[XM_{12}O_{40}]_n^-$, (M = W, Mo; X = Al, III). Journal of Physical Chemistry B, 2001, 123, 3749-3758.	6.6	219
9	Structure, Reactivity, and Growth Pathways of Metallo-carbocages and Transition Metal/Carbon Clusters and Nanocrystals: A Challenge to Computational Chemistry. Chemical Reviews, 2000, 100, 495-542.	23.0	207
10	Bonding within the Endohedral Fullerenes $Sc_3N@C_{78}$ and $Sc_3N@C_{80}$ as Determined by Density Functional Calculations and Reexamination of the Crystal Structure of $\{Sc_3N@C_{78}\} \cdot Co(OEP) \cdot 1.5(C_6H_6) \cdot 0.3(CHCl_3)$. Journal of Physical Chemistry A, 2002, 106, 12356-12364.	1.1	200
11	General Rule for the Stabilization of Fullerene Cages Encapsulating Trimetallic Nitride Templates. Angewandte Chemie - International Edition, 2005, 44, 7230-7233.	7.2	200
12	Electronic Properties of Polyoxometalates: A DFT Study of $[XM_{12}O_{40}]_n^-$ Relative Stability (M = W, Mo). Journal of Physical Chemistry B, 2001, 105, 1195-1200.	6.6	195
13	The Smallest Stable Fullerene, $M@C_{28}$ (M = Ti, Zr, U): Stabilization and Growth from Carbon Vapor. Journal of the American Chemical Society, 2012, 134, 9380-9389.	6.6	165
14	The maximum pentagon separation rule provides a guideline for the structures of endohedral metallofullerenes. Nature Chemistry, 2010, 2, 955-961.	6.6	162
15	Polyoxometalates with Internal Cavities: Redox Activity, Basicity, and Cation Encapsulation in $[X_nP_{5n}W_{30}O_{110}]^{n-}$ (15- and 18-membered) Preyssler Complexes, with X = Na, Ca, Y, La, Ce, and Th. Journal of the American Chemical Society, 2007, 129, 12241-12252.	6.6	152
16	Mechanistic Insights into Alkene Epoxidation with H_2O_2 by Ti- and other TM-Containing Polyoxometalates: Role of the Metal Nature and Coordination Environment. Journal of the American Chemical Society, 2010, 132, 7488-7497.	6.6	148
17	A seven atom cluster in a carbon cage, the crystallographically determined structure of $Sc_4(1/4)_3-O_3@h-C_{80}$. Chemical Communications, 2010, 46, 279-281.	2.2	123
18	$Sc_2S@C_{10528}-C_{72}$: A Dimetallic Sulfide Endohedral Fullerene with a Non Isolated Pentagon Rule Cage. Journal of the American Chemical Society, 2012, 134, 7851-7860.	6.6	123

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19	“Open Rather than Closed” Malonate Methano-Fullerene Derivatives. The Formation of Methanofulleroid Adducts of $Y_3N@C_{80}$. Journal of the American Chemical Society, 2007, 129, 10423-10430.	6.6	122
20	The Shape of the $Sc_2(I\frac{1}{4}2-S)$ Unit Trapped in C_{82} : Crystallographic, Computational, and Electrochemical Studies of the Isomers, $Sc_2(I\frac{1}{4}2-S)@C_3v(6)-C_{82}$ and $Sc_2(I\frac{1}{4}2-S)@C_3v(8)-C_{82}$. Journal of the American Chemical Society, 2010, 132, 6752-6760.	6.6	121
21	Sc ₂ (I ^{1/4} 2-O)@C _{3v} (6)-C ₈₂ and the Relevance of the Thermal and Entropic Effects in Fullerene Isomer Selection. Journal of the American Chemical Society, 2010, 132, 12098-12105.	6.6	119
22	Cobalt Polyoxometalates as Heterogeneous Water Oxidation Catalysts. Inorganic Chemistry, 2013, 52, 4753-4755.	1.9	118
23	ZrIV-Monosubstituted Keggin-Type Dimeric Polyoxometalates: Synthesis, Characterization, Catalysis of H ₂ O ₂ -Based Oxidations, and Theoretical Study. Inorganic Chemistry, 2006, 45, 7224-7234.	1.9	113
24	Relative basicities of the oxygen sites in [V10O ₂₈] ⁶⁻ . An analysis of the ab initio determined distributions of the electrostatic potential and of the Laplacian of charge density. Journal of the American Chemical Society, 1992, 114, 1136-1146.	6.6	112
25	On the Origin of Alternating Bond Distortions and the Emergence of Chirality in Polyoxometalate Anions. Journal of the American Chemical Society, 2008, 130, 8223-8233.	6.6	107
26	Synthesis of a new endohedral fullerene family, Sc ₂ S@C _{2n} (n = 40-50) by the introduction of SO ₂ . Chemical Communications, 2010, 46, 4818.	2.2	106
27	Redox properties of polyoxometalates: new insights on the anion charge effect. Dalton Transactions, 2006, , 1162-1167.	1.6	102
28	From Lindqvist and Keggin ions to electronically inverse hosts. Coordination Chemistry Reviews, 1998, 178-180, 1019-1049.	9.5	99
29	Unique Four-Electron Metal-to-Cage Charge Transfer of Th to a C_{82} Fullerene Cage: Complete Structural Characterization of $Th@C_3v(8)-C_{82}$. Journal of the American Chemical Society, 2017, 139, 5110-5116.	6.6	97
30	Polyoxometalates in Solution: Molecular Dynamics Simulations on the $\hat{\pm}$ -PW12O ₄₀ ³⁻ Keggin Anion in Aqueous Media. Journal of Physical Chemistry A, 2005, 109, 1216-1222.	1.1	96
31	Metal Nitride Cluster Fullerene $M_3N@C_{80}$ (M=Y, Sc) Based Dyads: Synthesis, and Electrochemical, Theoretical and Photophysical Studies. Chemistry - A European Journal, 2009, 15, 864-877.	1.7	96
32	$U_2@Ih(7)-C_{80}$: Crystallographic Characterization of a Long-Sought Dimetallic Actinide Endohedral Fullerene. Journal of the American Chemical Society, 2018, 140, 3907-3915.	6.6	96
33	Understanding the Stabilization of Metal Carbide Endohedral Fullerenes $M_2C_2@C_{82}$ and Related Systems. Journal of Physical Chemistry A, 2008, 112, 4550-4555.	1.1	90
34	Keggin Polyoxoanions in Aqueous Solution: Ion Pairing and Its Effect on Dynamic Properties by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2008, 112, 8591-8599.	1.2	87
35	Trimetallic Nitride Endohedral Fullerenes: Experimental and Theoretical Evidence for the $M_3N^{6+}@C_{2n}^{6-}$ model. Angewandte Chemie - International Edition, 2009, 48, 1425-1428.	7.2	86
36	Electronic Structure and Redox Properties of Metal Nitride Endohedral Fullerenes $M_3N@C_{2n}$ (M=Sc, Y, La, and Gd; $2n=80, 84, 88, 92, 96$). Chemistry - A European Journal, 2009, 15, 10997-11009.	1.7	84

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37	Nucleation Mechanisms of Molecular Oxides: A Study of the Assembly–Dissassembly of W_6O_{19} by Theory and Mass Spectrometry. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 5452-5456.	7.2	83
38	Polyoxopalladates Encapsulating Yttrium and Lanthanide Ions, $[X^{III}Pd^{II}]_{12}(AsPh)_8O_{32}$ ($X=Y, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu$). <i>Chemistry - A European Journal</i> , 2010, 16, 9076-9085.	1.7	81
39	Zigzag Sc_2C_2 Carbide Cluster inside a [88] Fullerene Cage with One Heptagon, $Sc_2C_2@C_{88}$ (hept- C_{88}): A Kinetically Trapped Fullerene Formed by C_2 Insertion?. <i>Journal of the American Chemical Society</i> , 2016, 138, 13030-13037.	6.6	81
40	Ammonolysis of Mono(pentamethylcyclopentadienyl) Titanium(IV) Derivatives. <i>Inorganic Chemistry</i> , 2000, 39, 642-651.	1.9	80
41	Dancing on a Fullerene Surface: Isomerization of $Y_3N@N$ -Ethylpyrrolidino- C_{80} from the 6,6 to the 5,6 Regioisomer. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 8176-8180.	7.2	80
42	Laplacian of charge density for binuclear complexes: terminal vs bridging carbonyls. <i>The Journal of Physical Chemistry</i> , 1993, 97, 6362-6366.	2.9	78
43	First Isolated Active Titanium Peroxo Complex: Characterization and Theoretical Study. <i>Inorganic Chemistry</i> , 2004, 43, 2284-2292.	1.9	77
44	$Sc_2S@C_{70}$ (7892) C_{70} : a metallic sulfide cluster inside a non-IPR C_{70} cage. <i>Chemical Science</i> , 2013, 4, 180-186.	3.7	77
45	Aerobic Carbon–Carbon Bond Cleavage of Alkenes to Aldehydes Catalyzed by First-Row Transition-Metal-Substituted Polyoxometalates in the Presence of Nitrogen Dioxide. <i>Journal of the American Chemical Society</i> , 2014, 136, 10941-10948.	6.6	77
46	Chemical Reactivity of D3h C_{78} (Metallo)Fullerene: Regioselectivity Changes Induced by Sc_3N Encapsulation. <i>Journal of the American Chemical Society</i> , 2008, 130, 6206-6214.	6.6	75
47	Gated and Differently Functionalized (New) Porous Capsules Direct Encapsulates' Structures: Higher and Lower Density Water. <i>Chemistry - A European Journal</i> , 2009, 15, 1844-1852.	1.7	74
48	Exohedral Reactivity of Trimetallic Nitride Template (TNT) Endohedral Metallofullerenes. <i>Journal of Organic Chemistry</i> , 2006, 71, 46-54.	1.7	73
49	Synthesis and Characterization of Non-Isolated-Pentagon-Rule Actinide Endohedral Metallofullerenes $U@C_{17418}-C_{76}$, $U@C_{28324}-C_{80}$, and $Th@C_{28324}-C_{80}$: Low-Symmetry Cage Selection Directed by a Tetravalent Ion. <i>Journal of the American Chemical Society</i> , 2018, 140, 18039-18050.	6.6	73
50	Electronic Structure of the Highly Reduced Polyoxoanion $[PMo_{12}O_{40}(VO)_2]^{5-}$: A DFT Study. <i>Inorganic Chemistry</i> , 1998, 37, 3444-3446.	1.9	71
51	Single crystal structures and theoretical calculations of uranium endohedral metallofullerenes ($U@C_{2n}$, $2n = 74, 82$) show cage isomer dependent oxidation states for U. <i>Chemical Science</i> , 2017, 8, 5282-5290.	3.7	71
52	Purification of Uranium-based Endohedral Metallofullerenes (EMFs) by Selective Supramolecular Encapsulation and Release. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 11294-11299.	7.2	70
53	Inductive Effects in Neutral Pentacoordinated Silicon Compounds Containing a Si–N Dative Bond. A Theoretical Study. <i>Organometallics</i> , 1999, 18, 5584-5593.	1.1	69
54	Current trends in the computational modelling of polyoxometalates. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 393-404.	0.5	69

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55	Bottom-up formation of endohedral mono-metallofullerenes is directed by charge transfer. <i>Nature Communications</i> , 2014, 5, 5844.	5.8	69
56	Real-time molecular scale observation of crystal formation. <i>Nature Chemistry</i> , 2017, 9, 369-373.	6.6	69
57	Ab Initio SCF and CI Investigations on Titanium-Carbon Clusters: Metallo-carbohedrenes Ti_8C_{12} and Cfc Crystallites $Ti_{14}C_{13}$. <i>Journal of the American Chemical Society</i> , 1995, 117, 508-517.	6.6	68
58	Polyoxometalates Paneling through $\{Mo_2O_2S_2\}$ Coordination: Cation-Directed Conformations and Chemistry of a Supramolecular Hexameric Scaffold. <i>Journal of the American Chemical Society</i> , 2012, 134, 1724-1737.	6.6	67
59	Cuprophilicity, a still elusive concept: a theoretical analysis of the ligand-unsupported $CuI \cdots CuI$ interaction in two recently reported complexes. <i>Chemical Communications</i> , 1998, , 1179-1180.	2.2	66
60	DFT Study on the Five Isomers of $PW_{12}O_{40}^{3-}$: Relative Stabilization upon Reduction. <i>Inorganic Chemistry</i> , 2004, 43, 6863-6865.	1.9	65
61	Self-Sorting of Heteroanions in the Assembly of Cross-Shaped Polyoxometalate Clusters. <i>Journal of the American Chemical Society</i> , 2018, 140, 2595-2601.	6.6	62
62	Large fullerenes stabilized by encapsulation of metallic clusters. <i>Chemical Communications</i> , 2007, , 4161.	2.2	61
63	Wheel-Shaped Cu_{20} -Tungstophosphate $[Cu_{20}X(OH)_{24}(H_2O)_{12}(P_8W_{48}O_{184})_{25}]^{25-}$ Ion (X = Cl, Br, I) and the Role of the Halide Guest. <i>Inorganic Chemistry</i> , 2009, 48, 11636-11645.	1.9	59
64	Alkaline Earth Guests in Polyoxopalladate Chemistry: From Nanocube to Nanostar via an Open Shell Structure. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 11974-11978.	7.2	59
65	Tetracobalt-polyoxometalate catalysts for water oxidation: Key mechanistic details. <i>Journal of Catalysis</i> , 2017, 350, 56-63.	3.1	59
66	Influence of the Heteroatom Size on the Redox Potentials of Selected Polyoxoanions. <i>Inorganic Chemistry</i> , 2010, 49, 7001-7006.	1.9	58
67	Polyoxopalladates Encapsulating 8-Coordinated Metal Ions, [MO₈Pd^{II}]₁₂L₈]ⁿ⁻ (M =) Tj ETQq1 1 0.784314 rgBT /Overlo	1.9	58
68	13214-13228. Photoreduction Mechanism of CO_2 to CO Catalyzed by a Rhenium(I)-Polyoxometalate Hybrid Compound. <i>ACS Catalysis</i> , 2016, 6, 6422-6428.	5.5	58
69	Electronic Structures of Scandium Oxide Endohedral Metallofullerenes, $Sc_4(I_{3/4}O)_n @ I_h-C_{80}$ ($n = 2, 3$). <i>Inorganic Chemistry</i> , 2009, 48, 5957-5961.	1.9	57
70	Quantifying the Donor-Acceptor Properties of Phosphine and N-Heterocyclic Carbene Ligands in Grubbs's Catalysts Using a Modified EDA Procedure Based on Orbital Deletion. <i>Organometallics</i> , 2009, 28, 4283-4287.	1.1	57
71	Bonding in Elongated Dihydrogen Complexes. Theoretical Analysis of the Electron Density in $[MLn(HA \cdots H)]$ Species. <i>Organometallics</i> , 1996, 15, 2947-2953.	1.1	55
72	Ab Initio Study of the Relative Basicity of the External Oxygen Sites in $M_2W_4O_{19}$ (M = Nb and V). <i>Inorganic Chemistry</i> , 1998, 37, 3071-3077.	1.9	55

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73	Are the solvent effects critical in the modeling of polyoxoanions?. Journal of Computational Chemistry, 2004, 25, 1542-1549.	1.5	55
74	Combined Theoretical and Mass Spectrometry Study of the Formation-Fragmentation of Small Polyoxomolybdates. Inorganic Chemistry, 2011, 50, 7811-7819.	1.9	53
75	Relevance of Protons in Heterolytic Activation of H ₂ O over Nb(V): Insights from Model Studies on Nb-Substituted Polyoxometalates. ACS Catalysis, 2018, 8, 9722-9737.	5.5	52
76	Reactivity differences of Sc ₃ N@C _{2n} (2n = 68 and 80). Synthesis of the first methanofullerene derivatives of Sc ₃ N@D _{5h} -C ₈₀ . Chemical Communications, 2016, 52, 64-67.	2.2	51
77	Sc ₂ O@C _{2v} (5)-C ₈₀ : Dimetallic Oxide Cluster Inside a C ₈₀ Fullerene Cage. Inorganic Chemistry, 2015, 54, 9845-9852.	1.9	50
78	Probing Polyoxometalate-Protein Interactions Using Molecular Dynamics Simulations. Chemistry - A European Journal, 2016, 22, 15280-15289.	1.7	50
79	Investigating the Transformations of Polyoxoanions Using Mass Spectrometry and Molecular Dynamics. Journal of the American Chemical Society, 2016, 138, 8765-8773.	6.6	50
80	DFT Studies of Uranyl Acetate, Carbonate, and Malonate, Complexes in Solution. Inorganic Chemistry, 2003, 42, 6136-6141.	1.9	49
81	Reactivity of Metallic Nitride Endohedral Metallofullerene Anions: Electrochemical Synthesis of a Lu ₃ N@Ih-C ₈₀ Derivative. Journal of the American Chemical Society, 2011, 133, 2760-2765.	6.6	49
82	Full Exploration of the Diels-Alder Cycloaddition on Metallofullerenes M ₃ N@C ₈₀ (M=Sc, Lu, Gd): The D _{5h} versus I _h Isomer and the Influence of the Metal Cluster. Chemistry - A European Journal, 2012, 18, 8944-8956.	1.7	49
83	A DFT Study of the Electronic Spectrum of the Keggin Anion [CoIIW ₁₂ O ₄₀] ⁶⁻ . Inorganic Chemistry, 2002, 41, 1883-1888.	1.9	48
84	A DFT study on the effect of metal, anion charge, heteroatom and structure upon the relative basicities of polyoxoanions. Journal of Molecular Catalysis A, 2007, 262, 236-242.	4.8	48
85	Structural and Electrochemical Property Correlations of Metallic Nitride Endohedral Metallofullerenes. Journal of Physical Chemistry C, 2010, 114, 13003-13009.	1.5	48
86	Alkene oxidation by Ti-containing polyoxometalates. Unambiguous characterization of the role of the protonation state. Chemical Communications, 2012, 48, 9266.	2.2	48
87	Bingel-Hirsch Reactions on Non-IPR Gd ₃ N@C _{2n} (2n = 82 and 84). Journal of Organic Chemistry, 2010, 75, 8299-8302.	1.7	46
88	Lanthanide Polyoxocationic Complexes: Experimental and Theoretical Stability Studies and Lewis Acid Catalysis. Chemistry - A European Journal, 2011, 17, 14129-14138.	1.7	46
89	Sc ₂ O@Td(19151)-C ₇₆ : Hindered Cluster Motion inside a Tetrahedral Carbon Cage Probed by Crystallographic and Computational Studies. Chemistry - A European Journal, 2015, 21, 11110-11117.	1.7	46
90	Small endohedral metallofullerenes: exploration of the structure and growth mechanism in the Ti@C _{2n} (2n = 26-50) family. Chemical Science, 2015, 6, 675-686.	3.7	45

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91	Sc ₂ O@C ₃ v<i>(8)</i>-C ₈₂ : A Missing Isomer of Sc ₂ O@C ₈₂ . <i>Inorganic Chemistry</i> , 2016, 55, 1926-1933.	1.9	45
92	Catalyst Design for Alkene Epoxidation by Molecular Analogues of Heterogeneous Titanium-Silicalite Catalysts. <i>ACS Catalysis</i> , 2020, 10, 4737-4750.	5.5	45
93	Geometric and electronic structure of metal-cage fullerenes, C ₅₉ M (M = Pt, Ir) obtained by laser ablation of electrochemically deposited films. <i>Chemical Communications</i> , 1999, , 493-494.	2.2	44
94	Connecting theory with experiment to understand the initial nucleation steps of heteropolyoxometalate clusters. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20136.	1.3	44
95	¹⁷ O NMR chemical shifts in oxometalates: from the simplest monometallic species to mixed-metal polyoxometalates. <i>Chemical Science</i> , 2014, 5, 2031.	3.7	44
96	Ti ₈ C ₁₂ : a polytopal molecule with 36 Ti-C bonds. <i>Journal of the Chemical Society Chemical Communications</i> , 1993, , 1182-1185.	2.0	43
97	Construction of Heterometallic Cubanes [Ti ₃ Cp(1/3-CR)](1/3-O) ₃ [Mo(CO) ₃] (R=H, Me; Cp*= ¹ -5-C ₅ Me ₅) and [Ti ₃ Cp(1/3-N)](1/3-NH) ₃ [M(CO) ₃] (M=Cr, Mo, W); Crystal Structure of [Ti ₃ Cp(1/3-CMe)](1/3-O) ₃ [Mo(CO) ₃]. <i>Angewandte Chemie - International Edition</i> , 2000, 39, 534-537.		43
98	In Quest of Factors That Control the Enantioselective Catalytic Markovnikov Hydroboration/Oxidation of Vinylarenes. <i>Chemistry - A European Journal</i> , 2004, 10, 6456-6467.	1.7	42
99	Epoxidation of Alkenes with H ₂ O ₂ Catalyzed by Ditungsten-Containing Tungstodiarsonate(III): Experimental and Theoretical Studies. <i>European Journal of Inorganic Chemistry</i> , 2010, 2010, 5312-5317.	1.0	42
100	Electrosynthesis of a Sc ₃ N@Ih-C ₈₀ Methano Derivative from Trianionic Sc ₃ N@Ih-C ₈₀ . <i>Journal of the American Chemical Society</i> , 2012, 134, 7480-7487.	6.6	42
101	Bingel-Hirsch Addition on Endohedral Metallofullerenes: Kinetic Versus Thermodynamic Control. <i>Chemistry - A European Journal</i> , 2013, 19, 5061-5069.	1.7	42
102	Ti ₂ S@D _{3h} (24109)-C ₇₈ : a sulfide cluster metallofullerene containing only transition metals inside the cage. <i>Chemical Science</i> , 2013, 4, 3404.	3.7	41
103	Molecular Nitrides Containing Group 4 and 5 Metals: Single and Double Azatitanocubanes. <i>Chemistry - A European Journal</i> , 2003, 9, 2337-2346.	1.7	40
104	Relative Stability in ¹ - and ² -Wells Dawson Heteropolyanions: A DFT Study of [P ₂ M ₁₈ O ₆₂] _n (M = W and Tj ETQg0 0 0 rgBT /Overlo	1.9	40
105	On the Origin of Regio- and Stereoselectivity in the Rhodium-Catalyzed Vinylarenes Hydroboration Reaction. <i>Journal of Organic Chemistry</i> , 2004, 69, 2669-2680.	1.7	40
106	Density Functional Theory and ab Initio Study of Electronic and Electrochemistry Properties of the Tetranuclear Sandwich Complex [FeII ₄ (H ₂ O) ₂ (PW ₉ O ₃₄) ₂] ₆ -. <i>Inorganic Chemistry</i> , 2007, 46, 4022-4027.	1.9	40
107	Fullerenes: formation, stability, and reactivity. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011, 1, 350-367.	6.2	40
108	Alkene Epoxidation Catalyzed by Ti-Containing Polyoxometalates: Unprecedented ¹ -Oxygen Transfer Mechanism. <i>Inorganic Chemistry</i> , 2016, 55, 6080-6084.	1.9	40

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109	Mass Spectrometric and Computational Studies of Heterofullerenes ([C58Pt] ⁻ , [C59Pt] ⁺) Obtained by Laser Ablation of Electrochemically Deposited Films. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2192-2198.	1.1	39
110	Ammonia Activation by $\frac{1}{4}$ -Alkylidyne Fragments Supported on a Titanium Molecular Oxide Model. <i>Inorganic Chemistry</i> , 2011, 50, 6269-6279.	1.9	39
111	Influence of polyoxometalate ligands on the nature of high-valent transition metal nitrido species. A theoretical analysis of experimentally known and unprecedented compounds. <i>Dalton Transactions</i> , 2008, , 5166.	1.6	38
112	Supramolecular Recognition Influences Magnetism in [X@HV^{IV}₈V^V₁₄O₅₄]<sup>6⁻ Self-Assemblies with Symmetry-Breaking Guest Anions. <i>Chemistry - A European Journal</i> , 2015, 21, 2387-2397.	1.7	38
113	(2 + 2) Cycloaddition of Benzyne to Endohedral Metallofullerenes M₃N@C₈₀ (M = Sc, Y): A Rotating-Intermediate Mechanism. <i>Journal of the American Chemical Society</i> , 2015, 137, 6820-6828.	6.6	38
114	A New Class of Molecular Electrocatalysts for Hydrogen Evolution: Catalytic Activity of M₃N@C<sub>2ⁿ (2ⁿ = 68, 78, and 80) Fullerenes. <i>Journal of the American Chemical Society</i> , 2021, 143, 6037-6042.	6.6	37
115	Effective Storage of Electrons in Water by the Formation of Highly Reduced Polyoxometalate Clusters. <i>Journal of the American Chemical Society</i> , 2022, 144, 8951-8960.	6.6	37
116	Assembly of titanium embedded polyoxometalates with unprecedented structural features. <i>Dalton Transactions</i> , 2010, 39, 11599.	1.6	36
117	Why Does Nb(V) Show Higher Heterolytic Pathway Selectivity Than Ti(IV) in Epoxidation with H₂O₂? Answers from Model Studies on Nb- and Ti-Substituted Lindqvist Tungstates. <i>ACS Catalysis</i> , 2019, 9, 6262-6275.	5.5	36
118	Polyoxometalates as alternative Mo precursors for methane dehydroaromatization on Mo/ZSM-5 and Mo/MCM-22 catalysts. <i>Catalysis Science and Technology</i> , 2019, 9, 5927-5942.	2.1	36
119	New dithiolate-bridged rhodium complexes. <i>Journal of the Chemical Society Dalton Transactions</i> , 1993, , 2689-2696.	1.1	34
120	Diversity in the Electronic Structures of Metallocarbohedrenes: Ab Initio Study of M8C12 (M = Ti, V), $\frac{1}{3}$ ETQqO O O rgBT /Overlock 10 Tf 5	2.9	34
121	Synthetic and Theoretical Study of the Incorporation of Metal Halides in [Ti($\frac{1}{5}$ -C5Me5)($\frac{1}{4}$ -NH)] ₃ ($\frac{1}{3}$ -N)]. <i>Chemistry - A European Journal</i> , 2005, 11, 1030-1041.	1.7	34
122	Characterization of a strong covalent Th3+–Th3+ bond inside an Ih(7)-C80 fullerene cage. <i>Nature Communications</i> , 2021, 12, 2372.	5.8	34
123	Multiple Metal Additions to C60. An ab Initio Study of [M(PH3)2] _n C60 (M = Pt and Pd; n = 1, 2, and 6). <i>The Journal of Physical Chemistry</i> , 1995, 99, 5914-5921.	2.9	33
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