

# Josep Maria Poblet

## List of Publications by Year in descending order

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Version: 2024-02-01

298  
papers

13,400  
citations

19608

61  
h-index

34900

98  
g-index

326  
all docs

326  
docs citations

326  
times ranked

7548  
citing authors

#	ARTICLE	IF	CITATIONS
1	Molecular Transition Metal Oxide Electrocatalysts for the Reversible Carbon Dioxide→Carbon Monoxide Transformation. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	15
2	When Identification of the Reduction Sites in Mixed Molybdenum/Tungsten Keggin-Type Polyoxometalate Hybrids Turns Out Tricky. <i>Inorganic Chemistry</i> , 2022, 61, 7700-7709.	1.9	3
3	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
4	Discovery and Supramolecular Interactions of Neutral Palladium→Oxo Clusters Pd <sub>16</sub> and Pd <sub>24</sub> . <i>Angewandte Chemie</i> , 2021, 133, 3676-3683.	1.6	9
5	Tuning Photoinduced Electron Transfer in POM→Bodipy Hybrids by Controlling the Environment: Experiment and Theory. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 6518-6525.	7.2	19
6	Reaction Pathway Discrimination in Alkene Oxidation Reactions by Designed Ti→Siloxo→Polyoxometalates. <i>ChemCatChem</i> , 2021, 13, 1220-1229.	1.8	13
7	Discovery and Supramolecular Interactions of Neutral Palladium→Oxo Clusters Pd <sub>16</sub> and Pd <sub>24</sub> . <i>Angewandte Chemie - International Edition</i> , 2021, 60, 3632-3639.	7.2	24
8	U <sub>2</sub> N@h(7)-C <sub>80</sub> : fullerene cage encapsulating an unsymmetrical U(IV) cluster. <i>Chemical Science</i> , 2021, 12, 282-292.	3.7	25
9	Understanding polyoxometalates as water oxidation catalysts through iron vs. cobalt reactivity. <i>Chemical Science</i> , 2021, 12, 8755-8766.	3.7	23
10	Oxidative detoxification of nerve agent VX simulant by polyoxoniobate: Experimental and theoretical insights. <i>Journal of Catalysis</i> , 2021, 394, 83-93.	3.1	6
11	Tuning Photoinduced Electron Transfer in POM→Bodipy Hybrids by Controlling the Environment: Experiment and Theory. <i>Angewandte Chemie</i> , 2021, 133, 6592-6599.	1.6	4
12	Density functional theory study of single-molecule ferroelectricity in Preyssler-type polyoxometalates. <i>APL Materials</i> , 2021, 9, .	2.2	5
13	A New Class of Molecular Electrocatalysts for Hydrogen Evolution: Catalytic Activity of M <sub>3</sub> N@C <sub>2n</sub> (2n = 68, 78, and 80) Fullerenes. <i>Journal of the American Chemical Society</i> , 2021, 143, 6037-6042.	6.6	37
14	Characterization of a strong covalent Th <sub>3</sub> +→Th <sub>3</sub> + bond inside an Ih(7)-C <sub>80</sub> fullerene cage. <i>Nature Communications</i> , 2021, 12, 2372.	5.8	34
15	An Ultra→Long→Lived Triplet Excited State in Water at Room Temperature: Insights on the Molecular Design of Tridecafullerenes. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 16109-16118.	7.2	8
16	An Ultra→Long→Lived Triplet Excited State in Water at Room Temperature: Insights on the Molecular Design of Tridecafullerenes. <i>Angewandte Chemie</i> , 2021, 133, 16245-16254.	1.6	2
17	Synthesis and Characterization of Two Isomers of Th@C <sub>82</sub> : Th@C <sub>2v</sub> (9)-C <sub>82</sub> and Th@C <sub>2</sub> (5)-C <sub>82</sub> . <i>Inorganic Chemistry</i> , 2021, 60, 11496-11502.	1.9	11
18	Activation of H <sub>2</sub> O <sub>2</sub> over Zr(IV). Insights from Model Studies on Zr-Monosubstituted Lindqvist Tungstates. <i>ACS Catalysis</i> , 2021, 11, 10589-10603.	5.5	25

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19	Crystallographic Characterization of U@C <sub>24</sub> (24 = 82): Insights about Metal-Cage Interactions for Mono-metallofullerenes. <i>Journal of the American Chemical Society</i> , 2021, 143, 15309-15318.	6.6	22
20	Unexpected Formation of Metallofulleroids from Multicomponent Reactions, with Crystallographic and Computational Studies of the Cluster Motion. <i>Angewandte Chemie</i> , 2021, 133, 25473-25477.	1.6	5
21	Unexpected Formation of Metallofulleroids from Multicomponent Reactions, with Crystallographic and Computational Studies of the Cluster Motion. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 25269-25273.	7.2	12
22	Unexpected formation of 1,2- and 1,4-bismethoxyl Sc <sub>3</sub> N@I <sub>h</sub> -C <sub>80</sub> derivatives via regioselective anion addition: an unambiguous structural identification and mechanism study. <i>Chemical Science</i> , 2021, 12, 8123-8130.	3.7	5
23	Photoreduction Mechanism of CO <sub>2</sub> to CO Catalyzed by a Three-Component Hybrid Construct with a Bimetallic Rhenium Catalyst. <i>ACS Catalysis</i> , 2021, 11, 1495-1504.	5.5	19
24	Th@D <sub>5h</sub> (6)-C <sub>80</sub> : a highly symmetric fullerene cage stabilized by a single metal ion. <i>Chemical Communications</i> , 2021, 57, 6624-6627.	2.2	13
25	Soluble Complexes of Cobalt Oxide Fragments Bring the Unique CO <sub>2</sub> Photoreduction Activity of a Bulk Material into the Flexible Domain of Molecular Science. <i>Journal of the American Chemical Society</i> , 2021, 143, 20769-20778.	6.6	30
26	Chemical Reactions of Cationic Metallofullerenes: An Alternative Route for Exohedral Functionalization. <i>Chemistry - A European Journal</i> , 2020, 26, 1748-1753.	1.7	15
27	Water-gas shift reaction co-catalyzed by polyoxometalate (POM)-gold composites: the magic role of POMs. <i>Catalysis Science and Technology</i> , 2020, 10, 8219-8229.	2.1	8
28	Origin of Selectivity in Protein Hydrolysis by Zr(IV)-Containing Metal Oxides as Artificial Proteases. <i>ACS Catalysis</i> , 2020, 10, 13455-13467.	5.5	13
29	Frontispiece: Structure-Activity Relationships for the Affinity of Chaotropic Polyoxometalate Anions towards Proteins. <i>Chemistry - A European Journal</i> , 2020, 26, .	1.7	0
30	Self-Assembly and Ionic-Lattice-like Secondary Structure of a Flexible Linear Polymer of Highly Charged Inorganic Building Blocks. <i>Journal of the American Chemical Society</i> , 2020, 142, 7295-7300.	6.6	12
31	Structure-Activity Relationships for the Affinity of Chaotropic Polyoxometalate Anions towards Proteins. <i>Chemistry - A European Journal</i> , 2020, 26, 5799-5809.	1.7	31
32	Catalyst Design for Alkene Epoxidation by Molecular Analogues of Heterogeneous Titanium-Silicalite Catalysts. <i>ACS Catalysis</i> , 2020, 10, 4737-4750.	5.5	45
33	±-DTC <sub>70</sub> fullerene performs significantly better than <sup>2</sup> -DTC <sub>70</sub> as electron transporting material in perovskite solar cells. <i>Journal of Materials Chemistry C</i> , 2020, 8, 6813-6819.	2.7	5
34	(Invited) Actinide-Based Buckyball Maracas: Fullerene Cages As Nanocontainers That Stabilize Monometallic and Actinide Clusters inside. <i>ECS Meeting Abstracts</i> , 2020, MA2020-01, 780-780.	0.0	0
35	(Invited) Electronic Structure and Bonding in Endohedral Actinidofullerenes. <i>ECS Meeting Abstracts</i> , 2020, MA2020-01, 782-782.	0.0	0
36	Tetravalent Metal Ion Guests in Polyoxopalladate Chemistry: Synthesis and Anticancer Activity of [MO <sub>8</sub> Pd <sub>12</sub> (PO <sub>4</sub> ) <sub>8</sub> ] <sup>12-</sup> (M =) Tj ETQq0 0 0 rgBI.9 Overlock 10 Tf 50		

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37	Peroxo-Cerium(IV)-Containing Polyoxometalates: $[Ce^{IV}_6(O_9)(GeW_{10}O_{37})_3]^{24-}$ as a Recyclable Homogeneous Oxidation Catalyst. <i>Inorganic Chemistry</i> , 2019, 58, 11300-11307.		24
38	9-Cobalt(II)-Containing 27-Tungsto-3-germanate(IV): Synthesis, Structure, Computational Modeling, and Heterogeneous Water Oxidation Catalysis. <i>Inorganic Chemistry</i> , 2019, 58, 11308-11316.	1.9	23
39	Th@C <sub>1</sub> (11)-C <sub>86</sub> : an actinide encapsulated in an unexpected C <sub>86</sub> fullerene cage. <i>Chemical Communications</i> , 2019, 55, 9271-9274.	2.2	30
40	Why Does Nb(V) Show Higher Heterolytic Pathway Selectivity Than Ti(IV) in Epoxidation with H <sub>2</sub> O <sub>2</sub> ? Answers from Model Studies on Nb- and Ti-Substituted Lindqvist Tungstates. <i>ACS Catalysis</i> , 2019, 9, 6262-6275.	5.5	36
41	How Does the Redox State of Polyoxovanadates Influence the Collective Behavior in Solution? A Case Study with $[V_8O_{42}]^{q-}$ (q = 3, 5, 7, 11, and 13). <i>Inorganic Chemistry</i> , 2019, 58, 3881-3894.	1.9	18
42	Small Cage Uranofullerenes: 27 Years after Their First Observation. <i>Helvetica Chimica Acta</i> , 2019, 102, e1900046.	1.0	4
43	Highly selective encapsulation and purification of U-based C <sub>78</sub> -EMFs within a supramolecular nanocapsule. <i>Nanoscale</i> , 2019, 11, 23035-23041.	2.8	19
44	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
45	Controlling the Activity and Stability of Electrochemical Interfaces Using Atom-by-Atom Metal Substitution of Redox Species. <i>ACS Nano</i> , 2019, 13, 458-466.	7.3	29
46	(Invited) Uranium-Based Endohedral Fullerenes: Completely Unexpected and Unusual Cage Structures Dictated By the Tetracationic Lanthanide Metal Ion. <i>ECS Meeting Abstracts</i> , 2019, , .	0.0	0
47	(Invited) Temperature Works Against Symmetry but "Fortunately" It Does Not Always Win: The Example of Formation of Actinide Endohedral Metallofullerenes. <i>ECS Meeting Abstracts</i> , 2019, , .	0.0	0
48	(Invited) Electronic Structure and Properties of Boron-Doped Endohedral Metalloheterofullerenes. <i>ECS Meeting Abstracts</i> , 2019, MA2019-01, 792-792.	0.0	2
49	(Invited) The Growth of Endohedral Metallofullerenes. <i>ECS Meeting Abstracts</i> , 2019, , .	0.0	0
50	(Invited) Intramolecular Reactions for Gas-Phase Formation of Carbon-Entrapped Clusterfullerenes. <i>ECS Meeting Abstracts</i> , 2019, , .	0.0	0
51	Understanding Electrochemical Interface Using Atom-By-Atom Metal Substitution of Redox Species. <i>ECS Meeting Abstracts</i> , 2019, , .	0.0	0
52	Formation of C <sub>2v</sub> -C <sub>72</sub> (11188)Cl <sub>4</sub> : A Particularly Stable Non-IPR Fullerene. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2288-2296.	1.1	3
53	U <sub>2</sub> @Ih(7)-C <sub>80</sub> : Crystallographic Characterization of a Long-Sought Dimetallic Actinide Endohedral Fullerene. <i>Journal of the American Chemical Society</i> , 2018, 140, 3907-3915.	6.6	96
54	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

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55	Probing the formation of halogenated endohedral metallofullerenes: Predictions confirmed by experiments. <i>Carbon</i> , 2018, 129, 750-757.	5.4	5
56	Self-assembly study of nanometric spheres from polyoxometalate-phenylalanine hybrids, an experimental and theoretical approach. <i>Dalton Transactions</i> , 2018, 47, 6304-6313.	1.6	30
57	Polyoxometalate electrocatalysts based on earth-abundant metals for efficient water oxidation in acidic media. <i>Nature Chemistry</i> , 2018, 10, 24-30.	6.6	375
58	Double functionalization of a fullerene in drastic arc-discharge conditions: synthesis and formation mechanism of C <sub>2v</sub> (2)-C <sub>78</sub> Cl <sub>6</sub> (C <sub>5</sub> Cl <sub>6</sub> ). <i>Carbon</i> , 2018, 129, 286-292.	5.4	7
59	Synthesis and Characterization of Non-Isolated-Pentagon-Rule Actinide Endohedral Metallofullerenes U@C <sub>1</sub> (17418)-C <sub>76</sub> , U@C <sub>1</sub> (28324)-C <sub>80</sub> , and Th@C <sub>1</sub> (28324)-C <sub>80</sub> : Low-Symmetry Cage Selection Directed by a Tetravalent Ion. <i>Journal of the American Chemical Society</i> , 2018, 140, 18039-18050.	6.6	73
60	Modeling the Oxygen Vacancy at a Molecular Vanadium(III) Silica-Supported Catalyst. <i>Journal of the American Chemical Society</i> , 2018, 140, 14903-14914.	6.6	26
61	Relevance of Protons in Heterolytic Activation of H <sub>2</sub> O <sub>2</sub> over Nb(V): Insights from Model Studies on Nb-Substituted Polyoxometalates. <i>ACS Catalysis</i> , 2018, 8, 9722-9737.	5.5	52
62	Mixed Dimetallic Cluster Fullerenes: ScGdO@C <sub>3v</sub> (8)-C <sub>82</sub> and ScGdC <sub>2</sub> @C <sub>2v</sub> (9)-C <sub>82</sub> . <i>Inorganic Chemistry</i> , 2018, 57, 11597-11605.	1.9	9
63	Purification of Uranium-based Endohedral Metallofullerenes (EMFs) by Selective Supramolecular Encapsulation and Release. <i>Angewandte Chemie</i> , 2018, 130, 11464-11469.	1.6	17
64	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
65	Tetracobalt-polyoxometalate catalysts for water oxidation: Key mechanistic details. <i>Journal of Catalysis</i> , 2017, 350, 56-63.	3.1	59
66	Single crystal structures and theoretical calculations of uranium endohedral metallofullerenes (U@C <sub>2n</sub> , 2n = 74, 82) show cage isomer dependent oxidation states for U. <i>Chemical Science</i> , 2017, 8, 5282-5290.	3.7	71
67	Current status of oxide clusterfullerenes. <i>Inorganica Chimica Acta</i> , 2017, 468, 91-104.	1.2	22
68	Counterintuitive Adsorption of [PW <sub>11</sub> O <sub>39</sub> ] <sup>7-</sup> on Au(100). <i>Inorganic Chemistry</i> , 2017, 56, 3961-3969.	1.9	18
69	Unique Four-Electron Metal-to-Cage Charge Transfer of Th to a C <sub>82</sub> Fullerene Cage: Complete Structural Characterization of Th@C <sub>3i</sub> v(8)-C <sub>82</sub> . <i>Journal of the American Chemical Society</i> , 2017, 139, 5110-5116.	6.6	97
70	Assembly Mechanism of Zr-Containing and Other TM-Containing Polyoxometalates. <i>Inorganic Chemistry</i> , 2017, 56, 4148-4156.	1.9	15
71	Transformation of doped graphite into cluster-encapsulated fullerene cages. <i>Nature Communications</i> , 2017, 8, 1222.	5.8	20
72	Size and charge effect of guest cations in the formation of polyoxopalladates: a theoretical and experimental study. <i>Chemical Science</i> , 2017, 8, 7862-7872.	3.7	20

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73	Deciphering the Role of Long-Range Interaction in Endohedral Metallofullerenes: A Revisit to Sc <sub>2</sub> C <sub>70</sub> . Journal of Physical Chemistry C, 2017, 121, 20481-20488.	1.5	6
74	Dimerization of Endohedral Fullerene in a Superatomic Crystal. Chemistry - A European Journal, 2017, 23, 13305-13308.	1.7	13
75	Unusual <i>c</i> -C <sub>2h</sub> -Symmetric <i>trans</i> -1-(Bispyrrolidine)-tetra-malonate Hexa-Adducts of C <sub>60</sub> : The Unexpected Regio- and Stereocontrol Mediated by Malonate-Pyrrolidine Interaction. Chemistry - A European Journal, 2017, 23, 15937-15944.	1.7	7
76	Understanding the Regioselectivity of Aromatic Hydroxylation over Divanadium-Substituted $\hat{I}^3$ -Keggin Polyoxotungstate. ACS Catalysis, 2017, 7, 8514-8523.	5.5	23
77	Real-time molecular scale observation of crystal formation. Nature Chemistry, 2017, 9, 369-373.	6.6	69
78	Diskrete Silber(I)-Palladium(II)-Oxo-Nanocluster, {Ag <sub>4</sub> Pd <sub>13</sub> } und {Ag <sub>5</sub> Pd <sub>15</sub> }, sowie die Rolle der Metall-Metall-Bindung induziert durch Kationen-Einschluss. Angewandte Chemie, 2016, 128, 15998-16002.	1.6	7
79	Discrete Silver(I)-Palladium(II)-Oxo Nanoclusters, {Ag <sub>4</sub> Pd <sub>13</sub> } and {Ag <sub>5</sub> Pd <sub>15</sub> }, and the Role of Metal-Metal Bonding Induced by Cation Confinement. Angewandte Chemie - International Edition, 2016, 55, 15766-15770.	7.2	31
80	Alkene Epoxidation Catalyzed by Ti-Containing Polyoxometalates: Unprecedented $\hat{I}^2$ -Oxygen Transfer Mechanism. Inorganic Chemistry, 2016, 55, 6080-6084.	1.9	40
81	Zigzag Sc <sub>2</sub> C <sub>2</sub> Carbide Cluster inside a [88] Fullerene Cage with One Heptagon, Sc <sub>2</sub> C <sub>2</sub> @C <sub>88</sub> (hept-C <sub>88</sub> ): A Kinetically Trapped Fullerene Formed by C <sub>2</sub> Insertion?. Journal of the American Chemical Society, 2016, 138, 13030-13037.	6.6	81
82	Synthesis, Structure, and Antibacterial Activity of a Thallium(III)-Containing Polyoxometalate, [Tl <sub>2</sub> {B $\hat{I}^2$ -SiW <sub>8</sub> O <sub>30</sub> (OH)} <sub>2</sub> ] <sup>12-</sup> . Inorganic Chemistry, 2016, 55, 10118-10121.	1.9	9
83	Direct Observation of the Formation Pathway of [Mo <sub>132</sub> ] Keplerates. Inorganic Chemistry, 2016, 55, 8285-8291.	1.9	15
84	Photoreduction Mechanism of CO <sub>2</sub> to CO Catalyzed by a Rhenium(I)-Polyoxometalate Hybrid Compound. ACS Catalysis, 2016, 6, 6422-6428.	5.5	58
85	Probing Polyoxometalate-Protein Interactions Using Molecular Dynamics Simulations. Chemistry - A European Journal, 2016, 22, 15280-15289.	1.7	50
86	Mixed-Metal Hybrid Polyoxometalates with Amino Acid Ligands: Electronic Versatility and Solution Properties. Inorganic Chemistry, 2016, 55, 12329-12347.	1.9	14
87	Sc <sub>3</sub> O@I <sub>h</sub> -C <sub>80</sub> : A Trimetallic Oxide Clusterfullerene Abundant in the Raw Soot. Journal of Physical Chemistry C, 2016, 120, 26159-26167.	1.5	16
88	Capturing the Fused-Pentagon C <sub>74</sub> by Stepwise Chlorination. Inorganic Chemistry, 2016, 55, 6861-6865.	1.9	20
89	Investigating the Transformations of Polyoxoanions Using Mass Spectrometry and Molecular Dynamics. Journal of the American Chemical Society, 2016, 138, 8765-8773.	6.6	50
90	Regio-, Stereo-, and Atropselective Synthesis of C <sub>60</sub> Fullerene Bisadducts by Supramolecular-Directed Functionalization. Angewandte Chemie - International Edition, 2016, 55, 11020-11025.	7.2	26

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91	Preparation of $\text{Ru}^{\text{I}}$ - and $\text{Ru}^{\text{II}}$ -isomers of mono-Ru-substituted Dawson-type phosphotungstates with an aqua ligand and comparison of their redox potentials, catalytic activities, and thermal stabilities with Keggin-type derivatives. <i>Dalton Transactions</i> , 2016, 45, 3715-3726.	1.6	16
92	$\text{La}_3\text{N@C}_{92}$ : An Endohedral Metallofullerene Governed by Kinetic Factors?. <i>Inorganic Chemistry</i> , 2016, 55, 3302-3306.	1.9	5
93	$\text{Sc}_2\text{O}@C_{82}(8)$ - $\text{C}_{82}$ : A Missing Isomer of $\text{Sc}_2\text{O}@C_{82}$ . <i>Inorganic Chemistry</i> , 2016, 55, 1926-1933.	1.9	45
94	On the formation of gold nanoparticles from $[\text{Au}^{\text{III}}\text{Cl}_4]^{\text{+}}$ and a non-classical reduced polyoxomolybdate as an electron source: a quantum mechanical modelling and experimental study. <i>New Journal of Chemistry</i> , 2016, 40, 1029-1038.	1.4	9
95	Reactivity differences of $\text{Sc}_3\text{N@C}_{2n}$ ( $2n = 68$ and $80$ ). Synthesis of the first methanofullerene derivatives of $\text{Sc}_3\text{N@D}_{5h}\text{-C}_{80}$ . <i>Chemical Communications</i> , 2016, 52, 64-67.	2.2	51
96	$\text{Sc}_2\text{O}@T_d(19151)\text{-C}_{76}$ : Hindered Cluster Motion inside a Tetrahedral Carbon Cage Probed by Crystallographic and Computational Studies. <i>Chemistry - A European Journal</i> , 2015, 21, 11110-11117.	1.7	46
97	Mechanism of Thioether Oxidation over Di- and Tetrameric Ti Centres: Kinetic and DFT Studies Based on Model Ti-Containing Polyoxometalates. <i>Chemistry - A European Journal</i> , 2015, 21, 14496-14506.	1.7	27
98	Different Factors Govern Chlorination and Encapsulation in Fullerenes: The Case of $\text{C}_{66}$ . <i>Inorganic Chemistry</i> , 2015, 54, 7562-7570.	1.9	9
99	Accuracy of Embedded Fragment Calculation for Evaluating Electron Interactions in Mixed Valence Magnetic Systems: Study of 2e-Reduced Lindqvist Polyoxometalates. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 550-559.	2.3	12
100	Cubane oxides inside middle-size fullerenes: the next endohedrals to be detected?. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	3
101	Supramolecular Recognition Influences Magnetism in $[\text{X}^{\text{IV}}\text{V}_8\text{V}_4\text{O}_{54}]^{6-}$ Self-Assemblies with Symmetry-Breaking Guest Anions. <i>Chemistry - A European Journal</i> , 2015, 21, 2387-2397.	1.7	38
102	(2 + 2) Cycloaddition of Benzyne to Endohedral Metallofullerenes $\text{M}_3\text{N@C}_{80}$ (M = Sc, Y): A Rotating-Intermediate Mechanism. <i>Journal of the American Chemical Society</i> , 2015, 137, 6820-6828.	6.6	38
103	Accurate calculation of $^{31}\text{P}$ NMR chemical shifts in polyoxometalates. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 8723-8731.	1.3	25
104	$\text{Sc}_2\text{O}@C_{82}(5)$ - $\text{C}_{80}$ : Dimetallic Oxide Cluster Inside a $\text{C}_{80}$ Fullerene Cage. <i>Inorganic Chemistry</i> , 2015, 54, 9845-9852.	1.9	50
105	Managing the Computational Chemistry Big Data Problem: The <b>ioChem-BD</b> Platform. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 95-103.	2.5	403
106	Small endohedral metallofullerenes: exploration of the structure and growth mechanism in the $\text{Ti@C}_{2n}$ ( $2n = 26-50$ ) family. <i>Chemical Science</i> , 2015, 6, 675-686.	3.7	45
107	Bottom-up formation of endohedral mono-metallofullerenes is directed by charge transfer. <i>Nature Communications</i> , 2014, 5, 5844.	5.8	69
108	Modular Molecules: Site-Selective Metal Substitution, Photoreduction, and Chirality in Polyoxometalate Hybrids. <i>Chemistry - A European Journal</i> , 2014, 20, 14102-14111.	1.7	30

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109	Magnetochemical Complexity of Hexa- and Heptanuclear Wheel Complexes of Late- $d$ Ions Supported by N-Donor Pyridyl-Methanolate Ligands. <i>Chemistry - A European Journal</i> , 2014, 20, 3769-3781.	1.7	15
110	ABILITY OF DFT CALCULATIONS TO CORRECTLY DESCRIBE REDOX POTENTIALS AND ELECTRON (DE)LOCALIZATION IN POLYOXOMETALATES. <i>Journal of Molecular and Engineering Materials</i> , 2014, 02, 1440004.	0.9	9
111	A fast metal-metal bonded water oxidation catalyst. <i>Journal of Catalysis</i> , 2014, 315, 25-32.	3.1	20
112	Dicobalt- $\mu_4$ -oxo Polyoxometalate Compound, $[(\mu_2\text{-P}_2\text{W}_{17}\text{O}_{61}\text{Co})_2\text{O}]^{14-}$ : A Potent Species for Water Oxidation, C-H Bond Activation, and Oxygen Transfer. <i>Inorganic Chemistry</i> , 2014, 53, 1779-1787.	1.9	30
113	Design and fabrication of memory devices based on nanoscale polyoxometalate clusters. <i>Nature</i> , 2014, 515, 545-549.	13.7	301
114	Maximum aromaticity or maximum pentagon separation; which is the origin behind the stability of endohedral metallofullerenes?. <i>Faraday Discussions</i> , 2014, 173, 201-13.	1.6	10
115	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
116	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
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