

Pere Miro

List of Publications by Year in descending order

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times ranked

5899
citing authors

#	ARTICLE	IF	CITATIONS
1	Computational Insights into Iron Heterometal Installation in Polyoxovanadate-Alkoxide Clusters. <i>Inorganic Chemistry</i> , 2023, 62, 1797-1803.	1.9	1
2	Computational Insights into the Nucleation of Mixed-Valent Polyoxovanadate Alkoxide Clusters. <i>Inorganic Chemistry</i> , 2021, 60, 7262-7268.	1.9	1
3	O ₂ Activation with a Sterically Encumbered, Oxygen-Deficient Polyoxovanadate-Alkoxide Cluster. <i>Inorganic Chemistry</i> , 2021, 60, 13833-13843.	1.9	8
4	Plausible Emergence and Self Assembly of a Primitive Phospholipid from Reduced Phosphorus on the Primordial Earth. <i>Origins of Life and Evolution of Biospheres</i> , 2021, 51, 185-213.	0.8	6
5	Computational investigation of KICl ₂ iodination of thiophene and its electron-poor derivatives. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4190.	0.9	0
6	Physicochemical implications of surface alkylation of high-valent, Lindqvist-type polyoxovanadate-alkoxide clusters. <i>Nanoscale</i> , 2021, 13, 6162-6173.	2.8	3
7	Actinide arene-metalates: ion pairing effects on the electronic structure of unsupported uranium-arene sandwich complexes. <i>Chemical Science</i> , 2021, 12, 13360-13372.	3.7	13
8	Prediction of optoelectronic properties of Cu ₂ O using neural network potential. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 14910-14917.	1.3	2
9	Application of Symmetry Functions to Large Chemical Spaces Using a Convolutional Neural Network. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1928-1935.	2.5	5
10	Suzuki coupling catalyzed by chloro({2-[mesityl(quinolin-8-yl- <i>l</i> -N)boryl]-3,5-dimethylphenyl}methyl- <i>l</i> -C)palladium(II). <i>Tetrahedron</i> , 2019, 75, 2365-2370.	1.0	7
11	Tuning the electronic structure of graphene through alkali metal and halogen atom intercalation. <i>Solid State Communications</i> , 2018, 272, 22-27.	0.9	9
12	A Single-Material Logical Junction Based on 2D Crystal PdS ₂ . <i>Advanced Materials</i> , 2016, 28, 853-856.	11.1	85
13	Self-Assembly of Uranyl-Peroxide Nanocapsules in Basic Peroxidic Environments. <i>Chemistry - A European Journal</i> , 2016, 22, 8571-8578.	1.7	32
14	Water oxidation catalysis with ligand substituted Ru-bpp type complexes. <i>Catalysis Science and Technology</i> , 2016, 6, 5088-5101.	2.1	23
15	Colloidal Synthesis of Single-Layer MSe ₂ (M = Mo, W) Nanosheets via Anisotropic Solution-Phase Growth Approach. <i>Journal of the American Chemical Society</i> , 2015, 137, 7266-7269.	6.6	147
16	Tandem intercalation strategy for single-layer nanosheets as an effective alternative to conventional exfoliation processes. <i>Nature Communications</i> , 2015, 6, 5763.	5.8	137
17	Noble-Metal Chalcogenide Nanotubes. <i>Inorganics</i> , 2014, 2, 556-564.	1.2	7
18	Hexagonal Transition-Metal Chalcogenide Nanoflakes with Pronounced Lateral Quantum Confinement. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 12624-12628.	7.2	9

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19	Oxygenation by Ruthenium Monosubstituted Polyoxotungstates in Aqueous Solution: Experimental and Computational Dissection of a Ru(III)â€Ru(V) Catalytic Cycle. Chemistry - A European Journal, 2014, 20, 10932-10943.	1.7	11
20	Uranylâ€Peroxide Nanocapsules in Aqueous Solution: Force Field Development and First Applications. Journal of Physical Chemistry C, 2014, 118, 24730-24740.	1.5	22
21	Two Dimensional Materials Beyond MoS ₂ : Nobleâ€Transitionâ€Metal Dichalcogenides. Angewandte Chemie - International Edition, 2014, 53, 3015-3018.	7.2	215
22	An atlas of two-dimensional materials. Chemical Society Reviews, 2014, 43, 6537-6554.	18.7	1,159
23	Encapsulated Water Inside Mo ₁₃₂ Capsules: The Role of Long-Range Correlations of about 1 nm. Journal of Physical Chemistry C, 2014, 118, 5545-5555.	1.5	11
24	Carbon Dioxide Reduction Catalyzed by Dinuclear Ruthenium Polypyridyl Complexes. ChemCatChem, 2013, 5, 3897-3903.	1.8	11
25	Synthesis and Characterization of the First ² D Neptunyl Structure Stabilized by Sideâ€on Cationâ€Cation Interactions. Chemistry - A European Journal, 2013, 19, 2937-2941.	1.7	21
26	Water clusters to nanodrops: a tight-binding density functional study. Physical Chemistry Chemical Physics, 2013, 15, 1837-1843.	1.3	40
27	Understanding Electronic Ligand Perturbation over Successive Metalâ€Based Redox Potentials in Mononuclear Rutheniumâ€Aqua Complexes. ChemPlusChem, 2013, 78, 235-243.	1.3	17
28	Spontaneous Ripple Formation in MoS ₂ Monolayers: Electronic Structure and Transport Effects. Advanced Materials, 2013, 25, 5473-5475.	11.1	97
29	Transition Metal Monolayers: Spontaneous Ripple Formation in MoS ₂ Monolayers: Electronic Structure and Transport Effects (Adv. Mater. 38/2013). Advanced Materials, 2013, 25, 5366-5366.	11.1	3
30	Selectivity in Ring-Opening Metathesis Polymerization of <i>Z</i> -Cyclooctenes Catalyzed by a Second-generation Grubbs Catalyst. ACS Catalysis, 2012, 2, 2547-2556.	5.5	55
31	Volatilities of Actinide and Lanthanide <i>N</i> , <i>N</i> -Dimethylaminodiboranate Chemical Vapor Deposition Precursors: A DFT Study. Journal of Physical Chemistry C, 2012, 116, 23194-23200.	1.5	19
32	Uranyl-Peroxide Nanocapsules: Electronic Structure and Cation Complexation in [(UO ₂) ₂₀ (¹ / ₄ O ₂) ₃₀] ²⁰⁺ . Inorganic Chemistry, 2012, 51, 3840-3845.	1.9	37
33	Effect of Axially Projected Oligothiophene Pendants and Nitro-Functionalized Diimine Ligands on the Lowest Excited State in Cationic Ir(III) bis-Cyclometalates. Inorganic Chemistry, 2012, 51, 5082-5094.	1.9	27
34	Electronic structure and bonding of lanthanoid(III) carbonates. Physical Chemistry Chemical Physics, 2012, 14, 14822.	1.3	38
35	Experimental and Computational Study of a New Wheel-Shaped {W ₅ O ₂₁ } ₃ [(U ^{VI} O ₂) ₂ (¹ / ₄ O ₂) ₃] ₃ Polyoxometalate. Inorganic Chemistry, 2012, 51, 8784-8790.	3.1	31
36	Polyoxometalates adsorbed on metallic surfaces: immediate reduction of [SiW ₁₂ O ₄₀] ⁴⁻ on Ag(100). Chemical Science, 2012, 3, 2020.	3.7	32

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37	A Journey inside the U ₂₈ Nanocapsule. Chemistry - A European Journal, 2012, 18, 8340-8346.	1.7	39
38	On the electronic structure of giant polyoxometalates: Mo ₁₃₂ vs. W ₇₂ Mo ₆₀ . Dalton Transactions, 2012, 41, 9984.	1.6	12
39	Encapsulated Water Molecules in Polyoxometalates: Insights from Molecular Dynamics. NATO Science for Peace and Security Series B: Physics and Biophysics, 2012, , 119-132.	0.2	0
40	Carbon dioxide reduction by mononuclear ruthenium polypyridyl complexes. Physical Chemistry Chemical Physics, 2011, 13, 19480.	1.3	23
41	Dynamics of Encapsulated Water inside Mo ₁₃₂ Cavities. Journal of Physical Chemistry B, 2011, 115, 5980-5992.	1.2	28
42	Electronic Structure of Oxidized Complexes Derived from cis-[Ru(bpy) ₂ (H ₂ O) ₂] ²⁺ and Its Photoisomerization Mechanism. Inorganic Chemistry, 2011, 50, 11134-11142.	1.9	64
43	Current trends in the computational modelling of polyoxometalates. Theoretical Chemistry Accounts, 2011, 128, 393-404.	0.5	69
44	On the Nature of Actinide ^{IV} and Lanthanide ^{III} Metal Bonds in Heterobimetallic Compounds. Chemistry - A European Journal, 2011, 17, 8424-8433.	1.7	112
45	Electronic structure and surface properties of the mixed-valence doughnut shaped polyoxomolybdate nanocapsule Mo ₅₇ V ₆ . Inorganica Chimica Acta, 2010, 363, 4368-4373.	1.2	4
46	On the Origin of the Cation Templated Self-Assembly of Uranyl-Peroxide Nanoclusters. Journal of the American Chemical Society, 2010, 132, 17787-17794.	6.6	102
47	Gated and Differently Functionalized (New) Porous Capsules Direct Encapsulates' Structures: Higher and Lower Density Water. Chemistry - A European Journal, 2009, 15, 1844-1852.	1.7	74
48	Supramolecular Chemistry on a Cluster Surface: Fixation/Complexation of Potassium and Ammonium Ions with Crown Ether Like Rings. Angewandte Chemie - International Edition, 2009, 48, 5934-5937.	7.2	25
49	Water Oxidation at a Tetraruthenate Core Stabilized by Polyoxometalate Ligands: Experimental and Computational Evidence To Trace the Competent Intermediates. Journal of the American Chemical Society, 2009, 131, 16051-16053.	6.6	195
50	Towards a computational treatment of polyoxometalates in solution using QM methods and explicit solvent molecules. Canadian Journal of Chemistry, 2009, 87, 1296-1301.	0.6	26
51	Flexible Pores of a Metal Oxide-Based Capsule Permit Entry of Comparatively Larger Organic Guests. Journal of the American Chemical Society, 2009, 131, 6380-6382.	6.6	102
52	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