Pere Miro

List of Publications by Year in descending order

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52 papers	3,334 citations	236833 25 h-index	175177 52 g-index
58 all docs	58 docs citations	58 times ranked	5899 citing authors

#	Article	IF	Citations
1	An atlas of two-dimensional materials. Chemical Society Reviews, 2014, 43, 6537-6554.	18.7	1,159
2	Two Dimensional Materials Beyond MoS₂: Nobleâ€Transitionâ€Metal Dichalcogenides. Angewandte Chemie - International Edition, 2014, 53, 3015-3018.	7.2	215
3	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
4	Colloidal Synthesis of Single-Layer MSe₂ (M = Mo, W) Nanosheets via Anisotropic Solution-Phase Growth Approach. Journal of the American Chemical Society, 2015, 137, 7266-7269.	6.6	147
5	Tandem intercalation strategy for single-layer nanosheets as an effective alternative to conventional exfoliation processes. Nature Communications, 2015, 6, 5763.	5.8	137
6	On the Nature of Actinideâ€“ and Lanthanideâ€“Metal Bonds in Heterobimetallic Compounds. Chemistry - A European Journal, 2011, 17, 8424-8433.	1.7	112
7	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
8	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
9	Spontaneous Ripple Formation in MoS₂ Monolayers: Electronic Structure and Transport Effects. Advanced Materials, 2013, 25, 5473-5475.	11.1	97
10	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
11	A Singleâ€Material Logical Junction Based on 2D Crystal PdS₂. Advanced Materials, 2016, 28, 853-856.	11.1	85
12	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
13	Current trends in the computational modelling of polyoxometalates. Theoretical Chemistry Accounts, 2011, 128, 393-404.	0.5	69
14	Electronic Structure of Oxidized Complexes Derived fromcis-[RuII(bpy)2(H2O)2]2+and Its Photoisomerization Mechanism. Inorganic Chemistry, 2011, 50, 11134-11142.	1.9	64
15	Selectivity in Ring-Opening Metathesis Polymerization of Z-Cyclooctenes Catalyzed by a Second-generation Grubbs Catalyst. ACS Catalysis, 2012, 2, 2547-2556.	5.5	55
16	Water clusters to nanodrops: a tight-binding density functional study. Physical Chemistry Chemical Physics, 2013, 15, 1837-1843.	1.3	40
17	A Journey inside the U₂₈ Nanocapsule. Chemistry - A European Journal, 2012, 18, 8340-8346.	1.7	39
18	Electronic structure and bonding of lanthanoid(iii) carbonates. Physical Chemistry Chemical Physics, 2012, 14, 14822.	1.3	38

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19	Uranyl-Peroxide Nanocapsules: Electronic Structure and Cation Complexation in [(UO₂)₂₀(Î¼-O₂)₃₀]^{20â€“}. Inorganic Chemistry, 2012, 51, 3840-3845.	1.9	37
20	Experimental and Computational Study of a New Wheel-Shaped {[W₅O₂₁]₃[(U^{VI}O₂)₂(Î¼-O₂₃} Polyoxometalate. Inorganic Chemistry, 2012, 51, 8784-8790.	1.9	35
21	Polyoxometalates adsorbed on metallic surfaces: immediate reduction of [SiW12O40]4â^' on Ag(100). Chemical Science, 2012, 3, 2020.	3.7	32
22	Selfâ€Assembly of Uranylâ€“Peroxide Nanocapsules in Basic Peroxidic Environments. Chemistry - A European Journal, 2016, 22, 8571-8578.	1.7	32
23	Dynamics of Encapsulated Water inside Mo₁₃₂ Cavities. Journal of Physical Chemistry B, 2011, 115, 5980-5992.	1.2	28
24	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
25	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
26	Supramolecular Chemistry on a Cluster Surface: Fixation/Complexation of Potassium and Ammonium Ions with Crownâ€Etherâ€Like Rings. Angewandte Chemie - International Edition, 2009, 48, 5934-5937.	7.2	25
27	Carbon dioxide reduction by mononuclear ruthenium polypyridyl complexes. Physical Chemistry Chemical Physics, 2011, 13, 19480.	1.3	23
28	Water oxidation catalysis with ligand substituted Ruâ€“bpp type complexes. Catalysis Science and Technology, 2016, 6, 5088-5101.	2.1	23
29	Uranylâ€“Peroxide Nanocapsules in Aqueous Solution: Force Field Development and First Applications. Journal of Physical Chemistry C, 2014, 118, 24730-24740.	1.5	22
30	Synthesis and Characterization of the First 2â€‰D Neptunyl Structure Stabilized by Sideâ€on Cationâ€“Cation Interactions. Chemistry - A European Journal, 2013, 19, 2937-2941.	1.7	21
31	Volatilities of Actinide and Lanthanide N,N-Dimethylaminodiboranate Chemical Vapor Deposition Precursors: A DFT Study. Journal of Physical Chemistry C, 2012, 116, 23194-23200.	1.5	19
32	Understanding Electronic Ligand Perturbation over Successive Metalâ€Based Redox Potentials in Mononuclear Rutheniumâ€“Aqua Complexes. ChemPlusChem, 2013, 78, 235-243.	1.3	17
33	Actinide arene-metalates: ion pairing effects on the electronic structure of unsupported uraniumâ€“arenide sandwich complexes. Chemical Science, 2021, 12, 13360-13372.	3.7	13
34	On the electronic structure of giant polyoxometalates: Mo132vs. W72Mo60. Dalton Transactions, 2012, 41, 9984.	1.6	12
35	Carbon Dioxide Reduction Catalyzed by Dinuclear Ruthenium Polypyridyl Complexes. ChemCatChem, 2013, 5, 3897-3903.	1.8	11
36	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

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37	Encapsulated Water Inside Mo₁₃₂ Capsules: The Role of Long-Range Correlations of about 1 nm. Journal of Physical Chemistry C, 2014, 118, 5545-5555.	1.5	11
38	Hexagonal Transitionâ€Metal Chalcogenide Nanoflakes with Pronounced Lateral Quantum Confinement. Angewandte Chemie - International Edition, 2014, 53, 12624-12628.	7.2	9
39	Tuning the electronic structure of graphene through alkali metal and halogen atom intercalation. Solid State Communications, 2018, 272, 22-27.	0.9	9
40	O₂ Activation with a Sterically Encumbered, Oxygen-Deficient Polyoxovanadate-Alkoxide Cluster. Inorganic Chemistry, 2021, 60, 13833-13843.	1.9	8
41	Noble-Metal Chalcogenide Nanotubes. Inorganics, 2014, 2, 556-564.	1.2	7
42	Suzuki coupling catalyzed by chloro({2-[mesityl(quinolin-8-yl-ÎºN)boryl]-3,5-dimethylphenyl}methyl-ÎºC)palladium(II). Tetrahedron, 2019, 75, 2365-2370.	1.0	7
43	Plausible Emergence and Self Assembly of a Primitive Phospholipid from Reduced Phosphorus on the Primordial Earth. Origins of Life and Evolution of Biospheres, 2021, 51, 185-213.	0.8	6
44	Application of Symmetry Functions to Large Chemical Spaces Using a Convolutional Neural Network. Journal of Chemical Information and Modeling, 2020, 60, 1928-1935.	2.5	5
45	Electronic structure and surface properties of the mixed-valence doughnut shaped polyoxomolybdate nanocapsule Mo57V6. Inorganica Chimica Acta, 2010, 363, 4368-4373.	1.2	4
46	Transition Metal Monolayers: Spontaneous Ripple Formation in MoS2Monolayers: Electronic Structure and Transport Effects (Adv. Mater. 38/2013). Advanced Materials, 2013, 25, 5366-5366.	11.1	3
47	Physicochemical implications of surface alkylation of high-valent, Lindqvist-type polyoxovanadate-alkoxide clusters. Nanoscale, 2021, 13, 6162-6173.	2.8	3
48	Prediction of optoelectronic properties of Cu₂O using neural network potential. Physical Chemistry Chemical Physics, 2020, 22, 14910-14917.	1.3	2
49	Computational Insights into the Nucleation of Mixed-Valent Polyoxovanadate Alkoxide Clusters. Inorganic Chemistry, 2021, 60, 7262-7268.	1.9	1
50	Computational Insights into Iron Heterometal Installation in Polyoxovanadateâ€“Alkoxide Clusters. Inorganic Chemistry, 2023, 62, 1797-1803.	1.9	1
51	Computational investigation of KICl 2 iodination of thiophene and its electronâ€poor derivatives. Journal of Physical Organic Chemistry, 2021, 34, e4190.	0.9	0
52	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