

WG1 Catalysis and Energy

A Lewis Acid Catalytic Core Sandwiched by Inorganic Polyoxoanion Caps: Selective H₂O₂ based Oxidations with [Al^{III}₄(H₂O)₁₀(β-XW₉O₃₃H)₂]⁶⁻ (X = As^{III}, Sb^{III}).
M. Carraro, B. Bassil, A. Sorarù, S. Berardi, A. Suchopar, U. Kortz, M. Bonchio
Chem. Commun., **2013**, 49, 7914-7916
pubs.rsc.org/en/Content/ArticleLanding/2013/CC/c3cc44077j

Improved Synthesis, Structure, and Solution Characterization of the Cyclic 48-Tungsto-8-Arsenate(V), [H₄As₈W₄₈O₁₈₄]³⁶⁻.
Mbomekallé, I.-M.; Bassil, B. S.; Suchopar, A.; Keita, B.; Nadjjo, L.; Ammam, M.; Haouas, M.; Taulelle, F.; Kortz, U.
J. Clust. Sci. **2014**, 25, 277-285.
link.springer.com/article/10.1007%2Fs10876-013-0656-2

Oxygenation by Ruthenium Monosubstituted Polyoxotungstates in Aqueous Solution: Experimental and Computational Dissection of a Ru(III)–Ru(V) Catalytic Cycle
A. Sartorel, P. Mirò, M. Carraro, S. Berardi, O. Bortolini, A. Bagno, C. Bo, and M. Bonchio.
Chem. Eur. J., **2014**, 20, 10932-10943
onlinelibrary.wiley.com/doi/10.1002/chem.201404088/abstract

Photocatalytic Water Oxidation by a Mixed-Valent Mn^{III}3Mn^{IV}O₃ Manganese Oxo Core that Mimics the Natural Oxygen-Evolving Center
R. Al-Oweini, A. Sartorel, B. S. Bassil, M. Natali, S. Berardi, F. Scandola, U. Kortz, and M. Bonchio.
Angew. Chem, Int. Ed. **2014**, 53, 11182-11185.
onlinelibrary.wiley.com/doi/10.1002/anie.201404664/abstract

Electrochemical behaviour of mixed d metal-iron containing Wells-Dawson sandwich-type complexes: [(FeOH₂)₂M₂(X₂W₁₅O₅₆)₂]ⁿ⁻ and [(MOH₂)₂Fe₂(X₂W₁₅O₅₆)₂]ⁿ⁻ (M = Cr^{III}, Mn^{III}, Mn^{II}, Co^{II}, Ni^{II}, Cu^{II}, Zn^{II}, X = As or P and n = 12 or 14),
Doungmene, F.; Aparicio, P.A.; Ntienoue, J.; Ayingone Mezui, Ch. S.; de Oliveira, P.; López, X.; Mbomekallé, I.-M. (2014)
Electrochimica Acta, **2014**, 125, 674-682.
sciencedirect.com/science/article/pii/S0013468614002849

Synthesis, Magnetism, and Electrochemistry of the Ni₁₄- and Ni₅-Containing Heteropolytungstates

*[Ni₁₄(OH)₆(H₂O)₁₀(HPO₄)₄(P₂W₁₅O₅₆)₄]³⁴⁻ and *[Ni₅(OH)₄(H₂O)₄(β-GeW₉O₃₄)(β-GeW₈O₃₀(OH))]¹³⁻**

Ibrahim, M.; Xiang, Y.; Bassil, B. S.; Lan, Y.; Powell, A. K.; de Oliveira, P.; Keita, B.; Kortz, U.

Inorg. Chem. **2013**, *52*, 8399-8408

pubs.acs.org/doi/abs/10.1021/ic400943j

Tetradecanuclear Iron(III)-Oxo Nanoclusters Stabilized by Trilacunary Heteropolyanions;

Ibrahim, M.; Haider, A.; Xiang, Y.; Bassil, B. S.; Carey, A. M.; Rullik, L.; Jameson, G. B.; Doungmene, F.; Mbomekallé, I. M.; de Oliveira, P.; Mereacre, V.; Kostakis, G. E.; Powell, A. K.; Kortz, U.;

Inorg. Chem. **2015**, *54*, 6136-6146

pubs.acs.org/doi/abs/10.1021/acs.inorgchem.5b00124

Heptanickel(II) Double-Cubane Core in Wells-Dawson Heteropolytungstate, [Ni₇(OH)₆(H₂O)₆(P₂W₁₅O₅₆)₂]¹⁶⁻

Bassil, B. S.; Xiang, Y.; Haider, A.; Hurtado, J.; Novitchi, G.; Powell, A. K.; Bossoh, A. M.; Mbomekallé, I. M.; de Oliveira, P.; Kortz, U.

Chem. Commun. **2016**, *52*, 2601-2604

<http://pubs.rsc.org/en/content/articlepdf/2016/cc/c5cc09823h>

Alkaline Earth Guests in Polyoxopalladate Chemistry: From Nanocube to Nanostar via an Open-Shell Structure.

Yang, P.; Xiang, Y.; Lin, Z.; Bassil, B. S.; Cao, J.; Fan, L.; Fan, Y.; Li, M.; Jiménez-Lozano, P.; Carbó, J. J.; Poblet, J. M.; Kortz, U.;

Angew. Chem. Int. Ed. **2014**, *53*, 11974-11978.

onlinelibrary.wiley.com/doi/10.1002/anie.201407090/abstract

Electrocatalysis by crown-type polyoxometalates multi-substituted by transition metal ions; Comparative study

Naseer, R.; Mal, S. S.; Kortz, U.; Armstrong, G.; Laffir, F.; Dickinson, C.; Vagin, M.; McCormac, T.

Electrochimica Acta **2015**, *176*, 1248-1255.

http://ac.els-cdn.com/S001346861530219X/1-s2.0-S001346861530219X-main.pdf?_tid=65dbacb0-e7dc-11e6-a834-0000aab0f27&acdnat=1485884627_0fa50f3fb4c6b5cbd9c1bd84d6166f56

Effect of electron (de)localisation and pairing in the electrochemistry of polyoxometalates. Study of Wells-Dawson molybdotungstophosphate derivatives

L. Parent, P. A. Aparicio, P. de Oliveira, A.-L. Teillout, J. M. Poble, X. Lopez, I. M. Mbomekalle

Inorg. Chem., **2014**, 53, 5941 – 5949.

pubs.acs.org/doi/abs/10.1021/ic500087t

A Dicobalt- μ -oxo Polyoxometalate Compound, $[(\alpha_2\text{-P}_2\text{W}_{17}\text{O}_{61}\text{Co})_2\text{O}]^{14-}$, A Potent Species for Water Oxidation, C-H Bond Activation and Oxygen Transfer

D. Barats-Damatov; L. J. W. Shimon; L. Weiner; R. Schreiber; P. Jiménez-Lozano; **J. M. Poble**; C. de Graaf; **R. Neumann**,

Inorganic Chemistry, **2014**, 53, 1779–1787.

pubs.acs.org/doi/abs/10.1021/ic402962c

Aerobic Carbon–Carbon Bond Cleavage of Alkenes to Aldehydes Catalyzed by First-Row Transition-Metal-Substituted Polyoxometalates in the Presence of Nitrogen Dioxide.

A. Rubinstein, P. Jiménez-Lozano, **J. J. Carbó**, **J. M. Poble** and **R. Neumann**

J. Am. Chem. Soc. **2014**, 136, 10941–10948

pubs.acs.org/doi/abs/10.1021/ja502846h

Photoreduction Mechanism of CO₂ to CO Catalyzed by a Rhenium(I) Polyoxometalate Hybrid Compound

C. Ci, **J. J. Carbó**, **R. Neumann**, C. de Graaf, **J. M. Poble**

ACS Catalysis, **2016**, 6, 6422–6428

pubs.acs.org/doi/abs/10.1021/acscatal.6b01638

Real-time molecular scale observation of crystal formation

R. E Schreiber, L. Houben, S. G Wolf, G. Leitus, Z.-L. Lang, **J. J Carbó**, **J. M Poble**, **R. Neumann**

Nature Chemistry online **2016**, doi:10.1038/nchem.2675

nature.com/nchem/journal/vaop/ncurrent/full/nchem.2675.html

¹⁷O NMR chemical shifts in oxometalates: from the simplest monometallic species to mixed-metal polyoxometalates.

M. Pascual-Borràs, X. López, A. Rodríguez-Forteza, R. J. Errington and J. M. Poble

Chem. Sci., **2014**, 5, 2031-2042.

pubs.rsc.org/en/Content/ArticleLanding/2014/SC/c4sc00083h

Mechanism of thioether oxidation over di- and tetrameric Ti centers: Kinetic and DFT studies based on model Ti-containing polyoxometalates.

I.Y. Skobelev, O. V. Zalomaeva, O.A. Kholdeeva, J. M. Poble, J. J. Carbó,

Chem. Eur J., **2015**, 21, 14496 –14506.

onlinelibrary.wiley.com/doi/10.1002/chem.201501157/abstract

Synthesis, Structural and Electrochemical Properties of the $[\text{Sb}^{\text{III}}_2\text{SiMo}_{12}\text{O}_{40}]^{4-}$ anion, a Bicapped Keggin Polyoxometalate.

R. Canioni, E. Cadot, R. J. Errington, N. Leclerc-Laronze, and C. Roche-Marchal.

Curr. Inorg. Chem. submitted

<http://benthamscience.com/journal-files/special-issue-details/CIC-SII20161028-01.pdf>

WG2 Hybrid POMs for Electronics

Electron Transfer to Covalently Immobilized Keggin Polyoxotungstates on Gold.

Yaqub, M.; Walsh, J.; Keyes, T.; Proust, A.; Rinfray, C.; Izzet, Guillaume; McCormac, T.; Forster, R., *Langmuir*, **2014**, *30*, 4509-4516.
<http://pubs.acs.org/doi/abs/10.1021/la4048648>

Hybrid Polyoxometalate Materials for Photo(electro-) chemical Applications.

J. Walsh, A.M. Bond, R.J. Forster, T.E. Keyes,
Coord. Chem Rev. **2016**, *306*, 217-234.
sciencedirect.com/science/article/pii/S0010854515002210

Covalent Attachment of Thiophene Groups to Polyoxomolybdates or Polyoxotungstates for the Formation of Hybrid Films

A. Saad, G. Rousseau, P. Mialane, J. Marrot, M. Haouas, F. Taulelle, N. Anwar, T. McCormac, A. Dolbecq,
Eur. J. Inorg. Chem., **2015**, 4775-4782.
onlinelibrary.wiley.com/doi/10.1002/ejic.201500660/abstract

Design and fabrication of memory devices based on nanoscale polyoxometalate clusters.

C. Busche, L. Vila-Nadal, J. Yan, H. N. Miras, D.-L. Long, V. P. Georgiev, A. Asenov, R. H. Pedersen, N. Gadegaard, M. M. Mirza, D. J. Paul, J. M. Poblet, L. Cronin.
Nature, **2014**, *515*, 545-549
nature.com/nature/journal/v515/n7528/full/nature13951.html

Polyoxometalate $\{W_{18}O_{56}XO_6\}$ Clusters with Embedded Redox-Active Main-Group Templates as Localized Inner-Cluster Radicals

L. Vilà-Nadal, K. Peuntinger, C. Busche, J. Yan, D. Lüders, D. -L. Long, J. M. Poblet, D. M. Guldi, L. Cronin.
Angew. Chem. Int. Ed., **2013**, *52*, 9695-9699.
onlinelibrary.wiley.com/doi/10.1002/anie.201303126/abstract

Surface Immobilization of a Tetra-Ruthenium Substituted Polyoxometalate Water Oxidation Catalyst Through the Employment of Conducting Polypyrrole and the Layer-by-Layer (LBL) Technique

N. Anwar, A. Sartorel, M. Yaqub, K. Wearen, F. Laffir, G. Armstrong, C. Dickinson, M. Bonchio, and T. McCormac

ACS Appl. Mater. Interfaces, **2014**, *6*, 8022-8031

pubs.acs.org/doi/abs/10.1021/am405295c

Redox, surface and electrocatalytic properties of layer-by-layer films based upon Fe(III)-substituted crown polyoxometalate $[P_8W_{48}O_{184}Fe_{16}(OH)_{28}(H_2O)_4]^{20-}$.

Naseer, R.; Mal, S. S.; Ibrahim, M.; Kortz, U.; Armstrong, G.; Laffir, F.; Dickinson, C.; Vagin, M.; McCormac, T.

Electrochim. Acta, **2014**, *134*, 450-458

sciencedirect.com/science/article/pii/S0013468614006124

Charge transfer interactions in self-assembled single walled carbon nanotubes/Dawson-Wells polyoxometalate hybrids

C. Bosch-Navarro, B. Matt, G. Izzet, C. Romero-Nieto, K. Dirian, A. Raya, S. I. Molina, A. Proust, D. M. Guldi, C. Martí-Gastaldo, E. Coronado

Chem. Sci., **2014**, *5*, 4346-4354

pubs.rsc.org/en/Content/ArticleLanding/2014/SC/C4SC01335B

Phosphomolybdate@Carbon-Based Nanocomposites as Electrocatalysts for Oxygen Reduction Reaction

M. Nunes, D. M. Fernandes, I. M. Rocha, M. F.R. Pereira, I.-M. Mbomekalle, P. de Oliveira, C. Freire.

Chemistry Select **2016**, *1*, 6257-6266.

<http://onlinelibrary.wiley.com/wol1/doi/10.1002/slct.201601370/abstract>

Polyoxometalate – conductive polymer composites for energy conversion, energy storage and nanostructured sensors

S. Herrmann, **C. Ritchie**, **C. Streb**,

Dalton Trans., **2015**, *44*, 7092-7104

pubs.rsc.org/en/Content/ArticleLanding/2015/DT/C4DT03763D

WG3 Molecular Magnetism and Spintronics

Modeling the Magnetic Properties and Mossbauer Spectra of Multifunctional Magnetic Materials Obtained by Insertion of a Spin-Crossover Fe(III) Complex into Bimetallic Oxalate-Based Ferromagnets.

Ostrovsky, S. M., Reu, O. S.; **Palii, A. V.**; Clemente-Leon, M.; **Coronado, E.**; Waerenborgh, J. C.; Klokishner, S. I.

Inorg. Chem., **2013**, 52, 13536-13545.

pubs.acs.org/doi/abs/10.1021/ic401997w

SIMPRES: A software package to calculate crystal field parameters, energy levels, and magnetic properties on mononuclear lanthanoid complexes based on charge distributions.

Baldovi, J. J.; Cardona-Serra, S.; Clemente-Juan, J. M.; **Coronado, E.**; Gaita-Arino, A.; **Palii, A.**

J. Comput. Chem. **2013**, 34, 1961-1967.

onlinelibrary.wiley.com/doi/10.1002/jcc.23341/abstract

Self-trapping of charge polarized states in four-dot molecular quantum cellular automata: bi-electronic tetrameric mixed-valence species

B. Tsukerblat, A. Palii, J.M. Clemente-Juan,

Pure and Applied Chemistry, **2015**, 87, 271–282.

degruyter.com/view/j/pac.2015.87.issue-3/pac-2014-0904/pac-2014-0904.xml

Electric field control of spin-dependent dissipative electron transfer dynamics in mixed-valence molecules

A. Palii, J. M. Clemente-Juan, **E. Coronado**, **B. Tsukerblat**,

J. Phys. Chem. C, **2015**, 119, 7911-7921.

pubs.acs.org/doi/abs/10.1021/jp512102n

Dissipative electron transfer dynamics in mixed valence dimers: Microscopic approach to the solid state problem.

Palii, A.; Bosch-Serrano, C.; Modesto Clemente-Juan, J.; **Coronado, E.**; **Tsukerblat, B.**

J. Chem. Phys., **2013**, 139, article 044304.

aip.scitation.org/doi/10.1063/1.4813855

Electric Field Control of the Optical Properties in Magnetic Mixed-Valence Molecules

A. Palii, J. M. Clemente-Juan, B. Tsukerblat, E. Coronado,
Chem. Sci, **2014**, 3598-3602.

pubs.rsc.org/en/Content/ArticleLanding/2014/SC/C4SC01056F

Symmetry Assisted Consideration of the Dynamic Pseudo Jahn-Teller Problem in Mixed-Valence Species with Square Topology: Intervalence Optical Bands

J. M. Clemente-Juan, A. Palii, E. Coronado, B. Tsukerblat,
Optics and Spectroscopy, **2014**, 116, 159-166.

link.springer.com/article/10.1134%2FS0030400X14050075

Mixed-valence molecular four-dot unit for quantum cellular automata: vibronic self-trapping and cell-cell response

B. Tsukerblat, A. Palii, J.M. Clemente-Juan, E. Coronado,
J. Chem. Physics, **2015**, 143, 134307-15.

aip.scitation.org/doi/full/10.1063/1.4932106

Spin-switching in molecular quantum cellular automata based on mixed-valence tetrameric units.

A. Palii, B. Tsukerblat, J. M. Clemente-Juan, E. Coronado,
J. Phys. Chem. **2016**, 120, 16994–17005.

pubs.acs.org/doi/abs/10.1021/acs.jpcc.6b02587

Mixed-Valence Molecular Unit for Quantum Cellular Automata: Beyond the Born-Oppenheimer Paradigm through the Symmetry Assisted Vibronic Approach.

J.M. Clemente-Juan, A. Palii, E. Coronado, B. Tsukerblat,
J. Chem. Theory and Computations, **2016**, 12, 3545–3560.

pubs.acs.org/doi/abs/10.1021/acs.jctc.6b00267

Modelling electric field control of the spin state in the mixed-valence polyoxometalate $[\text{GeV}_{14}\text{O}_{40}]^{8-}$
Cardona-Serra, S.; Clemente-Juan, J. M.; Gaita-Arino, A.; **Suaud, N.**; Svoboda, O.; **Coronado, E.**
Chem. Commun., **2013**, 49, 9621-9623.
pubs.rsc.org/en/Content/ArticleLanding/2013/CC/c3cc44859b

Molecular spin qubits based on lanthanide ions encapsulated in cubic polyoxopalladates: design criteria to enhance quantum coherence;
Baldoví, J. J.; Rosaleny, L. E.; Ramachandran, V.; Christian, J.; Dalal, N. S.; **Clemente-Juan, J. M.**; Yang, P.; **Kortz, U.**; **Gaita-Ariño, A.**;
Coronado, E.;
Inorg. Chem. Front. **2015**, 2, 893-897.
pubs.rsc.org/en/Content/ArticleLanding/2015/QI/C5QI00142K

Ln_{12} -Containing 60-Tungstogermanates: Synthesis, Structure, Luminescence, and Magnetic Studies;
Wang, K.-Y.; Bassil, B. S.; Lin, Z.; Römer, I.; Vanhaecht, S.; **Parac-Vogt, T. N.**; de Pipaón, C. S.; **Galán-Mascarós, J. R.**; Fan, L.; Cao, J.;
Kortz, U.
Chem. Eur. J. **2015**, 21, 18168-18176.
onlinelibrary.wiley.com/doi/10.1002/chem.201502457/abstract

Effect of Electron (De)localization and Pairing in the Electrochemistry of Polyoxometalates: Study of Wells-Dawson Molybdotungstophosphate Derivatives,
L. Parent, P. A. Aparicio, **P. de Oliveira**, A.-L. Teillout, **J. M. Poblet**, **X. Lopez**, **I. M. Mbomekalle**.
Inorg. Chem. **2014**, 53, 5941-5949.
pubs.acs.org/doi/abs/10.1021/ic500087t

Supramolecular Recognition Influences Magnetism in $[\text{X}@\text{HV}^{\text{V}}_8\text{VV}_{14}\text{O}_{54}]^{6-}$ Self-Assemblies with Symmetry-Breaking Guest Anions.
K. Y. Monakhov, O. Linnenberg, P. Kozłowski, J. van Leusen, C. Besson, T. Secker, A. Ellern, **X. López**, **J. M. Poblet**, and **P. Kögerler**.
Chem. Eur. J. **2015**, 21, 2387 – 2397
onlinelibrary.wiley.com/doi/10.1002/chem.201403858/abstract

Accuracy of Embedded Fragment Calculation for Evaluating Electron Interactions in Mixed Valence Magnetic Systems: Study of 2e-Reduced Lindqvist Polyoxometalates

N. Suaud, X. López, N. Ben Amor, N. A. G. Bandeira, C. de Graaf, and J. M. Poblet

J. Chem. Theory Comput., **2015**, *11*, 550–559

pubs.acs.org/doi/abs/10.1021/ct5010005

Single ion magnets based on lanthanoid polyoxomolybdate complexes

J. Baldovi, Y. Duan, C. J. Bustos, S. Cardona-Serra, P. Gouzerh, R. Villanneau, G. Gontard, J.-M. Clemente-Juan, A. Gaita-Arino, C. Giménez-Saiz, A. Proust and E. Coronado.

Dalton Trans., **2016**, *45*, 16653-16660.

pubs.rsc.org/en/Content/ArticleLanding/2016/DT/C6DT02258H

WG4 Biological Applications and Emergent Systems

Crystallization and preliminary X-ray crystallographic analysis of latent isoform PPO4 mushroom (Agaricus bisporus) tyrosinase

Mauracher, S. G.; Molitor, C.; Al-Oweini, R.; Kortz, U.; Rompel, A.

Acta Crystallogr. Sect. F: Struct. Biol. Commun. **2014**, *70*, 263-266

<http://scripts.iucr.org/cgi-bin/paper?S2053230X14000582>

Latent and active abPPO4 mushroom tyrosinases cocrystallized with hexatungstotellurate(VI) in a single crystal.

Mauracher, S. G.; Molitor, C.; Al-Oweini, R.; Kortz, U.; Rompel, A.;

Acta Cryst. **2014**, *D70*, 2301-2315.

<http://scripts.iucr.org/cgi-bin/paper?S1399004714013777>

Hen Egg White Lysozyme Crystallisation: Protein Stacking and Structure Stability Enhanced by a Tellurium(VI)-Centered Polyoxotungstate.

Bijelic, A.; Molitor, C.; Mauracher, S. G.; Al-Oweini, R.; Kortz, U.; Rompel, A.;

ChemBioChem. **2015**, *16*, 233-241

onlinelibrary.wiley.com/doi/10.1002/cbic.201402597/abstract

Hydrolysis of Tetraglycine by a Zr(IV)-Substituted Wells-Dawson Polyoxotungstate Studied by Diffusion Ordered NMR Spectroscopy

K. Stroobants, G. Absillis, P. S. Shestakova, R. Willem, T. N. Parac-Vogt

J. Clust. Sci. **2014**, *25*, 855-866

link.springer.com/article/10.1007%2Fs10876-013-0664-2

Integrating ³¹P DOSY NMR Spectroscopy and Molecular Mechanics as a Powerful Tool for Unraveling the Chemical Structures of Polyoxomolybdate Based Amphiphilic Nano-Hybrids in Aqueous Solutions

P. S. Shestakova, G. Absillis, F. J. Martin-Martinez, F. De Proft, R. Willem, T. N. Parac-Vogt

Chem. Eur. J. **2014**, *20*, 5258-5270.

onlinelibrary.wiley.com/doi/10.1002/chem.201304969/abstract

Hydrolysis of the RNA model substrate catalyzed by a binuclear ZrIV-substituted Keggin polyoxometalate.

T. K.N. Luong, G. Absillis, P. Shestakova, T. N. Parac-Vogt.

Dalton Trans., **2015**, 44, 15690-15696.

pubs.rsc.org/en/Content/ArticleLanding/2015/DT/C5DT02077H

Multinuclear Diffusion NMR Spectroscopy and DFT Modeling: A Powerful Combination for Unraveling the Mechanism of Phosphoester Bond Hydrolysis Catalyzed by Metal-Substituted Polyoxometalates.

T. K. N. Luong, P. Shestakova, T. T. Mihaylov, G. Absillis, K. Pierloot and T. N. Parac-Vogt,

Chem. Eur. J. **2015**, 21, 4428-4439.

onlinelibrary.wiley.com/wol1/doi/10.1002/chem.201405810/abstract

Solution Speciation of the Dinuclear Zr(IV)-Substituted Polyoxometalate [$\{\alpha\text{-PW11O39Zr}(\mu\text{-OH})(\text{H}_2\text{O})\}_2\}^{8-}$] and its Reactivity towards DNA-Model Phosphodiester Hydrolysis

T. K. N. Luong, T.K.N., G. Absillis, P. Shestakova, T. N. Parac-Vogt

Eur. J. Inorg. Chem. **2014**, 5276-5284.

onlinelibrary.wiley.com/wol1/doi/10.1002/ejic.201402735/abstract

Probing Polyoxometalate-Protein Interactions Using Molecular Dynamics Simulations

Albert Solé-Daura, V. Goovaerts, K. Stroobants, G. Absillis, P. Jiménez-Lozano, J. M Poblet, J. D Hirst, T. N. Parac-Vogt, J. J Carbó

Chem. Eur. J. **2016**, 22, 15280-15289

onlinelibrary.wiley.com/doi/10.1002/chem.201602263/abstract

Gallium(III)-Containing, Sandwich-type Heteropolytungstates: Synthesis, Solution Characterization and Hydrolytic Studies Towards Phosphoester and Phosphoanhydride Bond Cleavage

Kandasamy, B.; Vanhaecht, S.; Nkala, F. M.; Beelen, T.; Bassil, B. S.; Parac-Vogt, T. N.; Kortz, U.

Inorg. Chem. **2016**, 55, 9204-9211

<http://pubs.acs.org/doi/abs/10.1021/acs.inorgchem.6b01030>

Polyoxometalate $\{W_{18}O_{56}XO_6\}$ Clusters with Embedded Redox-Active Main-Group Templates as Localized Inner-Cluster Radicals
Vilà-Nadal, L.; Peuntinger, K.; Busche, C.; Yan, J.; Lüders, D.; Long, D.L.; **Poblet, J.M.**; Guldi, D.M.; **Cronin, L.**,
Angew. Chem. Int. Ed., **2013**, *52*, 9695-9699.
onlinelibrary.wiley.com/wol1/doi/10.1002/anie.201303126/abstract

Hydrophobic effect as driving force for host-guest chemistry of a multireceptor Keplerate-type capsule.
N. Watfa, **D. Melgar**, M. Haouas, F. Taulelle, A. Hijazi, D. Naoufal, J. Bonet Avalos, **S. Floquet**, **C. Bo**, **E. Cadot**.
J. Am. Chem. Soc. **2015**, *137*, 5845–5851
pubs.acs.org/doi/abs/10.1021/jacs.5b01526

Encapsulated Water Inside Mo_{132} Capsules: The Role of Long-Range Correlations of about 1 nm
M. Garcia-Rates, P. Miro, **A. Müller**, **C. Bo**, and J. Bonet Avalos
J. Phys. Chem., **2014**, *118*, 5545-5555.
<http://pubs.acs.org/doi/abs/10.1021/jp411240u>

An unstable paramagnetic isopolyoxomolybdate intermediate non-homogeneously reduced at different sites and trapped in a host based on chemical adaptability
Merca, A.; Garai, S.; Bögge, H.; Haupt, E.T.K.; Ghosh, A.; **López, X.**; **Poblet, J.M.**; Averseng, F.; Che, M.; **Müller, A.**,
Angew. Chem. Int. Ed., **2013**, *52*, 11765-11769.
onlinelibrary.wiley.com/wol1/doi/10.1002/anie.201305402/abstract

Anisotropy of the molecular magnet V_{15} spin Hamiltonian detected by high-field electron spin resonance
M. Martens, J. van Tol, N. S. Dalal, S. Bertaina, B. Barbara, **B. Tsukerblat**, **A. Müller**, S. Garai, S. Miyashita, I. Chiorescu
Phys. Rev. B, **2014**, *89*, 195439
<http://journals.aps.org/prb/abstract/10.1103/PhysRevB.89.195439>

Stepwise-Resolved Thermodynamics of Hydrophobic Self-Assembly

A. Grego, A. Müller, I. A. Weinstock

Angew. Chem. Int. Ed., **2013**, 52, 8358-8362

<http://onlinelibrary.wiley.com/wol1/doi/10.1002/anie.201303083/abstract>

Tracking "Apolar" NMe₄⁺ Ions within Two Polyoxothiomolybdates Having the Same Building Blocks: Smaller Clathrate and Larger Highly Porous-Type Cluster in Action.

V. S. Korenev, A. G. Boulay, M. Haouas, F. Bannani, V. P. Fedin, M. N. Sokolov, E. Terazzi, S. Garai, A. Müller, F. Taulelle, J. Marrot, N. Leclerc, S. Floquet, and E. Cadot,

Chem. Eur. J., **2014**, 20, 3097 – 3105.

onlinelibrary.wiley.com/wol1/doi/10.1002/chem.201303719/abstract

Biomolecules Electrochemical Sensing Properties of a PMo₁₁V@N-Doped Few Layer Graphene Nanocomposite.

D. M. Fernandes, M. Nunes, R. J. Carvalho, R. Bacsa, I.-M. Mbomekalle, P. Serp, P. de Oliveira, C. Freire.

Inorganics **2015**, 3, 178-193.

<http://www.mdpi.com/2304-6740/3/2/178>

Tin(II)-functionalization of the archetypal {P₈W₄₈} polyoxotungstate.

N. V. Izarova, L. Kläß, P. de Oliveira, I.-M. Mbomekalle, V. Peters, F. Haarmann, P. Kögerler.

Dalton Trans. **2015**, 44, 19200-19206

pubs.rsc.org/en/Content/ArticleLanding/2015/DT/C5DT03164H

Cation-Directed Dimeric vs. Tetrameric Assemblies of Lanthanide-Stabilized Dilacunary Keggin Tungstogermanates.

Artetxe, B.; Reinoso, S.; San Felices, L.; Lezama, L.; Gutiérrez-Zorrilla, J. M.; García, J. A.; Galán-Mascarós, J. R.; Haider, A.; Kortz, U.; Vicent, C.

Chem. Eur. J. **2014**, 20, 12144-12156

onlinelibrary.wiley.com/wol1/doi/10.1002/chem.201403028/abstract

Cyclic Tungstoselenites Based on {Se₂W₁₂} Unit.

Kalinina, I. V.; Peresyphkina, E. V.; **Izarova, N. V.**; Nkala, F. M.; **Kortz, U.**; Kompankov, N. B.; Moroz, N. K.; **Sokolov, M. N.**;
Inorg. Chem. **2014**, *53*, 2076-2082
pubs.acs.org/doi/abs/10.1021/ic402668v

Synthesis, Structure and Antibacterial Activity of a Thallium(III)-Containing Polyoxometalate, [Tl₂{B-β-SiW₈O₃₀(OH)}₂]¹²⁻

Ayass, W. W.; Fodor, T.; Lin, Z.; Smith R. M.; Xing, X.; Abdallah, K.; Tóth, I.; Zékány, L.; **Pascual-Borràs, M.**; Rodríguez-Forteza, A.;
Poblet, J. M.; Fan, L.; Cao, J.; Keita, B.; Ullrich M. S.; **Kortz, U.**
Inorg. Chem. **2016**, *55*, 10118–10121
<http://pubs.acs.org/doi/abs/10.1021/acs.inorgchem.6b01921>

Investigating the Transformations of Polyoxoanions Using Mass Spectrometry and Molecular Dynamics

J. M. Cameron, L. Vilà-Nadal; R. S. Winter; F. Iijima; J. C. Murillo, A. Rodríguez-Forteza; H. Oshio, **J. M. Poblet, L. Cronin**
J. Am. Chem. Soc., **2016**, *138*, 8765- 8773.
pubs.acs.org/doi/abs/10.1021/jacs.6b02245

Instantaneous formation of polyoxometalate-based cerium vanadium oxide gels

A. Seliverstov, M. Rangus, M. Hartmann, **S. G. Mitchell, C. Streb**
Inorg. Chem. Frontiers, **2017**, *4*, 160-164.
<http://pubs.rsc.org/en/Content/ArticleLanding/2016/QI/C6QI00457A#divAbstract>

Removal of Multiple Contaminants from Water by Polyoxometalate-Supported Ionic Liquid Phases (POM-SILPs)

S. Herrmann, L. De Matteis, Jesus M. de la Fuente, **S. G. Mitchell, C. Streb**
Angew. Chem. Int. Ed. **2017**, *56*, 1667-1670.
onlinelibrary.wiley.com/doi/10.1002/anie.201611072/abstract

Cr^{III}-substituted Heteropoly-16-Tungstates [Cr^{III}₂(B-β- X^{IV}W₈O₃₁)₂]¹⁴⁻ (X = Si, Ge): Magnetic, Biological, and Electrochemical Studies
Liu, W.; Al-Oweini, R.; Meadows, K.; Bassil, B. S.; Lin, Z.; Christian, J. H.; Dalal, N. S.; Bossoh, A. M.; Mbomekallé, I. M.; de Oliveira, P.; Iqbal, J.; Kortz, U.

Inorg. Chem. **2016**, *55*, 10936–10946.

pubs.acs.org/doi/abs/10.1021/acs.inorgchem.6b01458

Discrete Silver(I)-Palladium(II)-Oxo Nanoclusters, {Ag₄Pd₁₃} and {Ag₅Pd₁₅}, and the Role of Metal–Metal Bonding Induced by Cation Confinement

Yang, P.; Xiang, Y.; Lin, Z.; Lang, Z.; Jiménez-Lozano, P.; Carbó, J. J.; Poblet, J. M.; Fan, L.; Hu, C.; Kortz, U.

Angew. Chem. Int. Ed. **2016**, *55*, 15766–15770.

onlinelibrary.wiley.com/doi/10.1002/anie.201608122/full