

A century of Chemistry at Tsinghua and the rise of polyoxometalate and related cluster research

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As the Department of Chemistry at Tsinghua University celebrates its centennial anniversary in 2026, it is my distinct honor and privilege to introduce this special issue of *Polyoxometalates* dedicated to this remarkable milestone. One hundred years of chemical scholarship at Tsinghua represents not merely a chronological marker but a testament to the enduring pursuit of scientific excellence through profound societal transformations, global realignments, and paradigm shifts in chemical research. This special issue offers an opportunity to reflect on the intertwined histories of Tsinghua Chemistry and the field this journal serves, while showcasing the vibrant contributions of our community to polyoxometalates (POMs) and related clusters science.

Polyoxometalates Journal was established in 2022 as the first international interdisciplinary journal dedicated specifically to POMs and related clusters science. Sponsored by Tsinghua University and published by Tsinghua University Press, the journal emerged from a recognition that the rapidly expanding field of POM and related cluster chemistry—with its reach extending into catalysis, materials science, energy research, biology and medicine—required a dedicated platform for disseminating breakthrough discoveries and fostering scholarly exchange.

That this journal finds its home at Tsinghua is no coincidence. The Department of Chemistry has long nurtured excellence in inorganic chemistry, and POMs and related clusters science research has flourished here through decades of persistent investigation. Under the visionary leadership of pioneers who recognized the unique structural beauty and functional versatility of metal and metal-oxo clusters, Tsinghua has become one of the most recognized hubs for POMs and related clusters science research in China and increasingly on the global stage. The establishment of *Polyoxometalates* Journal represented a natural maturation of this research ecosystem—a commitment to serving not only our institutional community but the worldwide network of scholars who share our fascination with these kinds of remarkable molecules.


Since its launch, the *Polyoxometalates* Journal has experienced remarkable growth. We have been honored by our inclusion in major international databases including DOAJ, Scopus, CAS, Ei Compendex, and most recently the Emerging Sources Citation Index (ESCI), which ensures that all articles published since our inception will be recognized in the Web of Science Core Collection. With a CiteScore of 14.7 in 2024 and a real-time CiteScore reaching

17.4, the journal has quickly established itself as a significant voice in the fields of inorganic chemistry and interdisciplinary materials research. These metrics, while gratifying, reflect something more profound: the vibrant health of our field and the urgent need for continued communication and collaboration among POM and related cluster researchers worldwide.

Tsinghua Chemistry at one hundred: A century of transformation

The centennial of Tsinghua Chemistry invites reflection on how far Chinese chemical research has traveled. Founded in 1926, the department navigated the tumultuous decades of civil strife, war, and national reconstruction before emerging as a powerhouse of research and education in the reform era. This trajectory mirrors, in many ways, the evolution of POM and related cluster chemistry itself—from a specialized niche concerned primarily with structural characterization to a dynamic, application-oriented discipline addressing grand challenges in energy, sustainability, and human health.

Tsinghua's contributions to POM and related cluster research reflect broader strengths in synthetic inorganic chemistry, materials science, and interdisciplinary collaboration. Our faculty and students have pioneered new synthetic methodologies, elucidated complex self-assembly processes, and developed novel materials based on POMs and related clusters with applications ranging from molecular electronics to biomedicine. Recent work from Tsinghua laboratories exemplifies the field's expanding horizons: Chirality has been successfully induced in centrosymmetric Ag–Cu clusters through co-crystallization with chiral organic guests, which facilitates the development of circularly polarized luminescence (CPL) materials, with the resulting clusters exhibiting strong chiroptical activity and promising applications in 3D displays and encryption; a Ag⁰-doped Ag₁₄Cu₆ alloy nanocluster has been developed that demonstrates excellent photothermal conversion efficiency ($\eta \approx 31.2\%$), and in the second near-infrared (NIR-II) bio-window, these clusters enable high-spatial-resolution photoacoustic imaging and effective photothermal ablation of tumors *in vivo*, showcasing their potential as advanced theranostic agents; gold nanoclusters have been employed in visible-light-driven aerobic oxidation catalysis, in which the atomically precise structures allow for clear elucidation of structure–activity relationships, achieving high selectivity and conversion in organic transformations; the construction of atomically precise single-walled cluster nanotubes from giant Preyssler-type POMs, demonstrating exceptional catalytic activity for electrocatalytic transformations; the development of molecular-scale Schottky diodes based on POM

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monolayers achieving rectification ratios exceeding 3000; and the exploration of POM-based hybrids for antiviral applications, combining inorganic cluster chemistry with bioactive organic components.

These achievements represent not isolated discoveries but nodes in a growing network of POM and related cluster research that spans synthetic chemistry, theoretical modeling, advanced characterization, and application development. They also exemplify the collaborative spirit that has long characterized Tsinghua Chemistry—a willingness to bridge disciplinary boundaries and engage with colleagues across traditional divides.

The expanding universe of polyoxometalate science

As we celebrate this institutional milestone, it is worth considering the remarkable trajectory of POM chemistry as a field. Coincidentally, since Berzelius' discovery of the ammonium phosphomolybdate in 1826, this year also marks the second centenary of POM research. From the early crystallographic studies that revealed the elegant structures of Lindqvist, Keggin and Anderson cluster anions, POM research has expanded to encompass an extraordinary range of scientific questions and technological possibilities.

In synthesis and assembly, researchers have moved from simple salts to complex hierarchical structures. The ability to construct POM-based architectures with atomic precision—whether through coordination-driven self-assembly, covalent functionalization, or supramolecular organization—has opened new frontiers in materials design. Organophosphonate/organoarsenate-modified POMs, for example, combine the redox versatility of inorganic clusters with the tunable functionality of organic components, enabling applications that neither class of materials could achieve alone. The controlled assembly of POMs into nanowires, nanosheets, and nanotubes demonstrates the growing mastery over matter at the nanometer scale.

In catalysis, POMs continue to surprise and inspire. Their ability to undergo reversible multi-electron transfers without structural degradation makes them ideal candidates for redox catalysis, whether in solution, immobilized on supports, or integrated into electrochemical systems. The demonstration that POM-based nanotubes can achieve high selectivity and Faradaic efficiency for phenol hydrogenation—attributed to electron delocalization across the cluster array—illustrates how structural control at the molecular level can translate into enhanced function.

In energy research, POMs are finding roles in diverse contexts: as proton conductors in fuel cells, as components of batteries and supercapacitors, and as catalysts for water splitting and CO₂ reduction. The development of POM-based hybrid polymers for anhydrous proton conduction exemplifies the creative materials design that characterizes this field. As global energy demands intensify and the imperative for sustainable technologies grows, the unique properties of POMs—their stability, tunability, and redox activity—position them as valuable contributors to solutions.

In biology and medicine, POM research has entered an exciting phase. Long recognized for their antiviral and antibacterial activities, POMs are now being investigated for more sophisticated biomedical applications: enzyme inhibition, modulation of metabolic pathways, and intervention in protein misfolding diseases. Recent studies on POM regulation of mitochondrial

biosynthesis suggest potential applications in metabolic disorders including diabetes. The development of organic-POM hybrids with reduced cytotoxicity while retaining antiviral efficacy demonstrates the promise of rational design in biomedical applications. These investigations, while still at early stages, hint at future contributions to human health that would have seemed fanciful to earlier generations of POM chemists.

In molecular electronics, POMs offer distinctive advantages: their well-defined structures, multiple redox states, and ability to form ordered monolayers on surfaces. The demonstration of molecular-scale Schottky diodes based on POM self-assembled monolayers represents a significant advance, showing that phenomena typically associated with mesoscale materials can be realized at the molecular level through careful interface engineering. Such work bridges the gap between molecular chemistry and device physics, suggesting pathways toward functional molecular electronics.

This Special Issue: A snapshot of a vibrant field

The articles collected in this special issue reflect the breadth and depth of contemporary POM and related cluster research, with contributions from investigators intimately associated with the Department of Chemistry, Tsinghua University including faculty members, visiting scholars, post-doctors and graduated PhD students, and their collaborators across in the mainland of China. Readers will find reports spanning synthetic methodology, structural characterization, theoretical investigation, and application development—a testament to the multidimensional nature of these old yet youthful fields.

In this issue, POMs as an ultimate building block of sub-nanomaterials are highlighted in three excellent review papers on the following topics: cluster-nuclei co-assembled ultrathin materials (Peilei He), polyoxometalates-based one-dimensional subnanomaterials (Simin Zhang et al.), and the controllable preparation of polyoxometalate-based sub-1 nm materials and their applications in energy storage and conversion (Junli Liu et al.). Another two comprehensive reviews will shed light on the application of POMs in the hydrogen energy via water splitting with topics of recent advances and future research directions in polyoxometalates-based water electrolysis for hydrogen production (Jiangwei Zhang et al.) and polyoxometalate electrocatalysts on nickel foam for enhanced alkaline oxygen evolution reaction (Lubin Ni et al.), respectively. Thank for the importance of hydrogen energy, two research papers (Yichao Huang et al. and Pingfan Wu et al.) are focused on the hydrogen evolution with POMs as the precursor of promising electrocatalysts. Moreover, a polyoxometalate@copper based electrocatalyst will report by Dejin Zang et al. for the coupling of halo-(hetero)aromatic hydrocarbons and carbon dioxide to synthesize (hetero)aromatic acids.

Additionally, two papers discuss the POM-related clusters are collected in this issue too. One review by Dr. Zhen Lei and Prof. Quan-Ming Wang summarize well in detail the progress in the oxygen donor protection of atomically precise metal nanoclusters, and one research article presents Shang-Fu Yuan et al.'s newly discovery on dispersant collaborative metal chalcogenide semiconductor cluster photocatalysis in direct and green synthesis of dithioesters.

What unites these diverse contributions is a commitment to excellence and a recognition that fundamental understanding must precede technological translation. Whether exploring the intricacies

of cluster assembly, probing electronic structure through computation and spectroscopy, or demonstrating new functions in catalysis, the work presented here advances our collective understanding of these remarkable cluster molecules. However, due to space limitations, many excellent works have not been collected in this special issue and as will be seen, have to be published in subsequent issues.

Looking forward: The next century

As we commemorate one hundred years of chemistry at Tsinghua, it is natural to contemplate the century ahead. What will POM and related cluster chemistry look like in 2126? While prediction is hazardous, certain trajectories seem clear.

The integration of POMs and related clusters with other materials classes will deepen. Hybrid systems combining POMs and related clusters with polymers, metal-organic frameworks, carbon materials, and biological macromolecules will yield properties and functions inaccessible to any single component. The principles governing such integration—interfacial design, electronic coupling, cooperative phenomena—will become increasingly sophisticated.

Computational methods will play an expanding role. As algorithms improve and computing power grows, the ability to predict POM and related cluster's structure, stability, and reactivity from first principles will transform how ones design experiments and interpret results. The combination of high-throughput computation with targeted experimental validation promises to accelerate discovery dramatically.

Applications will multiply and mature. POMs and related clusters will find roles in commercial catalysts, energy storage devices, biomedical diagnostics and therapeutics, and environmental technologies. The path from laboratory discovery to practical application is rarely straight or short, but the fundamental

advantages of POMs and related clusters—their stability, tunability, and functional density—will ensure their place in the technological landscape.

Perhaps most importantly, the community of POM and related clusters researchers will continue to grow and diversify. The next generation of scientists, trained in interdisciplinary approaches and equipped with increasingly powerful tools, will ask questions we cannot yet formulate and develop applications we cannot yet imagine. Their creativity, dedication, and collaborative spirit will be the ultimate drivers of progress.

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As the guest editor, I am continually inspired by the quality and creativity of the work submitted to our pages. This special issue, marking a significant milestone in the history of Tsinghua Chemistry, offers particular cause for celebration—not merely of past achievements but of the vibrant present and promising future of POM science. May the next century of chemistry at Tsinghua bring discoveries as remarkable as those that have preceded it, and may *Polyoxometalates* Journal continue to serve as a worthy platform for sharing them.



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