Polyoxometalate-based Molecular Nanoscience

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The book deals with the molecular region of Nanoscience showing for the first time the unique possibilities offered by polyoxometalate (POM) chemistry to construct a common area of interest for supramolecular chemistry, molecular electronics, molecular magnetism and spintronics.

Molecular Nanoscience is still a region that has been scarcely explored in Nanoscience, maybe because the larger structural and electronic complexity of molecules, compared with that found in simpler atom-based nano-objects and nanostructures, make them more difficult to study at the nanoscale with available instrumental techniques. Albeit, it is in this molecular region where molecular chemists, biologists, physicists and engineers working in Nanosciences may find the best opportunities to interact and to converge.

Metal oxides are ubiquitous in modern technologies ranging from large-scale industrial catalysis to microelectronics, but the emerging area of Molecular Nanoscience, *i.e.* the study of advanced functional materials and nanometric systems based on *molecular* components, has involved mainly organic molecules and/or metal complexes. A key goal in the development of this are is therefore the incorporation of metal oxide components. In this regard, **polyoxometalates (POMs)** are archetypal *molecular metal oxides* and their uniquely diverse structural, electronic, magnetic and chemical properties provide a versatile platform for inorganic Molecular Nanoscience that has hardly been exploited. The uniquely versatile properties of POMs provide the basis for advances in catalysis, alternative energy sources, magnetic, electronic and photonic devices and medicine.

Encompassing some of the most exciting challenges facing modern chemists and materials scientists, POM-based Molecular Nanoscience is a truly interdisciplinary field in which areas such as supramolecular chemistry, molecular electronics and molecular magnetism converge. This field will allow the design, synthesis and full characterization of metal oxide components with specific properties prior to their incorporation into functional nanosystems, providing a wider diversity of materials and higher chemical precision than nanoscience that relies purely upon the manipulation of particle size, morphology and dimensionality of elements or simple compounds. For example, (i) the inorganic nature of POMs (lack of carbon-based components) makes them ideal candidates for catalysts under harsh conditions such as water oxidation, (ii) their unique electronic structures can be exploited for molecular electronics and spintronics with functionalities that potentially reach beyond the paradigms of von-Neumann architectures and binary logics, and (iii) self-assembly into molecule- based analogues of solid-state oxides produces complex architectures that can host numerous additional functional components and provide ‘soft’ routes to active oxide systems.

In this book we will illustrate the different aspects covered by Molecular Nanoscience in the context of POM chemistry. That incudes:

1) The design of functional molecules using POM chemistry;

2) The control of the self-assembling processes to prepare nanostructures of these chemical nano- objects on surfaces, and to prepare new materials based on these molecules;

3) The study of the properties exhibited by these nanomaterials/nanostructures, including the study of properties at the unimolecular level;

4) The development of applications (in catalysis and energy, molecular electronics, molecular nanomagnetism, spintronics and quantum computing, and in biology).

Proposed Content

1. **Introduction: What is molecular nanoscience? Why POMs?**
2. **Designing molecules: POM chemistry and reactivity**
3. **Assembling molecules: POM-based nanostructures, POM on surfaces and interfaces (organization/immobilization), POM-based materials**
4. **Observing, interrogating and manipulating molecules & assemblies at the nanoscale: Physical characterization (techniques) and theoretical modelling**
5. **POMs for catalysis and energy: water splitting, carbon dioxide reduction, multifunctional nanoscale catalytic assemblies**
6. **Molecular electronics: electronic devices based on POMs**
7. **Molecular Nanomagnetism, Spintronics and quantum computing**
8. **Biological applications**