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Spotlights on Recent *JACS* Publications

SIMPLIFYING IRON WITH RUTHENIUM

Heme proteins are involved in important biological processes, including oxygen transport in blood and catalysis of oxidation reactions. These proteins' heme groups consist of an iron atom bound in the center of a nitrogen-containing ring structure called a porphyrin. The iron also binds to sulfur atoms in the protein, and characterizing these interactions will contribute to a clearer understanding of heme protein function. However, reactions performed by heme proteins can be accompanied by complex changes in the chemical and electronic nature of the iron in the heme group, complicating the investigation of the iron−sulfur interactions in the proteins.

Now, Brian James and co-workers report the synthesis and characterization of 32 novel porphyrin complexes containing ruthenium instead of iron as models for exploring iron−sulfur interactions (DOI: 10.1021/ja211226e). Like iron, ruthenium binds to sulfur, but ruthenium does not experience the same complex chemical changes that iron undergoes. Structural analysis methods such as X-ray crystallography and nuclear magnetic resonance spectroscopy are used to characterize the interactions between various sulfur-containing molecules and ruthenium porphyrins.

This study illustrates the value of using ruthenium in place of iron to create heme mimics. Ruthenium porphyrins are easier to study than iron porphyrins and can provide valuable insight into the unique nature of the heme group and heme protein function as well as inform the design of small molecules that block heme protein activity. **Eva J. Gordon, Ph.D.**

CALCULATIONS EXPLAIN MEMRISTIVE SWITCHING IN NICKEL OXIDE

Electronic devices are constantly being improved upon, and new materials with properties on smaller length scales are necessary for these improvements. Memristors are materials that hold a memory of the last current or voltage seen by the material and can be used as switches in nanoelectronic devices. Devices made from memristors, much smaller in size than conventional transistors, can potentially replace such transistors or be used to create nonvolatile memory.

Nickel oxide (NiO) is one material that shows memristive behavior. Researchers Yanagida, Kawai, and co-workers have used density functional theory to explore the effect of nickel and oxygen vacancies, both alone and in conjunction with each other, on the electrical transport properties of NiO (DOI: 10.1021/ja2114344). The authors show that the coexistence of anion and cation defects affects the carrier concentration of holes. By inference, these calculations provide an explanation for observed cathode side switching properties for NiO.

This article provides a model for understanding the basis of memristive switching in p-type oxides, which can be used to guide NiO material synthesis and optimize device design. **Polly Berseth, Ph.D.**

GOING ORGANIC AND RADICAL FOR CONDUCTORS

Organic conductors with magnetic properties could be useful for electronics and spintronics, which utilize the magnetic moment from electron spin in addition to the transport of electric charge. Spintronics is an emerging field, but it has already led to major technological advancements. In the late 1990s, IBM used spintronics to increase the storage capacity of hard disks from 1 to 20 gigabits. While inorganic materials dominate in electronics and spintronics, there is a growing interest in using organic materials. Chemists can employ an arsenal of synthetic methods to create organic conductors for a variety of devices.

Richard Oakley and co-workers synthesized a neutral radical and characterized its properties as an organic conductor (DOI: 10.1021/ja209841z). Their neutral radical forms an adduct with acetonitrile which crystallizes in closely spaced π-stacks with strong overlap between the stacks. The packing pattern, coupled with favorable electrochemical properties of the radical, make the material a promising new molecular conductor. The unsolvated radical also adopts a π-stacked architecture, and is not only conductive but also orders magnetically.

The researchers have made major strides in the concept of neutral radical conductors, which may have valuable applications in electronics and spintronics. While the conductivity and magnetic properties of their compound are not comparable to metals, further improvements may be possible by chemical or physical modification. **Yun Xie, Ph.D.**

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