

## Spotlights on Recent JACS Publications

### ■ FOR QUANTUM DOT SOLAR CELLS, SIZE MAKES ALL THE DIFFERENCE

Solar energy is all about efficiency. To challenge fossil fuels, solar cells must convert more sunshine into electricity, at lower cost, than they can do today. Tiny particles of lead and sulfur called PbS quantum dots (QDs) show potential as solar cell components because, among other attributes, they are simple to produce and absorb sunlight well. But to optimize efficiency, researchers need to better understand how PbS QDs interact with sunlight to produce electrons.

Omar Mohammed and colleagues add a piece to the puzzle with a careful investigation into how light affects electrons at the space between PbS QDs and another material commonly used in solar cells (DOI: 10.1021/ja413254g). The researchers find that the dots' size distribution is critical. Their size determines not only what wavelength of light the QDs will absorb but also how quickly that light produces work-ready electrons at the interface.

With careful size control, researchers can tune PbS QDs to inject charge carriers into the surrounding material ultrafast, not at all, and every speed in between. Such information is essential to the design of solar-based devices if researchers hope to increase efficiency with quantum dots.

Jenny Morber, Ph.D.

### ■ MIXING UP THE METALS IN METALLO- $\beta$ -LACTAMASE

David L. Tierney and co-workers report a method for investigating the role of the metal ions in metallo- $\beta$ -lactamases, enzymes that hydrolyze  $\beta$ -lactam antibiotics such as penicillins and cephalosporins (DOI: 10.1021/ja410376s). Understanding the mechanism of metallo- $\beta$ -lactamases could contribute to the development of new strategies for combating antibiotic resistance, a global health threat.

The authors employ heterodimetallic analogues with a selectively placed paramagnetic cobalt (Co(II)) ion in one site or the other to study the metallo- $\beta$ -lactamase NDM-1. The presence of Co(II) enables the use of numerous spectroscopic techniques to probe the coordination environment of each of the two zinc binding sites. In addition, the investigators employ kinetic studies to determine the rate-limiting step of the hydrolysis reaction and explore how the acidity of the metal ion in the second zinc binding site affects the rate of formation of the product. Finally, they determine that the metal ions have functional roles throughout the hydrolysis reaction.

This study represents the first selective incorporation of Co(II) into the two metal binding sites of a metallo- $\beta$ -lactamase and highlights the utility of such heterodimetallic analogues to probe the structure and activity of these important enzymes.

Eva J. Gordon, Ph.D.

### ■ USING NEUTRONS TO EXPLORE THE DYNAMICS OF MYELIN

Myelin basic protein (MBP) is a major component of the myelin sheath in the central nervous system. Myelin has

tremendous medical importance, and many neurological disorders are related to MBP misfolding and malfunction. In aqueous solution, MBP is primarily unstructured and is classified as an intrinsically disordered protein (IDP). An IDP is flexible and can interact with various binding partners, so it functions adaptively in many essential biological processes. Andreas Stadler and colleagues present a study on the nature and extent of large conformational motions in MBP as a model for the role of these movements in IDP (DOI: 10.1021/ja502343b).

Using small-angle X-ray and neutron scattering experiments combined with coarse-grained structural ensemble modeling, the authors conclude that the structure of MBP is a central compact core with flexible ends. They find that the observed dynamics are governed by collective bending and stretching motion involving a large portion of the protein.

These large-scale conformational motions increase the accessibility of the protein surface and facilitate the interaction with binding partners. The results shed light on the biological mechanisms of intrinsically disordered proteins and demonstrate the utility of neutron scattering methodology in biomolecule dynamics experiments.

Hui Jin, Ph.D.

### ■ JOINED FORCES: UNDERSTANDING BIMETALLIC CATALYST NANOALLOYS

Alloying metals such as palladium and platinum with other transition metal elements is a common route to preparing low-cost, highly active, and stable catalysts. Palladium-based catalysts specifically have become a focus of research for use in a variety of important applications, including petrochemical processing, fuel cell reactions, and automotive exhaust treatments.

By combining experimental high-energy X-ray diffraction with theoretical reverse Monte Carlo simulations, Chuan-Jian Zhong and co-workers probe the critical structural factors of palladium–nickel nanoalloys in the model carbon monoxide oxidation reaction (DOI: 10.1021/ja5026744). They find a maximal catalytic activity at a palladium-to-nickel ratio of approximately 50:50. The researchers also elucidate the bonding and geometry of the surface atoms at this optimum composition and further explain how this geometry affects the electronic structure of the catalyst to promote binding and activation of the reagents.

These studies enable a better and more rational design of nanoalloy catalysts for a wide range of catalytic reactions.

Dalia Yablon, Ph.D.

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