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Spotlights on Recent *JACS* Publications

NEW MASS SPECTROMETRIC METHOD PROVIDES DETAILS ABOUT PROTEIN ASSEMBLIES

Large assemblies of proteins, such as ATP synthase and the coats of viruses, are critical for many biological functions. Researchers seek to identify the individual proteins and ligands inside these complicated assemblies and to understand how the individual components come together to carry out their functions. Although several mass spectrometric techniques have been developed to analyze large protein complexes, a drawback is that they do not allow researchers to get primary sequence information on individual components or information about how the individual components are held together.

To address the drawback, Jennifer S. Brodbelt and colleagues have developed a new mass spectrometric method (DOI: 10.1021/ja505217w). The investigators combine mass spectrometry with an approach called ultraviolet photodissociation. The photodissociation process provides detailed sequence information on each component and indicates where ligands bind to the complexes as well as the locations of the various protein−protein interfaces.

The investigators have applied the method to a number of proteins of differing complexity, such as myoglobin/heme and a translation factor bound with its nucleotide. They find that, unlike other mass spectrometric methods, ultraviolet photodissociation mass spectrometry provides them with primary sequence information as well as tertiary and quaternary structural data about the protein assemblies.

Rajendrani Mukhopadhyay, Ph.D.

GUANOSINE AND BORATE MIX TO FORM A STABLE HYDROGEL

Jeffery T. Davis and colleagues report a self-assembling, transparent guanosine−borate hydrogel that has potential for a variety of biomedical applications (DOI: 10.1021/ja507506c).

Chemists have taken advantage of the nucleoside guanosine in their efforts to make supramolecular hydrogels for use in drug delivery, cell culture, and tissue engineering. But researchers want to improve the stability of these hydrogels in physiological contexts, and to incorporate drugs and dyes into the gels. Now Davis and colleagues have made a highly stable hydrogel by mixing guanosine and potassium borate. The hydrogel remains intact for at over a year at physiological concentrations of potassium ion.

The hydrogel assembles into $G_4{\cdot}K^+$ quartets. Borate ions enhance its self-assembly by reacting with guanosine, the team finds by examining the hydrogel with cryogenic transmission electron microscopy, circular dichroism, and solid-state NMR spectroscopy.

The researchers also successfully introduce a cationic dye, as well as other nucleosides, into the gel. The gel's stability and adaptability to these additions suggest that it could be developed for a variety of clinical and research applications.

Deirdre Lockwood, Ph.D.

VAN DER WAALS INTERACTIONS CRUCIAL IN HETEROGENEOUS METAL CATALYSIS

The manufacture of many chemicals and fuels depends on heterogeneous catalysis on a metal surface. Additionally, chemical production is often a process requiring a significant energy input. Therefore, an important step in the future of heterogeneous metal catalysis is the development of highly selective catalysts that can function at lower energies, ideally using sustainable resources.

In order to create a catalyst that has high selectivity for a particular reaction, researchers must be able to determine the relative concentrations of intermediates at the surface, which may depend on the relative binding strengths of the intermediates. A team led by Cynthia Friend and Robert Madix has found a way to better predict these binding strengths, using both experimental and computational methods to take into account the van der Waals interactions between the reactants and the surface (DOI: 10.1021/ja506447y).

The authors find that, although these associations are weak, they affect the relative stability of the intermediates and, therefore, have an important impact on the conditions required for peak selectivity. The methods used are highly relevant to many catalytic applications. They give insight into the significant role of weak interactions in more complex chemical processes, and may lead to more efficient manufacture of important chemicals in the future.

Leigh Krietsch Boerner, Ph.D.

TURNING RED BLOOD CELLS TO STONE

Despite incredible progress in scientists' chemical control of nanostructures, in many ways our abilities still lag biology. Nonsymmetric structures, for example, which abound in biological systems in the form of multitudes of cells, enzymes, and more, remain difficult for researchers to create in large quantities. Here, Bryan Kaehr and colleagues co-opt biological structures to create new inorganic tools (DOI: 10.1021/ja506718z).

They start with red blood cells, the familiar, bendy, disk-like cells—but red blood cells can form other shapes, too. The authors coax the cells into new geometries by exposing them to solutions of different chemicals. One composition changes the cells into spikey balls, while another composition transforms them into cups or bowls. The researchers then impregnate the cells with amorphous silica to create inorganic structures that replicate the cells' biological form.

The work shows that a researcher does not have to figure out how to mimic biological structures to create new nanomaterials; she can simply change their chemistry. This medusa-like ability to turn animal into mineral, coupled with knowledge of how to direct structural changes in biology, creates a powerful new set of tools that researchers can use to develop new nanostructures.

Jenny Morber, Ph.D.

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COMPACTED BY COILING WITH THE HELP OF CROSS-LINKERS

In biology, a macromolecule's three-dimensional structure plays a pivotal role in determining its function, such as enzymatic activity or ligand recognition. Inspired by this natural phenomenon, researchers have sought to design synthetic materials that assemble into higher-order structures to perform a unique function. Numerous recent studies shed light on the relationship between a molecule's primary constituents and the shape it ultimately takes on in solution, including reports that "pseudo-tertiary" structures, also known as distinct compacted subdomains, can be formed within "soft" nanoparticles composed of single-chain foldable precursors. But control over the compaction and compartmentalization processes is often hard to achieve.

A new study by Raj Kumar Roy and Jean-François Lutz provides clues about how the compartmentalization of polymer single chains occurs—information that researchers can use to gain more control over the process (DOI: 10.1021/ja507889x). The team reports the design of single-chain molecules containing two regions that coil themselves into distinct subdomains. They use a sequence-controlled polymerization strategy that incorporates intramolecular cross-linking agents at precise locations, which helps drive the compartmentalization process. The strategy is not limited to only model morphologies like those in this report, the authors say, and should open the way to tailor-made polymer microstructures.
Christine Herman, Ph.D.