JACS
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
Spotlights
pubs.acs.org/JACS

Spotlights on Recent *JACS* Publications

CYCLIC POLYMERS AND METAL IONS JOIN FORCES

A new study combines cyclic polymers with metal ions to form a new class of organic/inorganic hybrid materials with tunable properties. Researchers led by Gregory Tew create cyclic polymer brushes and gels from novel metallo-supramolecular cyclic polymers and demonstrate the first direct visualization of cyclic brush polymers by transmission electron microscopy (DOI: 10.1021/ja407381f).

The team presents the first demonstration of supramolecular structures made of cyclic polymers that self-assemble on the basis of reversible metal−ligand interactions that render the materials both stable and dynamic. Cyclic polymers, which can have drastically different properties compared to their linear counterparts, have long served as the starting point for materials with interesting molecular topologies. But the majority of efforts in the field have involved completely organic molecules joined together with covalent bonds, which can limit the functionality of the resulting materials.

The researchers synthesize the cyclic polymer building block, presenting metal-chelating side chains composed of terpyridine that grab hold of metal ions in solution and lead to the formation of tunable polymer brushes and gels. The results open up a new research avenue focused on these new amphiphilic architectures, which may lead to the creation of advanced hybrid materials with unique properties.

Christine Herman, Ph.D.

TURNING ON AND OFF: PREDICTING RIBOSWITCH KINETICS

The time scales of conformational changes of riboswitches, which turn on and off important biochemical processes in gene expression, are mapped using simulations in a recent study by Jong-Chin Lin and Dave Thirumalai (DOI: 10.1021/ja408595e). Riboswitches are specific RNA elements that respond to an external event such as metabolite binding through a change in structural conformation, thereby regulating protein translation.

Like enzymes, riboswitches display activity that is complex in terms of the ability of some to turn biochemical processes "on" while others turn them "off". Understanding the conformational changes that riboswitches undergo is a first step toward understanding their diverse functions.

By simulating the application of mechanical force to a bacterial riboswitch, the researchers map its folding and unfolding landscape to explore the time scales of its structural changes. They find that the folding kinetics of the riboswitch are faster than the time scale of mRNA degradation, indicating that the switch may turn on and off multiple times before a decision is made, indicating a "thermodynamic control" mode of regulation (as opposed to kinetic control). These findings contribute to our understanding of the function—and potential sources of dysfunction—of riboswitches in gene expression.

Dalia Yablon, Ph.D.

REVERSING THE DRAWBACKS OF REVERSE TRANSCRIPTASE INHIBITORS

Millions of people across the globe rely on combination antiviral therapy for HIV. Key components of certain combination therapies are non-nucleoside inhibitors of HIV reverse transcriptase, the enzyme that makes a DNA copy of the virus's RNA. Despite the effectiveness of these regimens, non-nucleoside inhibitors do leave room for improvement in areas such as activity against common HIV mutant strains, undesirable side effects, and pharmacokinetic properties. A particular structural feature of the non-nucleoside inhibitors, the cyanovinylphenyl group, may be responsible for their less than ideal behavior. William Jorgensen and co-workers set out to replace this group with a less offensive but equally potent alternative (DOI: 10.1021/ja408917n).

The researchers use computer simulations to identify potential replacements for the troublesome cyanovinylphenyl group. Three promising heterobicyclic structures—indoles, indolizines, and benzofurans—exhibit encouraging interactions in silico. Chemical synthesis of the analogues and testing against wild-type virus and mutant strains confirm their potent activity against HIV, and structural characterization by X-ray crystallography affords a clear view of their interactions with reverse transcriptase.

This study highlights the immense power of computer simulations in drug discovery, in this case for facilitating the identification of potential next-generation HIV drugs with improved activity and reduced side effects.

Eva J. Gordon, Ph.D.

SEMICONDUCTOR SOLVENT SHAKES UP THIN-FILM PROCESSING

Thin films are vital to the proper production and function of semiconductors. These films are built up, etched down, and patterned to make just about any small machine in use today—including transistors, optical components, sensors, and memory devices. Currently, thin films are created by floating tiny particles of the desired material through a vacuum and onto a waiting platform. These processes require expensive equipment and work best in small batches. To lower cost and scale up, researchers envision a kind of thin-film printer, but the "ink" has been a problem. The only known semiconductor solvents are explosive and carcinogenic, and some semiconductors have no known solvents.

Remarkably, Richard Brutchey and David Webber report that they have found a relatively nonhazardous solvent mixture that dissolves a range of semiconductor materials, including technologically important ones such as bismuth sulfide and bismuth telluride (DOI: 10.1021/ja4084336). The researchers demonstrate that the dissolved semiconductors create good quality crystalline thin films with low contamination from organic molecules.

Published: October 29, 2013

dx.doi.org/10.1021/ja411008g | *J. Am. Chem. Soc.* 2013, 135, 16243−16244

In their Communication, the researchers examine nine different semiconductors. Their chemical insights into the solvation mechanism may enable the development of solvent mixtures for other chalcogenide semiconductors in the future. **Jenny Morber, Ph.D.**

dx.doi.org/10.1021/ja411008g | *J. Am. Chem. Soc.* 2013, 135, 16243−16244