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JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
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Spotlights on Recent *JACS* Publications

MOLECULAR ORIGINS OF THE "MAGNETIC SENSE"

It is thought that birds navigate using signals from light-detecting proteins in their eyes that also sense a magnetic field. Such proteins, called cryptochromes, influence plant growth as well, but scientists are not exactly sure how light waves activate cryptochrome's magnetic sensing. Current theories say light waves create a pair of radicals, known to be sensitive to magnetic fields, inside the protein.

Now Ilia Solov'yov, Tatiana Domratcheva, Abdul Rehaman Moughal Shahi, and Klaus Schulten use computer models to follow a radical pair in a plant cryptochrome. Their calculations track radical formation, stabilization due to structural changes inside the protein, and recombination (DOI: 10.1021/ja3074819).

This first study to follow the molecular movement of a radical pair through a cryptochrome can provide deeper insights into the origin of the mysterious magnetic sense. For example, animal cryptochromes have a slightly different structure than the plant protein, which means radical pairs in animal cryptochromes should behave slightly differently than those in the plant protein. However, a related electron transfer in the animal protein could create the stabilizing structural change needed for magnetic sensing, the researchers write. **Melissae Fellet**

BOXY COMPOUND WRAPS UP POLLUTANTS IN NEAT PACKAGES

Polycyclic aromatic hydrocarbons (PAHs) are an important class of fused-ring natural compounds that are under fire for being toxic. Evidence suggests PAHs, which occur naturally in oil (including edible oils), coal, and tar, may cause cancer or mutations in humans. Now, researchers have synthesized a chemical that sequesters a wide range of PAHs and may help remove the toxins from the environment.

Over the years, scientists have studied several chemicals that bind to PAHs, but each has drawbacks. Some are expensive, while others can bind to only a limited subset of PAHs. Fraser Stoddart, Jonathan Barnes, and Michal Juríček have synthesized a positively charged molecule made up of eight cyclically linked phenylene and pyridinium rings they call ExBox using standard chemistry and inexpensive starting materials (DOI: 10.1021/ja307360n). The compound could host a wide range of molecules, from azulene, a simple two-ring structure, up to coronene, which contains seven fused rings. Unlike other PAH sequestering reagents such as cyclodextrin, ExBox works in either water or oil, depending on the choice of anion. When it binds a PAH, the solution changes from colorless to yellow, orange, red, or brown, which could enable detection of PAHs via a simple visual color change. **Erika Gebel, Ph.D.** *C&EN*

ACHIRAL MOLECULES SELF-ASSEMBLE INTO CHIRAL SUPRAMOLECULAR STRUCTURES

Chiral supramolecular systems, made of achiral molecules assembled into structures with a preferred "handedness", have potential applications in disciplines ranging from biology to materials and separation sciences. While the field of asymmetric synthesis of chiral molecules is well-advanced, that of asymmetric noncovalent synthesis of self-assembled structures is still in its early stages.

Researchers led by E. W. Meijer demonstrate that achiral oligo(*p*-phenylenevinylene) ureidotriazine (AOPV3) monomers self-assemble into one-dimensional helical stacks with the assistance of a chiral auxiliary, or a helper molecule, which can later be removed while leaving the structures intact (DOI: 10.1021/ja3086005). The team has synthesized the monomers and performed spectroscopic measurements and molecular modeling simulations to understand the noncovalent self-assembly process. They find that, even after a heating–cooling cycle, which causes the stacks to depolymerize and polymerize anew, the structures retain the preferred helicity as long as they were not completely dissociated in the heating process. This study represents a significant advance in a budding field, providing insight into the kinetic and self-assembly properties of achiral molecules that enable them to form supramolecular structures that retain their chirality under various conditions. **Christine Herman, Ph.D.**

TUNABLE METHOD YIELDS STABLE DNA–QUANTUM DOT CONJUGATES

When researchers want to arrange or capture nanoparticles on solid surfaces, they often rely on complementarity between an oligonucleotide-conjugated particle and a DNA scaffold. The technology is particularly mature using DNA-coupled gold nanoparticles, which have been assembled via base complementarity into one-, two-, and three-dimensional structures. DNA-conjugated quantum dots, though, have proven tougher nuts to crack, as the particles tend to precipitate, have low quantum yield, and degrade. Now Yan Liu and colleagues report a method for creating stable core/shell particles that circumvent those issues (DOI: 10.1021/ja3081023).

The method relies on incorporating the DNA oligonucleotides into the quantum dots' outer layers during core/shell assembly. The oligonucleotides contain a stretch of 5–10 phosphorothiolated bases on their 3′ ends, and as the shell (e.g., CdS or ZnS) precipitates in a controlled manner on the quantum dot surface (~10 min/monolayer), the oligonucleotide's sulfur atoms are incorporated as well, anchoring the oligos into the shell.

The resulting conjugates are stable over a range of pH and ionic conditions and remain dispersed in solution. Using atomic force microscopy, the authors demonstrate their precise arrangement on triangular and rectangular DNA scaffolds. The quantum dots are also tunable based on their chemical composition and shell thickness, and the authors were able to produce a range of particles emitting throughout the visible spectrum. **Jeffrey M. Perkel**

Published: November 13, 2012

dx.doi.org/10.1021/ja310914q | *J. Am. Chem. Soc.* 2012, 134, 18881–18882

CHANGING UP THE RING OPENING OF BENZOCYCLOBUTENOLS

The stability of carbon−carbon bonds means chemists struggle to cleave them without affecting other reactive groups in a molecule. A carbon−carbon bond of benzocyclobutenol, a hydroxyl-containing cyclobutene ring attached to benzene, can be opened using heat, light, or base. Under these conditions, the bond of the cyclobutenol ring that is not attached to the benzene ring splits open, and this cleavage creates two double bonds that can react with an alkyne to form a new six-membered ring.

Now Masahiro Murakami and co-workers use a rhodium catalyst to open the cyclobutenol ring at a different place: along one of the bonds that connects the cyclobutenol to the benzene ring (DOI: 10.1021/ja309013a). A subsequent alkyne addition occurs between the benzene ring and the ketone-containing remnants of the cyclobutene.

This new reaction complements the known reactions of cyclobutenols due to the alternate location of the ring opening, the researchers write. It can be applied to build a variety of molecules with a dihydronaphthalene core. **Melissae Fellet**