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Spotlights

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Spotlights on Recent *JACS* Publications

WATCHING GROWTH ON A WIRE

Crystalline organic nanowires (CONs) are promising materials for a variety of applications, such as photovoltaics, field effect transistors, and memory devices. A relatively new method to grow CONs, known as a vapor−solid chemical reaction, produces thick arrays of these nanowires on metal films. However, limited knowledge of these materials' growth mechanisms has hampered efforts to control and improve their production. Kai Xiao, Mina Yoon, and co-workers expand understanding of the growth process by directly watching a lawn of CONs grow on a metal film in organic vapor and then explaining the results through atomistic modeling (DOI: 10.1021/ja301456p).

The growth kinetics of the organic nanowires was probed using X-ray diffraction spectroscopy and scanning electron microscopy. The results, together with calculations and computer modeling, suggested that the metal ions from the film diffuse along the nanowire to its tip where they react with the organic vapor to continue growth, an energetically favorable process. The selectivity of a metal for the vapor reactant is quite distinct. For example, deposit of nickel film on top of copper film may block copper diffusion, preventing nanowires from growing. This understanding of the growth process could lead to more effective incorporation of CONs into device fabrication. **Christen Brownlee**

ROUND OF APPLAUSE FOR TWO-HANDED GOLD−THIOL MIXTURE

Researchers are becoming increasingly interested in using gold nanoparticles covered in thiolates in a variety of applications including sensing, electronic devices, optics, catalysis, and biomedicine. Properties that make these applications possible largely depend on the nanoparticles' physical structure, including their handedness, or chirality. In a new study, Thomas Bürgi and co-workers demonstrate the ease of converting a pure, one-handed gold−thiolate material into a two-handed mixture using relatively low temperatures, a transformation that could potentially change its properties (DOI: 10.1021/ja3053865).

This group worked with nanoparticles that were covered with staple-like structures composed of gold and thiolates that spread in a fan formation in either a left- or right-handed fashion. Starting with a pure mixture of either left- or right-handed gold−thiolate nanoparticles, the researchers dissolved the material in solution and then heated it over a range of temperatures from 40 to 80 °C. Circular dichroism spectroscopy, a tool that assesses chirality, showed that the pure solutions gradually converted to mixtures of left- and right-handed varieties. Because this reaction did not require a high energy input, the researchers speculate that the structural rearrangement occurs without complete gold−thiolate bond-breaking. The authors suggest that gaining a further understanding of this reaction could have implications for gold−thiolate nanoparticle applications. **Christen Brownlee**

BUILDING BLOCK APPROACH TO SYNTHESIZING REACTIVE MOLECULAR CONTAINERS

Since the human body is over two-thirds water, low water solubility of some pharmaceutical candidates can hamper their performance as therapeutic drugs. In an effort to assist in drug solubilization, chemists have looked to the cucurbit[*n*]uril, or CB[*n*], class of water-soluble molecular containers. These barrel-shaped compounds have hydrophobic cavities that enable them to efficiently encapsulate and solubilize otherwise poorly soluble compounds.

Molecules in the CB[*n*] family of compounds might be even more useful if they could be incorporated into solid phases or attached to macromolecules, but previously CB[*n*] molecules could only be functionalized with multiple hydroxyl groups. Now, Lyle Isaacs and colleagues have developed a building block approach to the synthesis of CB[7] compounds and have synthesized the first CB[7] derivatives that are amenable to further modification through single functional groups such as azide or alkyl chloride (DOI: 10.1021/ja3058502).

The CB[7] derivatives synthesized and characterized by the research team bear reactive functional groups that would allow covalent attachment to other molecules or materials. Marrying the outstanding molecular recognition properties of the CB[7] container with the desirable properties of the other molecules or materials might enhance applications in not only drug delivery but also biomimetic systems, supramolecular polymers, and molecular machines. **Christine Herman, Ph.D.**

DATABASE GUIDES DESIGN OF NEXT-GENERATION ANTIMICROBIALS

Peptides—natural chains of amino acids—can puncture the membranes of harmful bacteria such as *Staphylococcus aureus*. Drug-makers may build such chains into antibiotics like methicillin, but as bacteria develop resistance, drug-makers must race to improve their peptide armament.

Now Biswajit Mishra and Guangshun Wang are using a database maintained by Wang of over 2000 existing peptides to learn which of seven selected traits of the peptides correlate with bacteria-killing activity and to design custom peptides combining the best traits (DOI: 10.1021/ja305644e). They identified the level of hydrophobicity that works best against methicillin-resistant *Staphylococcus aureus* (MRSA), allowing the other parameters to vary freely, and then they repeated the process for six other characteristics, including electrostatic charge and hydrophobicity. From the results they created a synthetic peptide combining the most successful of each of those characteristics and tested it against MRSA.

The synthetic, designed peptide burst the MRSA cells. The researchers write that their method should be generalizable and allow scientists to optimize and synthesize more new peptides capable of killing drug-resistant microbes, too, and then iterate until the peptides are even more effective. They demonstrated

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the idea by making an improved version of their first database-derived peptide. **Lucas Laursen**

LIPID RAFTS INFLUENCE ENZYME AFFINITY

It is well known among biologists that cellular membranes are not homogeneous. Certain proteins and lipids tend to segregate themselves into "rafts", patches of relatively high local concentration on the vast cell surface. The functional consequence that such rafts have on soluble enzymes and other molecules that interact with the membrane has been unclear, however. Now Simon Webb and colleagues address this question for an artificial *N*-acetylated lipid and the glycosyltransferase that acts upon it (DOI: 10.1021/ja302506t).

Using a mixture of fluorescent glycolipid and unlabeled phospholipid, with or without cholesterol, the team tweaked the ability of the glycolipid to aggregate into domains, an event they visualized via fluorescence microscopy. Forming these raft-like structures enhanced the rate of enzymatic modification of the lipid 9-fold, corresponding to more than a 5-fold increase in apparent affinity of the enzyme for its substrate.

There are several possible reasons for this, the authors note, including "phase boundary" effects and enzymatic "hopping" from substrate to substrate. Ultimately, though, they implicate structural factors: clustered lipids create a multimeric substrate that better interacts with the enzyme's "extended oligosaccharide binding site" than dispersed substrate lipids. "Given lipid rafts in cell membranes have high glycolipid densities, they could act as focal points for the action of exogenous enzymes," the researchers conclude. **Jeffrey M. Perkel**

HETERODITOPIC RECEPTORS WITH PECULIAR COMPLEXATION PROPERTIES TOWARD ION-PAIRS

For several decades, chemists have been interested in designing synthetic receptors that recognize ions with high specificity, for applications including salt extraction, salt solubilization, and sensing. However, breaking apart an ion-pair often has a high energetic cost, leading researchers to seek out heteroditopic ion-pair receptors that contain recognition sites for both ions in an anion−cation pair.

In a recent study, Pablo Ballester, Enrico Dalcanale, and co-workers demonstrate that making small changes to the chemical structures of an ion-pair receptor can have dramatic effects on its binding abilities (DOI: 10.1021/ja305684m).

The research team designed and synthesized three diastereomeric receptors, which belong to a new class of heteroditopic ion-pair receptors known as bis-phosphonate aryl-extended calix[4]pyrroles. The researchers characterized the compounds, each of which had a different arrangement of the bridging phosphonate groups, and showed their different abilities to bind alkylammonium ion-pairs. They found that the spatial orientation of the phosphonate groups affected both the binding affinity and the location of the cation in the resulting ion-paired complexes. This study is the first to demonstrate the synthesis and explore the ion-pair binding abilities of this unique class of heteroditopic receptors. **Christine Herman, Ph.D.**