

# Spotlights on Recent JACS Publications

## ■ FUNCTIONAL COLLOID MATERIALS MADE FROM LIQUID CRYSTAL-BASED EMULSIONS

Researchers led by Nicholas L. Abbott report a new method for the preparation of both spherical and non-spherical particles with one or two distinct chemical domains located at the particles' poles (DOI: 10.1021/ja4022182).

The approach begins with the creation of a liquid crystal-inwater emulsion to form micro-sized droplets containing defects at the particles' poles. The particles are prepared in bulk solution, making the method potentially scalable. The defects allow the team to attach organic or inorganic colloids to the particles in a controlled manner, resulting in functional colloid materials whose properties can be tailored by varying the composition of the colloids.

The ability to control the shape and functionality of colloidal materials could open the way to new scientific and technological advances in fields ranging from biology to materials engineering. Since particle shape can influence a variety of processes, the synthesis of particles with anisotropic, or ellipsoid-like shape, and patterned surface chemistry may enable advances in the study of intracellular particle delivery, colloidal interactions at interfaces, and Brownian motion. **Christine Herman,** Ph.D.

#### ANTICANCER COMPOUNDS: FROM THE OCEAN TO THE CLINIC

Carmen Cuevas and colleagues present the isolation, structural elucidation, total synthesis, and biological evaluation of a novel and highly promising class of marine natural products (DOI: 10.1021/ja404578u). The polyketides, PM050489 and PM060184, inhibit cell division by interacting with tubulin, one of the most effective anticancer targets to date. Paclitaxel is arguably the most well-known and commercially successful mitosis inhibitor; intriguingly, these new compounds isolated from the Madagascan sponge *Lithoplocamia lithistoides* show a distinct biochemical mechanism of interaction with tubulin.

To elucidate the structures, the researchers use a range of NMR techniques, as well as a number of decades-old chemical methods, to pinpoint the stereochemistry at key chiral centers. The structures are confirmed as the researchers construct the molecules—which comprise an  $\alpha,\beta$ -unsaturated  $\delta$ -lactone, a conjugated triene system, and a small natural amino acid—in a convergent synthesis. The polyketides display cytotoxicity at sub-nanomolar concentrations in human tumor cells lines, and PM060184 has entered clinical studies as a promising new drug for cancer treatment.

"The supply issue is often one of the biggest barriers to the successful [pharmaceutical] development of marine natural products," the authors note. They have surmounted that obstacle through the highly convergent synthesis reported, which can yield product on multi-gram scale and be used for the synthesis of new and possibly even more effective analogues. Sonja Krane, Ph.D.

# CARBON FIXATION THROUGH A TEMPORARY TUNNEL

Jochen Blumberger and colleagues solve a biophysical mystery regarding an important microbial carbon fixation pathway using molecular dynamics and density functional theory (DOI: 10.1021/ja403110s). Biochemists have long been intrigued by an anaerobic carbon fixation pathway that bacteria and archaea use to transform carbon dioxide to acetyl CoA, a precursor for carbohydrate synthesis. In this reaction, CO<sub>2</sub> is first reduced to CO. It has been unclear how the ligands are coaxed toward the active site of the metalloenzyme complex that catalyzes the first steps of the reaction.

Now Blumberger and colleagues show that  $CO_2$  diffuses through a temporary, dynamic channel to reach the active site of the enzyme. Earlier X-ray crystal structures could not detect this channel because of its transience. Once  $CO_2$  is reduced to CO, formation of an Fe-hydroxy ligand strengthens the enzyme's hydrogen-bonding network and traps CO within the protein. The researchers solve a diffusion reaction model to predict rates of  $CO_2$  diffusion and binding.

By clarifying how this enzyme works, this research could aid efforts to harness it for industrial applications. These include mitigating greenhouse gas concentrations by reducing  $CO_2$  to CO, an industrial feedstock, and photoelectrochemical reduction of  $CO_2$ . **Deirdre Lockwood**, Ph.D.

### DESIGNING EFFECTIVE SODIUM ION BATTERIES

Right now, lithium-based batteries lead the rechargeable battery market. Lithium batteries are lightweight, hold charge well, and can endure many recharging cycles. Sodium is abundant, more widely available, and less toxic than lithium, so in some applications—grid-level energy storage, for example—sodium ion batteries could provide an attractive alternative. The obstacle has been that sodium ion diffusion is slower than lithium, and a sodium anode results in a relative voltage loss.

Previous research has focused on either optimizing current battery materials or translating lithium technology to a sodium ion battery analogue. As an alternative, Kenneth Poeppelmeier and his team propose new materials and principles for effective sodium ion battery design (DOI: 10.1021/ja404189t). The researchers investigate a crystalline compound composed of silver, sodium, vanadium, oxygen, and fluorine. Fluorine replaces some oxygen atoms to offset the "toll" in potential introduced by sodium. Silver, another polarizable cation, drives anion and cation ordering and produces layers in which ion exchange can activate redox-active silver and vanadium cations.

The work introduces a baseline compound for new sodium ion battery materials and proposes a set of design rules for emerging sodium ion energy storage, distinct from lithium technologies. Jenny Morber, Ph.D.

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