

Spotlights on Recent JACS Publications

■ SURPRISING ARRANGEMENT FOR COMMON LIQUID CRYSTAL

The particles in liquid crystals arrange themselves based on interparticle interactions, creating various structures somewhere between the total disorder found in a liquid and the rigid order of a packed three-dimensional crystal. Increasing the concentration of particles shifts the liquid crystal structure into different phases dictated by the location and orientation of the particles.

In water, flakes of aluminum hydroxide, or gibbsite, form two concentration-controlled liquid crystalline phases, nematic and columnar, due to the particle anisotropic shape and particle interactions governed by ions in the water. When Dzina Kleshchanok and co-workers changed the solvent in a gibbsite liquid crystal, they found a surprising particle arrangement: the ordered layers of a phase called smectic B (DOI: 10.1021/ja300527w). The polar, yet non-ionizable, solvent dimethyl sulfoxide (DMSO) stabilizes long-range charge repulsion between the positively charged hexagonal flakes, causing the particles to organize in this unexpected fashion. Until now, only rod-shaped particles and molecules were known to assemble into this phase, and computer models did not predict that flake-like particles could form this structure.

Now scientists can shift between the structures of known liquid crystal phases, and even introduce new phases, by fine-tuning the particle interactions. Creating a particular structure on demand is important for controlling the shape of the growing polymer by templates from the liquid crystals. **Melissae Fellet, Ph.D.**

■ TUNING PROTEIN RESPONSE TO COLORED LIGHT

Rhodopsins are transmembrane proteins that use light energy to perform several vital functions. There are a variety of rhodopsins known, and they absorb light at UV- and visible wavelengths. The absorption properties of the protein can change with the introduction of an ion or mutations, and there is great interest in discovering how the response to light is affected by protein structure. Ideally, researchers would like to modify proteins to create a particular spectral response for application purposes.

Morokuma and co-workers use *ab initio* calculations to show that adding or removing a chloride ion from halorhodopsin causes a reordering of the hydrogen bond network of the protein (DOI: 10.1021/ja3009117). This in turn changes the position and orientation of polar and charged residues within the protein. The model shows how the electrostatic interactions of the halide ion in addition to the combination of shifts in the hydrogen bond network and polar and charged residues affect the spectral properties of the protein.

The authors found that charged residues up to 10 Å away from the chromophore (where light is absorbed) affect the absorption energy. Understanding the structure–response relationship is important as microbial rhodopsins are being investigated for optogenetic applications, which utilize light to control biological processes. The ultimate goal is to use

rhodopsins with a tuned spectral response *in vivo* to achieve a real-time response to light stimulus. **Polly Berseth, Ph.D.**

■ A NANO SANDWICH THAT MAKES ITSELF

Nanoscale fibrils consisting of stacked amphipathic peptides—which combine fat- and water-loving amino acids—are emerging as a versatile biomaterial. For example, they can form media for growing cells or scaffolds that facilitate biological signaling. These peptide structures are inspired by the β sheets found in the amyloid protein plaques behind Alzheimer's and other diseases.

Generally, researchers make peptide β sheet fibrils from only a single type of peptide. Bradley Nilsson and colleagues have now discovered that mirror-image peptides spontaneously create β sheet fibrils with alternating D- and L-peptides (DOI: 10.1021/ja301642c).

When the researchers mixed together amphipathic D- and L-peptides, they expected separate D- and L-fibrils to form. But to their surprise, images of the resulting fibrils looked different from those that assembled when D- and L-peptides were kept in separate test tubes. They confirmed that a hybrid structure had indeed formed using a clever isotope-edited infrared spectroscopy experiment. After labeling the peptides with heavy carbon atoms at specific locations, the researchers observed perturbations in the IR spectrum indicating that the D- and L-peptides were sandwiched together. This discovery opens the door to developing new, more complex self-assembling multifunctional biomaterials. **Erika Gebel, Ph.D.**

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