

Spotlights on Recent JACS Publications

■ DYNAMIC PERTURBATION OF HYDRATION WATER AROUND GFP

The water molecules surrounding proteins in solution are collectively referred to as “hydration water”, and they play an important role in protein function and stability. Many unanswered questions remain as to how exactly macromolecules in solution perturb the water molecules in which they are immersed. Now, Jonathan Nickels, Stefania Perticaroli, and colleagues shed light on this matter in an experimental study aimed at understanding the nature of the hydration water in a solution of the widely studied biomolecule, green fluorescent protein (GFP) (DOI: [10.1021/jacs.6b08845](https://doi.org/10.1021/jacs.6b08845)).

The researchers set out to determine a number of key differences between the characteristics of bulk water and hydration water. The team acquires spatiotemporal information about atomic motion on the scale of angstroms to nanometers using neutron scattering methods, finding that water molecules surrounding the proteins are perturbed up to a distance of two full shells of water (~ 5.5 Å) from the protein surface, and that the affected water molecules’ movements are slowed by a factor of 2–10, depending on both their distance from the surface and the length scale of the measurement technique. The findings deepen our understanding of water perturbation, which is of practical interest to researchers in food science, personal care, pharmaceuticals, and protein dynamics.

Christine Herman, Ph.D.

■ POKING HOLES IN MEMBRANES WITH PH-TRIGGERED PEPTIDES

Membranes are the guard walls that protect the insides of cells from unwanted guests that could cause harm. Large molecules, such as proteins, have a particularly difficult time breaching the membrane divide. Scientists would like to develop ways to poke holes in cell membranes, allowing, for example, macromolecular medications to enter the cytosol to either heal a cell or, in the case of cancer, eliminate it. The key to such an approach is to avoid universal cellular permeabilization and to target certain cells selectively.

William C. Wimley, Kalina Hristova, and colleagues focus on using pH to induce selectively a peptide to form macromolecule-sized pores in membranes (DOI: [10.1021/jacs.6b11447](https://doi.org/10.1021/jacs.6b11447)). The researchers screen a peptide library looking for candidates that form membrane pores at low pH, but not at physiological pH. Through multiple iterations, they hit on potent pore formers at pH 5–6 that are essentially inert at pH 7.

These pH-sensitive peptides could help deliver molecular cargo via endosomes, which have an acidic interior. Endosomes carry macromolecules captured via endocytosis through the cell. Typically, these molecules are disposed of, but pore formation would allow them to escape into the cytosol. Similarly, the microenvironment around cancer cells is acidic, offering an opportunity to poke holes in malignant cells to usher in chemotherapeutics.

Erika Gebel Berg, Ph.D.

■ “THAR SHE GLOWS!” LUMINESCENT COMPLEX FROM AN EARTH-ABUNDANT ELEMENT

Complexes based on precious metals, including ruthenium(II), iridium(III), osmium(II), and rhenium(I), have found a host of useful applications due to their long-lived, redox-active excited states when modified with suitable ligands. For example, these materials have previously been investigated as luminophores in light-emitting devices, as dyes in solar and photoelectrochemical cells, as sensitizers for photoredox reactions in organic chemistry, or as photosensitizers for the production of solar fuels. However, the scarcity of these precious metals and their corresponding high cost has spurred a quest to replace them with more Earth-abundant elements. Laura Büldt, Oliver Wenger, and co-workers report a new chromium(0)-based complex that generates robust luminescence at room temperature (DOI: [10.1021/jacs.6b11803](https://doi.org/10.1021/jacs.6b11803)).

The new complex consists of a chromium(0) center surrounded with chelating diisocyanide ligands that shield the metal atom from the chemical environment. Tests show that this complex has an excited-state lifetime of 2.2 ns in de-aerated THF at 20 °C, nearly 2 orders of magnitude longer than that of the best-performing isoelectronic iron(II) complexes currently being pursued as sensitizers in dye-sensitized solar cells. The authors suggest that this new complex is promising for the replacement of precious metals in dye-sensitized solar cells and in luminescent devices.

Christen Brownlee

Published: January 25, 2017