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Spotlights

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UNRAVELING THE SECRETS OF FIBRIL ASSOCIATIONS

At first glance, a ball of yarn consists of one long, never-ending piece of string. You might think the string is a continuous fiber, but you will notice it is a collection of smaller fibers assembled as you look closer. The act of smaller fibers assembling into larger ones is vital to many life processes, such as collagen fibers associating with soft tissues. These natural processes are referred to as fibril associations.

While fibril associations are known to exist, we have only begun to study and understand the factors that control their predictable self-assembly. Through both experimental and theoretical experiments, Guosong Chen and co-workers have made great strides in understanding them (DOI: 10.1021/jacs.1c01951). Looking at a family of glycoproteins composed of oligosaccharides and oligopeptides, they determined which components could regulate the growth and chirality of the fibrils. Some fibril associations were even shown to stick to tumor cells, paving the way for some exciting medical advances in the future. As we continue to understand the entire landscape of fibril associations, we will be able to design both unique materials based on them and materials that take advantage of naturally occurring fibril associations.

Rebecca Yardley Ph.D.

THROWING NON-NATURAL ENZYME REACTIVITY FOR A LOOP

Enzymes—proteins that catalyze chemical reactions in nature—have captured many researchers' attention as a highly selective, environmentally friendly way to do chemistry in the lab. Frances Arnold's "directed evolution" approach (which garnered her a share of the 2018 Nobel Prize in Chemistry) can be used to develop enzymes that facilitate reactions not seen in nature. For example, Arnold's team developed a modified cytochrome *c* which catalyzes Si−C bond formation. Now, Ken Houk and Marc Garcia-Borràs have teamed up with Arnold and co-workers to thoroughly investigate the reaction mechanism and the factors behind the modified enzyme's selectivity (DOI: 10.1021/jacs.1c02146).

The researchers used a combination of computations, kinetics experiments, and further mutations to explore the silylation mechanism and factors influencing the reaction rate. Using molecular dynamics simulations to model the protein conformation, the team uncovered how a specific loop in the enzyme makes the reaction selective for silylation over amination by affecting substrate binding. As a proof of concept, the researchers designed an enzyme variant with a loop conformation that favors amination. The study illuminates how mechanistic and conformation information can be used strategically to influence enzyme reactivity. More broadly, this knowledge could help design better non-natural enzymes for synthetic chemistry.

Brianna Barbu

ORGANOMETALLIC FILMS CHOOSE WHAT THEY LET THROUGH

Solar cells often have a thin protective film between the light-responsive layer and the conductive cathode. This film can interfere with the flow of electrons, limiting the electrical power the cell can produce. Finding protective film materials that also preserve power conversion efficiency (PCE) has proven challenging. Haiping Xia, Hsing-Lin Wang, and co-workers now report a versatile series of organometallic compounds that protect cathodes from air, moisture, and corrosive halogens that diffuse out of the light-sensitive layer, while allowing electrons to pass through efficiently (DOI: 10.1021/jacs.1c02118).

These organometallic compounds feature carbon chain structures that boost charge transport by forming electrical dipoles at the interface with the metal electrode surface. Devices with protected silver or gold cathodes achieved an impressive 21% or 20% PCE, respectively. In just over 10 days of exposure to air at 50% humidity, the difference in PCE between protected and unprotected cathodes became apparent. The difference was even more pronounced for cathodes stored for almost 6 months under nitrogen: protected silver cathodes lost less than 5% PCE, and gold cathodes were essentially unchanged.

These protective layers could provide a cost-efficient way to produce efficient solar cells, not only for power-generating plants but also for light-emitting devices and thin-film transistors.

Nancy McGuire Ph.D.

POINT-OF-CARE ANTIBIOTIC RESISTANCE DETECTION

Carbapenems are a type of antibiotic reserved by medical practitioners for treating infections that resist other antibiotics.

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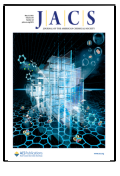

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But their long-term effectiveness depends on not creating more resistant microbes. Treating an infection with an antibiotic to which the microbe is already resistant not only fails to help the patient—it can spread resistant strains in the microbe population. Doctors want to know ahead of time how the strain of an infection they are treating will respond to their dwindling arsenal of antibiotics. Yet the approved activity-based diagnostic today for carbapenem resistance has sensitivity rates as low as 11% for an emerging resistant enzyme.

Now Dan Yang and co-workers report their development of a new, pan-carpabenemase reporter, CARBA-H (DOI: 10.1021/jacs.1c00462). The team found a common feature across several carbapenems that allowed them to design their reporter to detect a wider range of resistant bacteria than before. They tested their method via rapid test assays and got clear results in 15 min, about an eighth the time of the only approved phenotypic test. Application in bacteria-spiked urine that mimics UTI patient samples was also successful. This could enable clinics to offer point-of-care diagnostics with less culturing time or the need for a hospital setting.

Lucas Laursen

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