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Spotlights

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Spotlights on Recent *JACS* Publications

MULTILOOP PROTEIN SURFACES MIMIC ANTIBODIES

Researchers in fields ranging from biosensing to therapeutic design are always looking for better binding agents that recognize protein targets with high affinity and specificity. Antibodies have these properties and so have traditionally been sought out for such applications. Now, chemists are seeking to develop new classes of molecules that exhibit comparable or improved protein recognition properties.

Inspired by antibodies, which contain multiple peptide loops that afford complementarity toward their targets, researchers have sought to generate multiloop protein surfaces with specific functional domains. For the first time, Partha Ghosh and Andrew Hamilton report a noncovalent synthetic approach to the generation of multiloop protein surfaces by self-assembly of peptides onto a template (DOI: 10.1021/ja305360q).

The team mixed two different oligoguanosine-tagged peptides in the presence of metal ions. The peptides self-assembled via G-quadruplex formation onto the scaffold to produce both homo- and heterosequences. The team studied the kinetics of the self-assembly process and characterized the resulting multiloop protein surfaces. The authors envision this method will enable researchers to develop combinatorial libraries of multiloop structures by multicomponent self-assembly, which would be screened and fine-tuned to identify structures that can detect protein targets with high affinity and specificity. **Christine Herman, Ph.D.**

FACTORING PHYSICAL PROPERTIES INTO PHASE TRANSFER CATALYSIS

Phase transfer catalysts facilitate reactions between components in immiscible liquids. This kind of catalysis is useful in a “green chemistry” process because it helps reactions proceed in the presence of water, thereby reducing the need for organic solvents. Now, Scott Denmark and co-workers have quantified the effect of various physical properties on the kinetics of a phase transfer catalyzed phenol alkylation (DOI: 10.1021/ja304808u).

The researchers studied a series of six increasingly hydrophobic quaternary ammonium salts and compared the activities of the catalysts with the stoichiometric reactivities of the ammonium phenoxides. They evaluated the effect of the radius of the tetraalkylammonium cation and the lipophilicity of the catalysts on their activities. The catalytic activity was most affected by the hydrophobicity of the catalysts, with less dependence on the radius of the ammonium cation. Thus, the intrinsic reactivity of the ammonium phenoxide does not significantly contribute to the rate of the catalytic reaction.

Denmark and colleagues suggest that a complete understanding of the physical *and* chemical characteristics of a quaternary ammonium salt is not required to select a maximally active phase transfer catalyst. Rather, a simple model, based on ClogP, is sufficient to explain the catalytic activities accurately. The analysis simplifies the catalyst selection process, which is commonly done by trial-and-error. **Sonja Krane, Ph.D.**

MORE PHOTOCURRENT BY TWEAKING POLYMERS IN SOLAR CELLS

Organic solar cells are a promising source of energy because they are more flexible, more lightweight, and likely cheaper to manufacture than their inorganic counterparts. Although the creation of photocurrents is governed by similar physics, the conversion of photons into exitons and the breaking up of these exitons into charge carriers at the interface between the donor and an acceptor—a required step for solar cells to produce energy—operate at lower efficiency in organic solar cells than in silicon-based cells. As a result, the power conversion rate is currently about 3 times lower with organic solar cells.

Now, researchers led by René Janssen have designed and synthesized organic materials that are less affected by the problems that limit the photocurrents they can generate (DOI: 10.1021/ja305358z). These conjugated diketopyrrolopyrrole (DPP) donor polymers have small band gaps, allowing the absorption of photons in the near-infrared region of the solar spectrum. Extended, electron-rich π-conjugated segments attached to the DPP monomers provide the exitons with a surplus of free energy, increasing their dissociation rate and creation of charge carriers.

The group investigated eight DPP polymers and measured improved current densities, up to 16 mA/cm^2, corresponding to a power conversion rate of nearly 6%. These solar cells might someday become as ubiquitous as paint, producing energy on any imaginable surface exposed to the sun. **Alexander Hellemans**

SPINNING OUT INDIUM TIN OXIDES FOR FLEXIBLE SURFACES

Indium tin oxide (ITO) is commonly used as a material for transparent electrodes, for example in flat panel displays and organic light-emitting diodes, because it has good electrical conductivity and allows visible light to easily pass through. Generally, ITO films are deposited onto a surface by sputtering—spraying the material via vapor deposition onto the desired surface. However, in the past this dispersion method has only worked well on rigid surfaces. Sputtered ITO is not amenable to flexible substrates, which are preferred for bendable displays and devices, because ITO is brittle and can easily crack over repeated bending cycles, leading to a decrease in device performance. Conversely, using other deposition methods leads to ITO films with high resistivity that are not transparent, rendering them unusable for electronic devices that detect and control light.

Now Shouheng Sun and co-workers have successfully deposited ITO nanocrystals on a glass surface using a technique called spin-casting, resulting in a surface coating with excellent electrical conductivity and 93% transparency, the highest so far for this type of material (DOI: 10.1021/ja3044807). This result can be attributed to the high stability and homogeneous nature of the nanocrystals in solution, essential for making evenly

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dispersed and closely packed ITO layers on the glass support. Moreover, spin-casting can be used to deposit ITO nanocrystals onto polymer films, bringing technologies such as flexible displays closer to reality. **Leigh Krietsch Boerner, Ph.D.**

TRACKING A SINGLE-MOLECULE REACTION AT THE SOLID/SOLUTION INTERFACE OVER A RANGE OF TEMPERATURES

A number of critical processes, such as self-assembly, film growth, and catalysis, rely on temperature-dependent surface reactions at the solid/solution interface. Being able to study these processes at the single-molecule level is important for technological advances, and scanning tunneling microscopy (STM) is one way to analyze surfaces on molecular and atomic length scales.

In the first study of its kind, Ursula Mazur, Kerry W. Hipps, and colleagues monitor an interface reaction over a temperature range from 10 to 40 °C (DOI: 10.1021/ja304431b). Using STM, they study the reversible binding of oxygen to a cobalt porphyrin called CoOEP, which has the potential to be a gas sensor. The CoOEP molecule is positioned on a support known as highly oriented pyrolytic graphite (HOPG).

The free energy, enthalpy, and entropy changes associated with the oxygen binding process are determined for the first time. Interestingly, CoOEP, which is not expected to bind oxygen in the solution phase, forms a stable CoOEP–O_2 complex at the solid/solution interface. It is inferred from the thermodynamic data that HOPG, by donating electrons to the cobalt ion of CoOEP, increases the affinity of the compound for oxygen. The approach opens up a way to better understand the thermodynamic properties of a reaction system at the solid/solution interface at a molecular level. **Rajendrani Mukhopadhyay, Ph.D.**

DNA MAKES THE MECHANICAL AND ELECTRICAL SWITCH

Jason Thomas, Hua-Zhong Yu, and Dipankar Sen are bringing DNA far from its roots as a genetic blueprint, showing in a new study that DNA helices in a three-way junction can act as both a nanomachine and an electrical switch (DOI: 10.1021/ja303530y).

DNA has potential as a nanomachine, since it readily changes conformation with chemical stimuli. However, a useful mechanical switch needs reversibility, which no study on DNA switches fueled by simple chemicals had thus far demonstrated. Previous research had also suggested that DNA could act as an electrical switch, since it can conduct electricity depending on its conformation. Yet, the connection between mechanical and electrical switching had not been demonstrated unequivocally.

In the new study, the researchers fashioned a three-way junction in which one arm contained a base-paring mismatch, forming a bulge that pushed the other two arms together at an angle. By binding to added mercury cations, residues in the bulging arm paired, pulling the other two arms into a linear conformation, a phenomenon that can be reversed by chelating mercury ions. A series of tests linked this mechanical switching with electrical switching, demonstrating an increase in charge transport when the angular arms became linear. The authors suggest that this convenient switch offers a way to monitor a nanodevice's mechanical work through electronic measurement. **Christen Brownlee**