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Spotlights on Recent *JACS* Publications

NEW POLYMER DERIVATIVE TRANSPORTS ELECTRONS FASTER THAN EVER

The development of *n*-type polymers for applications in organic electronics has long been hampered by the polymers' inability to transport electrons efficiently under ambient conditions. Now, researchers led by Jian Pei present a compound that sets a new record for polymer electron transport under ambient conditions, with an electron mobility 4 orders of magnitude higher than those of other molecules of its kind (DOI: 10.1021/ja403624a).

The team designed the conjugated polymer, a benzodifurandione-based derivative of the widely studied poly(*p*-phenylene vinylene) (PPV) class of polymers. The new PPV derivative overcomes common PPV defects known to cause low electron mobility, including conformational disorder, weak inter-chain interactions, and a LUMO level too high to achieve stable electron transport. The researchers show that it has numerous desirable qualities, including increased stability under UV and visible light and a strong tendency to aggregate.

A field-effect transistor device based on the polymer is stable under ambient conditions for at least 30 days. The team is hopeful that the new electron-deficient polymer and its derivatives may pave the way for the development of electronic devices based on polymers, such as field-effect transistors and organic photovoltaics. **Christine Herman, Ph.D.**

ENGINEERING A NERVE AGENT-DESTROYING ENZYME

Name an interesting chemical, and there's probably an enzyme that can degrade it. Organophosphates—acetylcholinesterase inhibitors that have been used as both pesticides and chemical weapons—can be inactivated by organophosphate hydrolases, or phosphotriesterases. How, though, do such enzymes evolve? Frank Raushel and colleagues show just how readily such a reaction can happen by evolving a novel hydrolase from a structurally related lactonase (DOI: 10.1021/ja405911h).

Starting from a phosphotriesterase-like lactonase (PLL), which also has weak activity toward organophosphates, Raushel's team uses repeated rounds of mutagenesis and screening to obtain variants able to degrade a range of organophosphates up to 5 orders of magnitude more efficiently than the starting PLL (while still retaining weak lactonase activity, as well). The most active variant differs from the starting PLL by just seven amino acids, and using crystallography and molecular docking studies, the authors demonstrate how those changes alter protein function.

The results, the authors say, suggest that in nature, phosphotriesterases could have evolved from PLLs. In the lab, however, "the concerted efforts of directed evolution, structural biology, and computational docking enabled the design of a tailored and highly efficient enzyme," they conclude. **Jeffrey M. Perkel**

CLEARING UP A LONGTIME MYSTERY IN LOW-TEMPERATURE OXIDATION

William H. Green and colleagues determine new reaction pathways involved in the low-temperature oxidation of hydrocarbons using electronic structure calculations (DOI: 10.102/ja4034439). In doing so, they theoretically confirm a 30-year-old hypothesis about the kinetics of these reactions.

Understanding how hydrocarbons oxidize at low temperatures is important in fields as diverse as engine and materials design, biochemistry, and atmospheric science. But kinetic studies of these oxidation reactions are limited. Some of the greatest insights date 30 years to the work of Stefan Korcek and colleagues, who hypothesized that γ-ketohydroperoxides (KHP) are intermediates in the decomposition of long chain hydrocarbons to shorter carboxylic acids.

Now Green and co-workers have proven Korcek right. They show that KHP rearranges to a cyclic peroxide isomer, which then decomposes through two pathways to yield carboxylic acids and carbonyl compounds. The study clarifies a new class of reactions that have relevance for the atmospheric formation of secondary aerosols. It could also explain acid formation that has been observed in partial oxidation and engine combustion experiments. **Deirdre Lockwood, Ph.D.**

LIGHTING UP THE GOLGI OF CANCER CELLS

A new fluorescent probe offers a way to distinguish cancer cells from healthy cells by lighting up a key cellular structure called the Golgi apparatus (DOI: 10.1021/ja4056905). The new probe could be a tool for early cancer diagnosis or for guiding tumor surgery.

Jiangli Fan, Xiaojun Peng, and co-workers have designed a fluorescent probe that can get inside the Golgi apparatus, an organelle that modifies, transports, and secretes proteins once they come off the cell's protein synthesis machinery. Cancer cells often overproduce certain proteins such as cyclooxygenase-2 (COX-2), and the proteins accumulate in the Golgi. The team's probe can detect this buildup of COX-2.

To make their probe, the researchers connected an inhibitor of COX-2 to a fluorescent dye via a flexible hydrocarbon linker. In the absence of COX-2, the molecule folds up so that the inhibitor sits on top of the dye and quenches its fluorescence. However, when the inhibitor binds to COX-2, the probe unfolds and the dye can fluoresce, glowing green when hit with 800-nm light.

In addition to potential diagnostic applications, the probe—after some modification and improvement to make it ready for clinical applications—might be used to guide tumor resection during surgery, the authors say. Doctors could spray the probe on cancerous tissue and look for the glow to know where to cut. **Laura Cassiday,** *C&EN*

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