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Spotlights on Recent *JACS* Publications

TESTING MOLECULES FOR NANOELECTRONIC CIRCUITS

Molecular electronics is a developing application in nanotechnology that uses single molecules as electronic components. Hopes are high that individual molecules, or combinations of them, will perform functions such as switches, rectifiers, and even transistors in future nanoelectronic circuits. The geometric and electronic structural dynamics of a single-molecule junction is highly related to its function in molecular electronics, but these dynamics can be difficult to study due to sensitivity limits.

Manabu Kiguchi, Kei Murakoshi, and their team report surface-enhanced Raman scattering (SERS) of a single 4,4′-bipyridine molecule—a linear structure of two pyridine rings—between two gold nanoelectrodes that form a nanogap whose size is controlled by a piezoelectric crystal (DOI: 10.1021/ja307821u). While increasing the separation between the contacts, the researchers measure changes in the conductance (reciprocal of resistance) of the molecule, up to the point that the molecule becomes detached from one of the electrodes. Simultaneously, SERS allows the detection of changes in vibrational modes of the molecule caused by changes in its electronic and geometrical structure.

With density functional theory calculations, the researchers link the observed changes in the Raman spectra to changes in the tilting angle of the molecules caused by the increasing width of the nanogap. The observation broadens the knowledge needed in order to advance the development of molecular electronics. **Alexander Hellemans**

TWO METALS ARE BETTER THAN ONE

Heterogeneous catalysis using nanoclusters consisting of more than one metal is seeing more widespread application in chemistry, because these types of catalysts can be highly efficient or may have unusual properties. Particularly attractive are the gold/palladium bimetallic cluster alloys, due to their high catalytic turnover.

Masahiro Ehara, Hidehiro Sakurai, and co-workers have used this bimetallic alloy to activate the high-energy carbon−chlorine bond (DOI: 10.1021/ja309606k). They discover that the Au/Pd nanocluster can catalyze Ullmann coupling of chloroarenes at room temperature, a reaction that otherwise requires harsh conditions. The reaction does not progress with either gold or palladium single-metal nanoclusters alone, nor with a macroscopic mixture of the two metals. Through computational analysis, the researchers find that the high activity of the bimetallic nanocluster is due to the substrate being adsorbed onto the alloy surface, which is unlikely to occur with single-metal catalysts. In addition, the nanocluster is found to have higher activity toward chloroarenes than their bromo equivalents.

This straightforward method to activate the robust C−Cl bond may enable the design and synthesis of new multimetallic catalysts for similar high-energy activations. **Leigh Krietsch Boerner, Ph.D.**

FLUORESCENT SENSOR HOLDS PROMISE FOR RAPID CHIRAL ASSAYS

A new molecule may make chiral assays faster and easier. Researchers led by Lin Pu have discovered an enantioselective dual-emission fluorescent molecular sensor that can simultaneously determine both the enantiomeric composition and concentration of a chiral molecule in solution (DOI: 10.1021/ja3101165).

The researchers synthesized both enantiomers of a trifluoromethyl ketone-based molecular sensor. They studied the molecules' optical properties in the presence and absence of a chiral diamine compound. When treated with the chiral compound, the sensors undergo different enantiomer concentration-dependent changes in fluorescence intensity at two different wavelengths. The changes in intensity enable scientists to determine the enantiomeric composition of the chiral diamine, making this the first report of a compound that can determine both the concentration and enantiomeric composition of a chiral molecule at once with only one fluorescence measurement.

This work is an improvement over previous single-emission fluorescent sensors and sensor pairs and may help researchers more simply conduct analysis of chiral molecules. **Christine Herman, Ph.D.**

LASER BLAST TESTS EXTRATERRESTRIAL ORIGIN OF BIOMOLECULES

Even after scientists searched in hydrothermal vents, simulated early shallow seas, and provoked self-replicating crystal growth in mud, the sparks that bring inorganic molecules to life are elusive targets. Another possibility is that comets or asteroids carried the right combination of molecules and kinetic energy to spark life when they hit the Earth's atmosphere. To test that idea, Judit E. Šponer, Svatopluk Civiš, and colleagues simulated in a laboratory the atmospheric breakup of an icy extraterrestrial body (DOI: 10.1021/ja310421z).

The team focused on formamide mixed with FeNi materials common in comets and asteroids. In a previous study, researchers predicted that a high-energy reaction of formamide could produce some of the nucleobase components of deoxyribonucleic acid (DNA), crucial for the reproduction of living cells. The current study investigates a frozen formamide−FeNi mixture treated with laser sparks forming a plasma heated to 4500 K. The researchers analyzed the composition of the resulting gas with infrared spectroscopy and detected the precursors of diaminomaleonitrile, a compound which is generally believed to be a key player in the emergence of life-giving nucleobases. Using theoretical calculations, they show that all detected molecules can be derived from formamide by consecutive addition of $CN^{\bullet}$ radicals. **Lucas Laursen**

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■ ENHANCING APTAMER ABILITIES

Special types of biomolecules called aptamers have emerged as versatile materials for a variety of applications, including as biosensors for monitoring biological processes and as diagnostic, drug delivery, and therapeutic agents. Aptamers are made up of short strands of RNA or DNA that fold into precise three-dimensional structures, creating an architecture that can bind to other biomolecules with exquisite affinity and specificity. One challenge in this technology is the ability to manipulate and fine-tune these binding properties, which would improve and expand the utility of the aptamers for more sophisticated investigative and medical purposes.

Francesco Ricci and co-workers tackle this challenge by developing methods for tuning the binding affinities and specificities of DNA-based aptamers (DOI: 10.1021/ja310585e). They tweak the structure of the aptamers by incorporating mutations at locations distal to the binding site and using short DNA strands that inhibit aptamer folding. Combinations of these approaches enable the creation of sets of aptamers with varying affinities and dynamic ranges. This strategy will contribute to the continued development of aptamers with increasingly adaptable and refined capabilities. **Eva J. Gordon, Ph.D.**