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Spotlights on Recent *JACS* Publications

HOW TO MAKE A VAT OF GLOWING NANOPARTICLES

Shuit-Tong Lee, Yao He, and colleagues use simple "kitchen chemistry" to make large batches of fluorescent nanoparticles in water (DOI: 10.1021/ja4026227). Fluorescent silicon nanoparticles exhibit remarkable optical, electrical, and mechanical properties, and are nontoxic, which makes them excellent biomarkers and cellular probes. Though researchers have refined techniques for making these materials dispersible in water, the processing required to create and then modify the particles was complex and tedious.

The new approach is a "bottom-up" strategy that creates silicon nanoparticles in a single vessel by microwaving silicon-containing hydrophilic molecules. The chemistry represents a completely new route to the creation of silicon nanocrystals. Following an oxidation−reduction reaction, particles of silicon build up until they reach a diameter of around 2 nm. The particles are water dispersible, brightly luminescent (they glow blue), and biocompatible. They can be easily attached to proteins, and they remain luminous over lengthy storage periods without the need for special temperature or light protection. Assuming continuous production in smaller batches, the technique can produce approximately one gram every two hours.

This fast, cheap, and easy method to create high-quality fluorescent nanoparticles should drive costs down in applications ranging from biosensors to solar cells. **Jenny Morber, Ph.D.**

LIFE'S LEDS CHANGE COLOR IN SOLUTION

Fireflies light up the night, but at significant energetic cost. In their light-producing organs, a molecule called luciferin reacts with oxygen in the air and biology's basic unit of energy, adenosine triphosphate, or ATP, to form oxyluciferin in an excited state. As oxyluciferin returns to a resting state, it releases photons, but researchers still do not fully know how these so-called charge-transfer (CT) excitations work or how solvents, such as water, could change the color of the emerging light. Now Angel Rubio, Steen Brøndsted Nielsen, and colleagues report how water and two other types of solvents affect the light that emerges from a charge-transfer excitation (DOI: 10.1021/ja4025275).

The team uses *meta*-nitrophenolate as their model, since its two components, nitrite and phenolate, move apart when transferring charges between them. Predicting how nearby molecules would change that charge transfer, however, is the stuff of speculation and density functional theory. So the team generates charge transfers in *m*-nitrophenolate while parking it adjacent to three solvents: water, methanol, and acetonitrile. Because many CT excitations occur in small spaces within complex protein pockets, the team first experiments with just one adjacent solvent molecule and then again in bulk. Using a mass spectrometer, they make the surprising observation that a single solvent molecule can blue-shift the CT excitation by about half as much as the solvent in bulk form. **Lucas Laursen**

"ACSESS" TO VIRTUALLY ALL DRUGS

Weitao Yang, David Beratan, and co-workers develop a way to create a representative universal library of all drug-like compounds (DOI: 10.1021/ja401184g). "Algorithm for Chemical Space Exploration with Stochastic Search" (ACSESS) elevates chemical space exploration by enabling the search of uncharted domains of the vast universe of small molecules.

Using ACSESS, a virtual chemical library is seeded with simple molecules, and a series of structural modifications including addition, deletion, or change of specific atoms or bonds, while taking into consideration structural diversity, stability, and synthetic accessibility, leads to the generation of a representative, maximally diverse collection of compounds. In this study, the researchers create a representative universal library of 8.9×10^6 compounds with a molecular weight between 125 and 500 Da, a property common to a majority of pharmaceutical drugs.

ACSESS enables the large gaps in structural diversity between the known chemical universe and that identified using the algorithm to be systematically explored, and provides access to a nearly limitless source of new compounds for further investigation. This innovative approach can also be expanded to incorporate additional computational parameters for applications in other fields that rely on molecular discovery. **Eva J. Gordon, Ph.D.**

FLEXIBLE NANOCRYSTALS BEND, COIL, AND STACK

As building materials, inorganic nanocrystals can be difficult to work with. Conventional nanoparticles and nanowires are often rigid and brittle, and require careful coaxing to assemble into complex structures. If only inorganic nanomaterials were more like flexible organic proteins and other macromolecules, researchers could create much more sophisticated shapes for novel devices.

Now with a simple solution-based method, Xun Wang and co-workers have created indium sulfide (In_2S_3) nanocrystals that are so thin and long that they bend like flexible proteins (DOI: 10.1021/ja403065z). Even more interesting, the ultrathin nanocrystals are adaptive. They spontaneously coil in solution, and when left for several days the coils assemble into ordered chicken-wire-like arrays and three-dimensional supercrystals. High-resolution microscopy shows that the edges of some supercrystals form steps like those formed by atoms at the rough edges of natural crystals.

In_2S_3 is a potential replacement material for hazardous cadmium sulfide in solar cells. This technique's simplicity hints at the potential to form similar structures from other inorganic starting materials. The authors suggest that these ultrathin nanocoils may help researchers to bridge the gap between organic and inorganic nanomaterials, providing insights into superstructure self-assembly and polymer crystallization. **Jenny Morber, Ph.D.**

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