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Spotlights on Recent *JACS* Publications

FUELING THE FUTURE WITH METHANE IN METAL–ORGANIC FRAMEWORKS

Methane in natural gas is an attractive alternative to fossil fuels because its combustion generates significantly fewer pollutants. However, widespread use of natural gas as fuel for automotives has been hampered by a lack of practical ways to store and transport methane. In a new study, Pantelis Trikalitis and coworkers suggest a potential solution to this conundrum through a novel metal–organic framework (MOF) that can store high amounts of methane at easily achievable temperatures and pressures (DOI: 10.1021/jacs.5b11079).

The new MOF is topologically related to one previously explored for methane storage, known as HKUST-1. Using reticular synthesis and the supermolecular building layer (SBL) approach, preselected rigid and directional building blocks are assembled into predetermined tbo-MOF structures, a HKUST-1-like framework but now expanded and deliberately functionalized. The new tbo-MOF structure has higher gravimetric and volumetric surface areas than its parent HKUST-1 structure, as well as aromatic rings functionalized with methyl groups, features all designed to maximize methane storage.

Adsorption studies show that the novel MOF displays high total gravimetric and volumetric methane uptakes, reaching 372 and 221 cm^3 (STP) g^{-1}, respectively, at 85 bar and 298 K. The authors suggest that these results could provide new direction for the design and construction of future MOFs with even further improved methane storage properties.

Christen Brownlee

NEW DRUG DELIVERY STRATEGIES IMPROVE THERAPEUTIC EFFICACY

It takes more to make a good drug than mere potency; also critical is how that drug is delivered. Is it oral or injected, local or systemic? Is it delivered all at once, or released over time? These questions relate to drug delivery, a topic that Robert Langer and colleagues discuss in a new Perspective (DOI: 10.1021/jacs.5b09974).

Langer and colleagues focus on five key areas: controlled drug release, RNA therapeutics, localized drug delivery, oral administration of biologics (such as antibodies), and biologic drug delivery systems, including designs based on modified bacteria, vesicles, and red blood cells. The authors discuss the unique challenges posed by new genome-editing strategies, especially CRISPR/Cas9, as they make their way toward the clinic.

Drug delivery systems represent the intersection of such fields as synthetic and polymer chemistry, materials science, nanotechnology, and more. Yet no single design will work for every application, and successful strategies must factor in differences in chemical properties, tissue target, and drug release timing, among other variables.

Jeffrey M. Perkel

UNIVERSAL WAY TO SEE MOTIONS OF PROTEINS

Proteins do not simply sit still, and vibrational spectroscopy is a common method for studying various protein motions. But a significant problem with the method is that it is very difficult for scientists to isolate motions in different parts of a sizable protein.

Now Sebastian Peuker, Sebastian Westenhoff, and colleagues have come up with a way to pinpoint how different parts of a protein move (DOI: 10.1021/jacs.5b12680). Their method enables scientists to construct a protein made with a specific, isotopically labeled amino acid. This tagged amino acid makes it possible to determine by vibrational spectroscopy how a specific part of the protein moves.

As proof of concept, the researchers have made an analogue of a widely studied laboratory protein, called green fluorescent protein, with a critical tyrosine residue labeled with the isotopes oxygen-18 and carbon-13. They are able to make milligram amounts of the protein, which is ample for vibrational spectroscopy analysis. Through their spectroscopic analyses of the labeled protein, the investigators discover an important configuration that the protein takes on as it functions. The investigators say, "Our method lifts vibrational spectroscopy of proteins to a higher level of structural specificity."

Rajendrani Mukhopadhyay, Ph.D.

SUPERCOMPUTERS PROBE FULLERENE FORMATION

Bun Chan and colleagues have calculated precise heats of formation for carbon fullerenes, enabling researchers to better predict their properties and behavior (DOI: 10.1021/jacs.5b12518).

A compound's "heat of formation" is a fundamental thermodynamic value based on the energy required to create molecular bonds, and this information is essential to understanding how materials form and change. Despite a flurry of basic and applied research on soccer-ball-like carbon fullerenes since their discovery in 1993, researchers still did not have precise values for their heats of formation. The problem, in part, is that fullerenes are small enough to act unlike familiar bulk materials, but large enough that atomistic calculations become unwieldy.

Aided by advances in supercomputing, more efficient software, and improved quantum chemistry frameworks, the researchers have determined reliable heats of formation for fullerenes of up to 180 carbon atoms. They create a formula to compute heats of formation per carbon atom, enabling a general estimation for larger molecules. The calculations also hint at why fullerenes behave so differently from their graphene cousins—perhaps, the authors propose, it is because most of the fullerene bonds are associated with substantially higher strains.

Jenny Morber, Ph.D.

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