

## Spotlights on Recent JACS Publications

### ■ PINNING DOWN QUANTUM INTERFERENCE IN MOLECULAR CONDUCTOR

Quantum interference is one of the most intriguing phenomena in quantum physics. Single photons or electrons pass through a double slit and the matter waves interfere, either constructively or destructively, depending on the phases of the matter waves.

Recently, this phenomenon has been observed with electrons sent through single molecules, whereby differences in the conductance are attributed, at least in part, to quantum interference. However, because conductance measurements are performed on molecules with different chemical structures, it is impossible to measure the conductance resulting from quantum interference alone.

Now, Marius Bürkle, Nongjian Tao, Yoshihiro Asai, and co-workers report a way to pin down quantum interference of electrons passing through two identical isomers of tetraphenylbenzene (DOI: [10.1021/jacs.6b10837](https://doi.org/10.1021/jacs.6b10837)). The molecule consists of four benzene rings attached to a central benzene moiety that functions like a roundabout for electrons. In one configuration of the injection point, the electrons undergo constructive interference. With a different injection point, the conductance becomes 1 order of magnitude lower because of destructive interference. *Ab initio* calculations for the conductance show close concordance with the experimental results. The work presents a new approach to quantify quantum interference effects in molecular conductors.

Alexander Hellemans

### ■ ROOM FOR IMPROVEMENT: POSTSYNTHETIC CHEMISTRY IN METAL–ORGANIC FRAMEWORKS

Metal–organic frameworks (MOFs), a class of crystalline materials that consist of coordination bonds between metal ions and organic linkers, have garnered enormous interest over the past two decades. Although these materials have already found a bevy of applications as-is, including in catalysis, drug delivery, and fuel storage, MOFs' readily modifiable structures offer an opportunity to tweak and customize their composition after synthesis for a variety of purposes.

In a new Perspective, Seth Cohen details the history and recent advances in several different postsynthetic MOF-modification techniques (DOI: [10.1021/jacs.6b11259](https://doi.org/10.1021/jacs.6b11259)). The most well established technique for postsynthetic modification of MOFs involves chemically functionalizing the organic ligands. Additionally, the researchers describe four other methods including postsynthetic deprotection, postsynthetic exchange, postsynthetic insertion, and postsynthetic polymerization. Although each method maintains the crystallinity, porosity, and overall structural integrity of the original material, these techniques lead to very different end results. For example, recent studies in postsynthetic polymerization highlight the potential to integrate MOFs into polymer membranes capable of filtering toxic materials from aqueous solutions. The author notes that continued forward momentum in this field will lead

to even more exciting ways to transform MOFs into new and varied materials.

Christen Brownlee

### ■ COMBINATORIAL FLUORESCENT MOLECULAR SENSOR DIFFERENTIATES BETWEEN AMYLOID BETA AGGREGATES

The aggregation of amyloid  $\beta$  ( $A\beta$ ) peptides is believed to play a major role in the progression of Alzheimer's disease. But  $A\beta$  peptides can consist of different alloforms and their aggregation can lead to the creation of a variety of species, such as oligomers, protofibrils, and fibril, which are difficult to track using conventional techniques. Given that all these parameters can affect  $A\beta$  toxicity, much effort has been made to develop new analytical tools for differentiating between distinct forms of  $A\beta$ .

David Margulies and colleagues create a new fluorescent molecular sensor that, by generating a wide range of distinct emission patterns, is able to differentiate between different  $A\beta$  aggregates (DOI: [10.1021/jacs.6b10809](https://doi.org/10.1021/jacs.6b10809)) and track dynamic changes that occur in their composition. Other methods such as mass spectrometry, gel electrophoresis, and immunoblotting, can all effectively determine composition but require special expertise and are not high-throughput. The new approach is similar to an earlier, widely used fluorescence assay that can readily sense fibril formation, but it is unique in that it can distinguish among alloforms and identify additional  $A\beta$  aggregates through pattern recognition methods. This tool shows great promise in analyzing complex and dynamic mixtures to ultimately achieve a better understanding of  $A\beta$  aggregates' role in Alzheimer's disease.

Christine Herman, Ph.D.

### ■ HALOGEN BONDING DRIVEN HELIX THAT BUILDS ITSELF

Helices form the backbone of many important biological molecules including DNA and many proteins. Generating *de novo* helices in the laboratory is a goal of scientists interested in the design of self-assembling macromolecular materials with novel functions. Researchers led by Yun-Bao Jiang design a molecule that self-organizes into a supramolecular helix (DOI: [10.1021/jacs.6b13171](https://doi.org/10.1021/jacs.6b13171)).

The basic unit of the supramolecular helix is an amidothiourea with a halogen atom, iodine, substituted at the *para*-position of the phenyl rings at both ends of the molecule. An intramolecular hydrogen bond generates a  $\beta$ -turn, which then induces the twist of the helix. The crystal structure shows that each amidothiourea molecule becomes a link in a chain of molecules, connected head to tail via halogen bonding interactions between the iodine and the center of the terminal phenyl ring (a halogen- $\pi$  bond).

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The combination of  $\beta$ -turns and head-to-tail halogen bonding generate a single-stranded left-handed helix, and additional halogen bonding between helices gives rise to a supramolecular helix. The structure forms spontaneously in solution at micromolar concentrations of amidothiurea. These findings suggest an overall approach to designing building blocks that, using halogen bonding, can generate functional supramolecular helices.

**Erika Gebel Berg**, Ph.D.