

Spotlights on Recent JACS Publications

■ THE GRAPHENE MIMIC OF THE FUTURE?

Since the discovery of graphene—a form of carbon in which the atoms are arranged in a single sheet like chicken wire researchers have sought and found many more novel planar materials. Driving the hunt for these materials are their unusual and often very useful properties. Some, for example, demonstrate extremely high thermal conductivity, while others promise tunable electronic conduction. Here, Li-Ming Yang and colleagues use computer simulations and calculations to predict a potential new single-layer material made of silicon and copper (DOI: 10.1021/ja513209c).

The calculations predict that the material should be stable, even at moderately high temperatures, and show metal-like fast electron conduction. Unlike previous two-dimensional materials, there is no analogue of such material featuring planar hexacoordinate copper and planar hexacoordinate silicon. The ability to engineer new low-dimensional materials is a recent and powerful development, made possible in part through theoretical examinations such as these, which provide experimentalists with worthwhile targets. Considering the rapid development of experimental techniques for new-material fabrication, the researchers are optimistic that a Cu_2Si monolayer can be created in the near future. Jenny Morber, Ph.D.

AUTOXIDATION INHIBITION IS ALL ABOUT THAT BASE

Hydrocarbons, such as those used in petroleum-derived lubricants and polymers, are susceptible to autoxidation, which puts wear and tear on the equipment in which these hydrocarbons are used. Manufacturers of such products often include radical-trapping additives such as phenols or diphenylamines to slow the hydrocarbon's oxidation. A team led by Derek A. Pratt of the University of Ottawa, Canada, has been exploring the use of heterocyclic analogues of diphenylamines as antioxidants in recent years, based their earlier observations that phenols could be made more effective upon exchanging the phenyl ring for a heterocycle.

Now Pratt's team has tested the antioxidant effects of several heterocyclic diarylamine compounds under real-world conditions and reports remarkable results (DOI: 10.1021/ ja5124144). They compare the rate of hydroperoxide formation—the primary product of autoxidation—at $160 \,^{\circ}C$ of six of their heterocyclic diarylamines and a standard industry additive. The team reports that when they add a base to their test compounds, to counter the buildup of carboxyl acids, they could delay hydroperoxide formation by more than a factor of 10. That improvement could make for less lubricant oxidation and less frequent maintenance for combustion engines, and offers many other possible applications where hydrocarbon oxidation is a big problem.

Lucas Laursen

POLYMER SOLAR CELLS: REDUCING ENERGY LOSS WITHOUT COMPROMISING EFFICIENCY

Although the loss of photon energy in solar cells is unavoidable, scientists are on the lookout for new materials that allow those losses to be minimized. The main challenge is the reduction of energy loss in polymer-based solar cells that often comes with a dramatic drop in quantum efficiency for charge generation. Now, Weiwei Li, René A. J. Janssen, and co-workers describe a new class of polymer solar cells that attains the minimum photon energy loss possible without allowing quantum efficiency to take a huge hit (DOI: 10.1021/ja5131897).

The newly designed solar cells are based on the conjugated polymer diketopyrrolopyrrole (DPP), which serves as the electron-deficient unit. By bridging DPP units to electron-rich units using thiazoles, the team achieves conjugated polymers with both a high ionization potential and a high electron affinity, which results in a material with efficient charge generation (>50%) and the minimum amount of energy loss possible for such a material ($\leq 0.6 \text{ eV}$). Prior to this report, the best organic solar cells reported have had energy losses of 0.7–0.8 eV. The results thus suggest it is possible to improve the performance of organic solar cells beyond the present efficiency limits.

Christine Herman, Ph.D.

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