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Spotlights on Recent *JACS* Publications

ON A ROLL: TURNING GRAPHENE FLAKES INTO CARBON NANOTUBES

Carbon nanotubes (CNTs) are often described as rolled-up layers of graphene—single-atom-thick sheets of carbon—but this description seemed to be more of an analogy than a true representation. In a new study, a group led by Mildred Quintana, Petra Rudolf, Francesco Zerbetto, and Maurizio Prato shows that it is indeed possible to create CNTs from graphene (DOI: 10.1021/ja303131j). Previously, CNTs have only been synthesized through chemical and physical means that did not use graphene as a starting material.

The researchers use ultrasound waves to partially peel apart multilayer graphene in the solvent dimethylformamide. They then perform the same process for a longer period after adding ferrocene aldehyde (Fc-CHO), a compound used in other CNT-synthesizing processes.

Analysis shows that the Fc-CHO causes the graphene flakes to curl, resulting in CNTs that are about 2 μm long, much longer than those created by the usual methods. The authors suggest that this new method adds to the CNT-synthesis repertoire and confirms that CNTs can indeed be derived from graphene. **Christen Brownlee**

THEORETICAL STUDIES SHED LIGHT ON ENERGETIC MATERIALS DEGRADATION

A new theoretical study led by Maija Kuklja sheds light on the relationship between crystal morphology and decomposition mechanisms of energetic materials (DOI: 10.1021/ja3044695).

In the field of energetic materials research, much emphasis is placed on the design and development of improved high energy density materials for use as fuels, propellants, and explosives. Lagging behind these discoveries is fundamental knowledge about the relationship between surface structure and the initiation of energy release. This knowledge is important in order to avoid accidental initiation and to enable researchers to design and create energetic materials with precisely defined decomposition mechanisms.

In this study, the researchers perform quantum-chemical simulations to model the decomposition of β-octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) crystals. While HMX has been extensively studied, this report is the first to provide insight into the relationship between a material's decomposition mechanism and its morphology, including its surfaces, defects, and the size of the particles within it. The results would have been difficult to obtain from experiments alone and may help scientists better control fast, highly energetic chemical reactions. **Christine Herman, Ph.D.**

STRUCTURAL INSIGHT INTO RESISTING ANTIBIOTIC RESISTANCE

Natalie Strynadka and co-workers have solved the crystal structure of an enzyme called the New Delhi metallo-β-lactamase-1, a major player in the growing problem of antibiotic resistance (DOI: 10.1021/ja303579d).

Approximately 50% of all antibiotic prescriptions worldwide are for a group of drugs called β-lactams, which include such common medicines as penicillin and cephalosporin. Growing bacterial resistance to this class of drugs is an increasingly alarming global health concern. New Delhi metallo-β-lactamase-1 is one of a class of enzymes called β-lactamases that are produced by resistant bacteria and inactivate the β-lactam drugs. Understanding how β-lactamases interact with the antibiotics at the molecular level is critical to developing new strategies for combatting these dangerous microorganisms.

Now, the authors have characterized the structure of the β-lactamase in complex with four β-lactam antibiotics as well as with the blood pressure medication L-captopril, a promising inhibitor of the enzyme. The structures provide exquisite detail of key interactions between the enzyme and the drugs, including exposing a unique binding mechanism for L-captopril that will inform the design of new and improved β-lactamase inhibitor antibiotics. **Eva J. Gordon, Ph.D.**

NANOPARTICLES IN OXIDES ON NANOTUBES: IT'S A WRAP!

By arranging nanosized components into hierarchical structures, researchers are finding that end products can be far more useful and interesting than expected from the sum of individual pieces. That was indeed the case for Paolo Fornasiero and co-workers, who developed new nanomaterials-based catalysts that show promise for a variety of energy-related reactions (DOI: 10.1021/ja304398b).

Using multi-walled carbon nanotubes (MWCNTs) as a base, the researchers coat them with a mixture of individual metal oxides (TiO_2, ZrO_2, or CeO_2) and palladium or platinum nanoparticles, components traditionally used as catalysts on their own. They compare the finished composite materials with mixtures of the metal oxides and nanoparticles that were not supported by MWCNTs.

The results show that the MWCNTs cause the oxide/nanoparticle mixtures to crystallize into a porous coating, leading to better access to the catalysts' metal centers (or active sites) for reactions. In three different test reactions, the wrapped MWCNTs showed substantially greater catalytic performance than the unsupported mixtures, with the MWCNTs themselves providing a synergistic effect with the nanoparticles. The authors suggest that precisely organizing components could have important implications for a variety of catalytic applications. **Christen Brownlee**

LIFE ON THE EDGE CHANGES A POLLUTANT'S BEHAVIOR

Volatile organic compounds (VOCs), a class of pollutant, permeate the atmosphere in gas form and in liquid water droplets such in clouds. Yet classical models assume that the behavior of VOCs at the air−water interface of such droplets is intermediate between their behavior in gas or liquid phases.

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Now, Manuel Ruiz-Lopez and collaborators use a computer simulation of formaldehyde, a common VOC, to predict that the molecule accumulates at the air−water interface and that when there, it reacts more with free radicals such as $HO_2^{\bullet}$ than in formaldehyde's other states (DOI: 10.1021/ja304971e).

The researchers had previously simulated the behavior of $HO_2^{\bullet}$ and $O_2^{\bullet-}$ using quantum mechanics and molecular dynamics and found that those radicals exhibited unique acidity and other properties at the surface (DOI: 10.1002/anie.201200656). By applying their new simulation method to formaldehyde, they find that life on the edge is not just an average of life in water or gas form but that instead the molecule exhibits exotic electronic properties and might react more readily with $HO_2^{\bullet}$, which would neutralize the pollutant. In this article, the authors call for new experimental methods to test their predictions, and, in the meantime, they will study how formaldehyde at the interface might interact with still more atmospheric agents. **Lucas Laursen**