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Spotlights
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# Spotlights on Recent *JACS* Publications

## TRACKING PROTEIN MOVEMENTS ON A TUMBLING NANOPARTICLE

Protein motions are critical to their functions, facilitating interactions, catalysis, signaling, translocation, and more. NMR spectroscopy has proved indispensable to studying the dynamics of isolated proteins. However, many proteins perform their work while clinging to larger particles, such as cells, macromolecular assemblies, and organelles. Detecting the motions of proteins attached to such particles is challenging due to the particles' slow rotation, which is not compatible with standard NMR experiments that rely on rapid tumbling. Now, Marius Clore, Vital Tugarinov, and colleagues have developed a relaxation-based NMR spectroscopy approach for measuring the dynamics of proteins on the surface of nanoparticles (DOI: 10.1021/jacs.6b02654).

As a test case, the researchers study a small, relatively stable model protein—ubiquitin—on the surface of liposomes, nanosized vesicles that are frequently used as drug carriers. The liposomes are invisible in the NMR experiment, while the ubiquitin molecules are labeled with the NMR-active isotope $N^{15}$. The key to this approach is measuring the relaxation of ubiquitin attached to nanoparticles of drastically varying sizes, which allows the researchers to tease out the global dynamics and exchange kinetics of the ubiquitin molecule on the liposomes: that ubiquitin rotates on an internal axis roughly perpendicular to the liposome surface.

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

## CHALLENGES AND PROMISE OF SINGLE-WALL CARBON NANOTUBES

Single-wall carbon nanotubes (SWCNTs) are atom-thick tubular structures known for their ultra-high strength and chemical stability, excellent thermal and electrical conductivity, and high carrier mobility. Depending on their chiral angle and diameter, the tiny graphene roll-ups can be either semiconducting or metallic, each with their own unique properties: the metallic nanostructures are capable of ballistic electron transport, while the semiconducting counterparts have high current on/off ratios and high carrier mobilities.

In a new Perspective, Chang Liu and Hui-Ming Cheng present an overview of recent developments in the synthesis of both semiconducting and metallic SWCNTs (DOI: 10.1021/jacs.6b00838). They discuss the potential applications of SWCNTs, which range from flexible electronics to computer hardware, and explain the importance of various characteristics, such as chirality, dimensions, and electrical type, on their behavior and performance. The authors also discuss the various routes for preparing SWCNTs and emphasize the importance of uniform electrical type. The Perspective concludes with a look ahead at some of the biggest challenges in the field, which include achieving high sample purity, understanding the underlying mechanisms of SWCNT formation, and thoroughly characterizing the final products.

**Christine Herman**, Ph.D.

## COBALT(II)-BASED MOFS A BREATH OF FRESH AIR FOR AIR SEPARATION

Synthetic transition metal—dioxygen compounds mimic biological $O_2$ carriers and metalloenzymes by reversibly binding to $O_2$. This useful characteristic makes them good candidates for industrial air separation applications. While some of these compounds have been incorporated into the porous, crystalline structures known as metal—organic frameworks (MOFs) for this purpose, these materials have suffered from a number of drawbacks, including low thermal stability, a loss of performance over multiple cycles, and decomposition with humidity.

Seeking to overcome these challenges, Jeffrey Long and coworkers have synthesized two new MOFs capable of binding $O_2$ (DOI: 10.1021/jacs.6b03680). Using $O_2$-carrying cobalt(II) as the MOF nodes and electron-donating triazolate linkers as the MOF connectors, the researchers create Co-BTTri. Tests show a strong preference for binding $O_2$ over $N_2$ and reliable performance after repeated cycling, even in the presence of humidity.

Replacing one of the triazolate groups on the tritopic organic linker with a pyrazolate generates the analogous MOF, Co-BDTriP, which demonstrates markedly higher yet still fully reversible $O_2$ binding. The authors suggest that their stability, selectivity, and high $O_2$ capacity position these materials as frontrunners for use in air separation devices.

**Christen Brownlee**

## REVISING THE MECHANISM OF CHOLESTEROL OXIDATION

The in vivo oxidation of lipids and other biomolecules plays a critical role in health and disease. New research shows that the most pathogenic products of cholesterol oxidation can arise from a reaction with oxygen, rather than with ozone, a molecule whose natural occurrence in tissues remains controversial, or singlet oxygen, an electronically-excited form of oxygen, as has been previously suggested.

Cholesterol is one of the most common lipids in cell membranes, and it helps to regulate membrane fluidity; however, the molecule is probably most known for its relationship to disease. Cholesterol levels in the blood are linked to heart disease, and oxidation products that are formed after cholesterol reacts with ozone or singlet oxygen have been implicated in cancer, Alzheimer's disease, Parkinson's disease, and multiple sclerosis.

Zosia Zielinski and Derek Pratt have elucidated the product mixture that arises when cholesterol reacts with oxygen in organic media, finding four hydroperoxides; three previously unknown products of this reaction, of which two decompose into the same compounds observed in the reaction with ozone (DOI: 10.1021/jacs.6b03344). The results suggest that the cholesterol oxidation products linked to disease derive simply from aerobic oxidation, rather than reactions with ozone or singlet oxygen.

**Melissae Fellet**, Ph.D.

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