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Spotlights on Recent *JACS* Publications

TOOL FOR EXPLORING INTERFACIAL SOLVATED ELECTRONS

Solvated electrons are free electrons in an aqueous solution. They occur widely but are challenging to observe directly. Justin Wiens, Gilbert Nathanson, William Alexander, Timothy Minton, Lakshmi Sankaran, and George Schatz have collaborated to show that soft collisions of sodium atoms with the protic liquid glycerol can be a useful tool to explore the interfacial behavior of solvated electrons (DOI: 10.1021/ja4106144).

Collision of a sodium atom with a solvent is a gentle method to generate solvated electrons. These atoms rapidly ionize into Na^+ ions and solvated electrons at or near the surface of glycerol upon their gas-phase deposition onto the liquid. The researchers employ this technique to investigate reactions initiated by the collisions.

They combine molecular dynamics calculations with atomic beam surface-scattering experiments. The experiments measure the scattered Na beam with a mass spectrometer to show that reactive uptake of Na atoms into glycerol is greater than 75%. Electrons from the Na atoms then react with near-interfacial glycerol molecules. The simulations follow the Na atom after the collision as it begins to form the solvated electron and Na^+ on the surface of glycerol. The results illustrate the reorientation of the hydroxyl groups of glycerol to stabilize the electron and suggest that formation of a fully solvated electron occurs on time scales greater than a few picoseconds.

Dalia Yablon, Ph.D.

TWO-FACED PARTICLES ARE ACTUALLY PRETTY NICE

In Roman mythology, Janus is a two-faced god of transitions and gateways. Appropriately, nanoparticles made up of two materials fused together are called Janus particles. Wolfgang Tremel and his team create Janus nanoparticles that are part gold and part silica-coated molybdenum oxide (MnO/SiO) (DOI: 10.1021/ja410787u).

Gold is thermally conductive and optically active. Silica is stable, water-soluble, and biocompatible. MnO is highly magnetic. Together these materials make up a kind of ideal triumvirate for biomedical applications and magneto-optical detection. The researchers use a simple seeded nucleation and growth fabrication technique that affords precise control over particle shape, size, and surface properties. Importantly, the fabrication process creates a silica coating on the MnO section only, leaving the gold section untouched.

Experiments confirm that the nanoparticles are magnetic, water-soluble, stable, and strongly fluorescent. Customizable through easy addition of biomolecules such as antibodies or proteins, functionalized nanoparticles retain their attractive magnetic and optical attributes. Cell viability studies reveal that the Janus particles are also biocompatible. These Janus particles combine the attributes of several separate nanoparticles into one high potential package for medical imaging, bimolecular tagging, localized drug delivery, and magnetic separation.

Jenny Morber, Ph.D.

SEEKING SEQUENCE-SPECIFIC INHIBITORS OF DNA METHYLATION

DNA methylation, the attachment of a small chemical entity called a methyl group to DNA, generally occurs at the sequence CG. This seemingly modest covalent alteration has significant ramifications in gene transcription, the process in which DNA is copied into RNA. When DNA is methylated, transcription of certain genes is repressed, including those that stop tumor cells from growing, making DNA methylation an exciting therapeutic target for cancer.

One challenge in targeting DNA methylation is finding compounds that can inhibit the process in a sequence-specific manner, which would help gain control over which genes are blocked. Peter Dervan and co-workers tackle this challenge using a method called Bind-n-Seq to identify and design sequence-specific DNA-binding molecules (DOI: 10.1021/ja500211z). They program a specific compound, called a hairpin polyamide, that binds with high specificity to the sequence CGCG. They also suggest that binding of the hairpin polyamide in the minor groove of DNA acts as a stabilizing clamp that prevents the distortion of DNA necessary for the DNA methylation process to occur.

This study illuminates a path forward toward the design of improved DNA methylation inhibitors. The ability to manipulate DNA methylation with such compounds could lead to the development of effective new anticancer agents.

Eva J. Gordon, Ph.D.

PROTEINS “ZIP” TO METAL SURFACE AFTER ANCHORING

Proteins are ubiquitous in nature and are known to quickly coat solid surfaces. One example of this process is protein facilitation of biomineralization to create new bone in the body. Proteins also coat surfaces of medical devices inside the human body, and improved control over this process—through expanded understanding of protein affinity for solid surfaces and the details of how they adsorb to surfaces—could aid performance.

Mark Biggs and co-workers use molecular dynamics simulations to model interactions of peptides with a metal surface covered in water (DOI: 10.1021/ja411796e). Their study is comprehensive, with more than 240 simulations of two different peptides. They discover that peptide adsorption is preceded by biased diffusion toward the surface, where a hydrophilic group generally anchors the peptide to the interfacial water, allowing for its slow, stepwise adsorption to the surface.

This study is exciting in that it elucidates the mechanism of peptide adsorption at a molecular level, giving scientists a tool to design protein/surface interactions for biomedical and technological development. The possible uses and improvement on current technologies are numerous, including building nanoparticles by design, improved bone formation on implants, and better coating of medical implants to suppress immune response.

Polly Berseth, Ph.D.

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