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SILVER NANOCLUSTERS BUILT FOR BIGGER THINGS

Imagine if researchers could coax atoms and molecules to do their bidding; if people, rather than nature, could dictate binding patterns and molecular interactions. This capability is a goal of nanoparticle research: to engineer new molecular building blocks that confer precise control. One strategy is to create core−shell nanoparticle clusters with specific surface binding sites. Unfortunately, the particle's core is often highly disordered, which destroys the homogeneity and predictability of its interaction behaviors.

Now, Osman Bakr and colleagues fabricate a highly ordered core−shell silver nanocluster that crystallizes reliably in a cubic form (DOI: 10.1021/jacs.5b04547). The researchers present the synthesis, optical properties, and structure of these atomically precise building blocks. In a solution-based process, organic surface ligands trap and stabilize the nanocluster of 29 silver atoms, forming a stable and uniform two-layered structure. These structures can then combine with others, like pyramid-shaped blocks, to form optically interesting large crystals.

These synthetic crystals hint at larger things to come. The work offers a new, solution-based approach to create and stabilize nanoclusters into macroscopic-scale solids with unique properties. It brings us closer to a future in which we can create low-cost, high-quality, artificially produced solids, with dial-in properties for any application.

Jenny Morber, Ph.D.

BUILDING A BETTER PROTEIN CRYSTAL

The ability to design crystalline materials with tunable structural, chemical, and physical properties would be a boon to many different scientific disciplines. Proteins make especially attractive building blocks to incorporate into these engineered lattices, useful for their inherent functions including catalysis, electron transfer, and molecular recognition. However, forming ordered, 3D protein crystals is the rate-limiting step for protein crystallography, which is often a trial-and-error process. Successfully engineering 3D protein crystals has been rare, providing a strong impetus for their rational design.

Motivated by the success of metal−organic frameworks—constructs that use various metal centers as nodes and organic molecule linkers as struts interchangeably to create a variety of different crystalline lattices—F. Akif Tezcan and co-workers have developed a system that uses spherical proteins engineered with anchored metal ions as nodes that join together with organic linkers (DOI: 10.1021/jacs.5b07463). As proof of principle, the researchers adapt the octahedral iron storage enzyme ferritin to carry zinc ions. After adding the organic molecule benzene-1,4-dihydroxamic acid to the solution as a linker, the researchers find that the engineered proteins aggregate into crystals as large as 0.5 mm. The authors suggest that this system could be used with other proteins, metal ions, and organic linkers, forming a new class of hybrid materials.

Christen Brownlee

PROTEINS STAY FOLDED EVEN WHEN FLOATING IN AIR

Many scientists rely on electrospray ionization mass spectrometry to unravel protein identity and to provide insights into their biological function. Though the method has been around for over two decades, questions have remained on how proteins are ionized and whether proteins remain folded during the transition from the liquid to the gas phase. To get to the bottom of this mystery, Lars Konermann and co-workers perform experiments and molecular dynamics simulations on three compact globular proteins—ubiquitin, cytochrome *c*, and myoglobin (DOI: 10.1021/jacs.5b07913). The simulations begin with native proteins in tiny droplets containing excess positive charge. The researchers then track the molecules as the droplets dry out to release the gaseous proteins.

This first-of-its-kind simulation supports the charged-residue model of protein electrospray ionization: as a protein is desolvated, it becomes coated with charge carriers from the droplet. The researchers also monitor the simulated proteins' conformations throughout the electrospray process, confirming that the native structure remains largely intact. The results bolster the field of gas-phase structural biology, which uses mass spectrometry to explore interactions between macromolecules. Because the proteins maintain native-like conformations in the simulations, macromolecular interactions observed in the gas phase are likely to be biologically relevant.

Erika Gebel Berg, Ph.D.

FULL CATALYTIC PATHWAY DETERMINED FROM FIRST PRINCIPLES

Despite continuing advances in techniques to characterize catalytic reactions *in situ*, many important transformations with complicated, competing pathways remain poorly understood. The catalytic combustion of methane, for example, has generated renewed interest due to automotive and shale gas applications, but the mechanism remains unclear.

Now, Maxime Van den Bossche and Henrik Grönbeck use density functional theory and reaction kinetics models to calculate the reaction pathways of methane oxidation over a palladium oxide catalyst in a wide range of temperatures and pressures (DOI: 10.1021/jacs.5b06069). Their calculations compare favorably with the experimental observations, revealing important insights into the rate-limiting step at various temperatures and the inhibitory role played by water.

By directing attention to critical steps in the reaction pathways, this study provides new information that can be applied to the design of materials to improve the catalytic combustion of methane, and possibly other industrially important reactions.

Dalia Yablon, Ph.D.

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