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JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
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Spotlights on Recent *JACS* Publications

NEW METHOD EASILY CAPTURES ABSOLUTE CHIRAL CONFORMATIONS

Assigning chirality to mirror-image molecules is critical for a number of scientific disciplines, such as pharmacology and supramolecular chemistry. Vibrational circular dichroism (VCD) spectroscopy, combined with theoretical calculations, has been the preferred way in recent years to determine the chirality of various molecules, including nucleic acids and peptides. However, VCD, which detects differences in response to left and right circularly polarized infrared and near-infrared light, suffers from low sensitivity and is computationally demanding.

Tohru Taniguchi and Kenji Monde now have a novel take on VCD spectroscopy that makes it easier to determine the absolute chiral conformation of molecules (DOI: 10.1021/ja3001584). In their more general and sensitive method, the investigators track the interaction between two infrared chromophores on a molecule, which produces a special signal known as a vibrational circular dichroism couplet. This couplet is easy to detect, and its plus or minus sign indicates the absolute conformation of the molecule. Furthermore, the technique avoids theoretical calculations.

The investigators successfully applied their approach, which they call the VCD exciton chirality method, to a series of small chiral molecules that are typically hard to analyze, such as some types of natural products and drugs. They also demonstrated that the approach overcomes the sensitivity problem of conventional VCD spectroscopy by boosting the signals. **Rajendrani Mukhopadhyay, Ph.D.**

MD SIMULATIONS ON UNFOLDED PROTEINS

Protein folding and unfolding are important biological events that have been very difficult to characterize in detail. The unfolded state, where the process of protein folding begins, has long been a research subject for experimentalists and theoreticians in structural biology. Kresten Lindorff-Larsen, David E. Shaw, and co-workers have presented the use of molecular dynamics (MD) simulations as a tool for providing atomic-level insight into the structure and dynamics of an unfolded protein (DOI: 10.1021/ja209931w).

MD simulations, which track the motions of every atom in a larger molecule, are one of the principal tools for modeling larger biomolecules. Its application to unfolded proteins is limited by the enormous number of conformations associated. The researchers conducted simulations of the unfolded protein on a special supercomputer named Anton, which is 100 times faster than other current supercomputers. The results not only captured the local and global structural properties of the unfolded protein, which are in good agreement with NMR experimental data, but also supported the formation of contacts between amino acids residues that have been observed experimentally.

Their findings demonstrated the usefulness of MD simulation in the study of the unfolded protein, which is essential to understanding the mechanism by which a protein folds into its active state. **Lingling Chen, Ph.D.**

ENZYME AFFIXED TO CDS NANORODS MAKES HYDROGEN FUEL

Solar energy has been used experimentally to produce hydrogen gas since the 1940s, but the efficiency of light-based H_2 production methods is still not adequate for their widespread use as a fuel source for cars. To more effectively make hydrogen fuels, several laboratories are developing systems that mimic photosynthesis, sometimes by using semiconductor nanoparticles coupled to other materials.

Gordana Dukovic, Paul W. King, and their colleagues built a hydrogen-producing system by affixing an enzyme from *Clostridium acetobutylicum* onto cadmium sulfide nanorods (DOI: 10.1021/ja2116348). When the nanorods absorb light, they generate electrons that are taken up by the enzyme. The enzyme then reduces protons to create hydrogen gas. The team determined the optimal light levels, sacrificial donor concentrations, and ratio of nanorods to enzyme molecules.

During their best experiments, the photoconversion efficiencies reached 20%, and the nanomaterials were able to produce hydrogen for 6 hours with a turnover number of 1 million. Further kinetic studies showed that the main bottleneck in their system is the absorption of light by the nanorods. As efficiencies are improved and long-term stability issues are resolved, the full potential of photochemical solar energy conversion systems from enzyme-modified nanocrystals may be realized. **Aaron Rowe, Ph.D.**

Published: March 21, 2012

dx.doi.org/10.1021/ja302470c | *J. Am. Chem. Soc.* 2012, 134, 5005−5005