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Spotlights on Recent *JACS* Publications

UNRAVELING HETEROGENEOUS ZEOLITE CATALYSIS AT THE SINGLE MOLECULE LEVEL

Zeolites are microporous crystalline solids with cavities and channels of roughly the same size as small molecules. The unique combination of acidic and shape-selective properties has made zeolites a very important group of catalysts for industrial applications. The design of better-performing zeolites depends on further understanding of the single zeolite particle reactivity, which is inaccessible by traditional spatially averaged techniques. Maarten B. J. Roeffaers, Bert M. Weckhuysen, and colleagues apply super-resolution fluorescence microscopy, which has revolutionized biological research, to the study of heterogeneous catalysis by zeolites at the single molecule level (DOI: 10.1021/jacs.5b01698).

In this work, the researchers use a fluorogenic probe reaction, acid-catalyzed oligomerization of furfuryl alcohol, to observe individual catalytic turnovers with high spatiotemporal resolution. By capturing 3D images in the pores of zeolite single crystals, they obtain a wealth of new information on the impact of steaming at the molecular-level. The results show that mild steaming at 500 °C enhances reactant accessibility to catalytic sites, while severe steaming at 700 °C leads to significant loss of Brønsted acidity. The work demonstrates the power of single catalytic particle study in unraveling complex reactivity in zeolite-based catalyst materials.

Hui Jin, Ph.D.

WATCHING CANCER WORK WITH CARBON MRI

For most of human history, a knife has been required to peer beneath the skin. Now, magnetic resonance imaging (MRI) can create maps of internal anatomy using hydrogen atoms in water. However, these MRI pictures tend to be static and lack molecular detail. Lacing metabolites with MRI-active carbon-13 offers an opportunity to track individual molecules as they morph into different metabolites with each enzyme they encounter. *In vivo* ^{13}C imaging may provide new insights into tissue metabolism, including the processes underlying cancer.

The problem is that the signal from a small number of metabolites is not strong enough to light up a typical magnetic resonance image. In this Perspective, Kevin M. Brindle describes recent advances in dynamic nuclear spin polarization that increase signal strength from ^{13}C by orders of magnitude (DOI: 10.1021/jacs.5b03300). The polarization lasts at most a few minutes, yet the approach may still allow researchers to gain valuable clinical insight. In a clinical trial, researchers have detected the presence of prostate cancer, which showed increased conversion of ^{13}C-labeled pyruvate into lactate. This strategy may someday help doctors select the most effective anticancer therapy for a particular patient. The Perspective goes on to highlight multiple avenues by which imaging metabolism could revolutionize modern medicine.

Erika Gebel Berg, Ph.D.

INTERFACIAL ELECTROSTATIC FORCES COULD INFLUENCE ORGANIC PHOTOVOLTAIC DESIGN

The efficiency of an organic solar cell is related to how an electron−hole pair generated at the interface of donor and acceptor materials splits into individual charges. Here, Carl Poelking and Denis Andrienko have used computer simulations to identify electrostatic forces that can assist charge separation at the donor−acceptor interface (DOI: 10.1021/jacs.5b02130).

The researchers evaluate the electrostatic forces for several interfaces in a fullerene−based solar cell. They find that the long-range Coulomb interactions can provide electrostatic forces that drive the separation of electrons and holes. The strength of these forces depends on molecular orientation and degree of donor-acceptor mixing at the interface.

This relationship among electrostatic forces, molecular ordering, and nanoscale roughness provides clear rules for materials selection and processing that can be used to improve organic solar cell performance.

Melissae Fellet, Ph.D.

ADJUSTMENTS IN THE JUXTAMEMBRANE SEGMENT

Alanna Schepartz and co-workers uncover an unexpected structural difference between the naturally occurring form of the cell signaling molecule epidermal growth factor receptor (EGFR) and a mutated and drug-resistant variant, findings that could guide drug discovery efforts in non-small-cell lung cancer (DOI: 10.1021/jacs.5b02326). Surprisingly, the structural change occurs not in the active site of the protein but in the juxtamembrane segment, which links the extracellular and intracellular portions of the receptor.

The authors employ a method called bipartite tetracysteine display to interrogate the structure of the juxtamembrane segment of EGFR variants associated with drug resistance. They find that the structure is influenced by mutations in the active site of the protein as well as by binding interactions outside the cell, and these structural changes directly affect receptor activity. Essentially, the juxtamembrane segment, which can adopt two different helical conformations, acts as a mediator of signals on both sides of the cell membrane.

Understanding how structure in the juxtamembrane segment influences drug resistance is integral to the development of novel drugs that can circumvent resistance and prevent cancer cell growth when other treatments fail and offers valuable new insight that could be applied to evade drug resistance mechanisms in cell surface receptors.

Eva J. Gordon, Ph.D.

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