

Change Is the Only Constant: A Virtual Issue on Contemporary Catalysis

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Change Is the Only Constant: A Virtual Issue on Contemporary Catalysis

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Catalysts are now critical in all areas of chemistry, from
biochemistry to synthesis to energy to biomedical
devices. It is perhans not surprising then that the ACS Au devices. It is perhaps not surprising then that the ACS Au community journals have published a wealth of exciting content in the area of catalysis. From among these publications, we have chosen to highlight a few examples in this virtual issue to demonstrate the excellence and diversity of these contributions and the field, as representations of catalysis in the early 2020s.

Heterogeneous catalysis has been critical in improving modern life and environmental technologies, from the Haber− Bosch process, to the catalytic converter for cars, to upgrading chemicals. For example, 5-hydroxymethylfurfural (HMF) and levulinic acids can be upgraded to HMF levulinate for biorefining ([10.1021/acsorginorgau.2c00027\)](https://pubs.acs.org/doi/full/10.1021/acsorginorgau.2c00027). Recent efforts have focused on designing catalysts to increase product selectivity and sustainability ([10.1021/acsnanoscien](https://pubs.acs.org/doi/10.1021/acsnanoscienceau.2c00057)[ceau.2c00057](https://pubs.acs.org/doi/10.1021/acsnanoscienceau.2c00057)). There is a wealth of work on the conversion of carbon dioxide into fuels and value-added products, e.g., cyclic carbonate [\(10.1021/acsmaterialsau.1c00012\)](https://pubs.acs.org/doi/full/10.1021/acsmaterialsau.1c00012), and the abatement of other greenhouse gases like methane [\(10.1021/](https://pubs.acs.org/doi/10.1021/acsenvironau.1c00034) [acsenvironau.1c00034\)](https://pubs.acs.org/doi/10.1021/acsenvironau.1c00034). Researchers are also studying the development of heterogeneous catalysts for renewable fuel production, e.g., jet fuel via hydrodeoxygenation [\(10.1021/](https://pubs.acs.org/doi/full/10.1021/acsengineeringau.2c00015) [acsengineeringau.2c00015\)](https://pubs.acs.org/doi/full/10.1021/acsengineeringau.2c00015). Challenges in managing omnipresent polymer waste have motivated research on nextgeneration heterogeneous catalysts for chemical recycling of, e.g., PET ([10.1021/acsengineeringau.2c00029\)](https://pubs.acs.org/doi/full/10.1021/acsengineeringau.2c00029). Recently, zeolite and zeolite-supported catalysts have become popular for applications such as diesel oxidation [\(10.1021/acsengineer](https://pubs.acs.org/doi/full/10.1021/acsengineeringau.1c00016)[ingau.1c00016\)](https://pubs.acs.org/doi/full/10.1021/acsengineeringau.1c00016) and ethene dimerization ([10.1021/acsengi](https://pubs.acs.org/doi/10.1021/acsengineeringau.1c00014)[neeringau.1c00014](https://pubs.acs.org/doi/10.1021/acsengineeringau.1c00014)). It is important to note that although many of these new catalysts are focused on moving the chemical and fuel industry toward better sustainability, there is also a wealth of effort in making the catalysts themselves more sustainable by moving to catalysts made from earth abundant elements instead of precious metals.

Homogeneous catalysts are integral to the chemical, polymer, and pharmaceutical industries. These catalysts are used to both increase reaction rates and improve selectivity. In the polymer field, researchers have designed organometallic catalysts for making hyperbranched ethylene oligomers and ethylene/methyl acrylate co-oligomers ([10.1021/acspolymer](https://pubs.acs.org/doi/10.1021/acspolymersau.1c00039)[sau.1c00039](https://pubs.acs.org/doi/10.1021/acspolymersau.1c00039)) and have studied borate cocatalysts for ethylene copolymerization [\(10.1021/acsorginorgau.2c00020\)](https://pubs.acs.org/doi/10.1021/acsorginorgau.2c00020). In the pharmaceutical area, researchers have been interested in biscyclometalated chiral-at-iridium/rhodium complexes for asymmetric catalysis in organic synthesis ([10.1021/acsorginor](https://pubs.acs.org/doi/full/10.1021/acsorginorgau.1c00032)[gau.1c00032](https://pubs.acs.org/doi/full/10.1021/acsorginorgau.1c00032)). Researchers have also been studying trinuclear complexes enabling more efficient C−C bond-forming transformations [\(10.1021/acsorginorgau.2c00029](https://pubs.acs.org/doi/10.1021/acsorginorgau.2c00029)). Recently, organocatalysts have also become popular, including the use of diphenylprolinol silyl ether for catalyzing the asymmetric Michael reaction [\(10.1021/acsorginorgau.1c00054\)](https://pubs.acs.org/doi/10.1021/acsorginorgau.1c00054). Depending on the application, some of these homogeneous catalysts are utilized "as-is" in industry, but there has also been considerable effort in the past decade at "heterogenizing" molecular catalysts.

Electrocatalysts can be heterogeneous, homogeneous, or biological, but recently have been widely studied for energy conversion and electrosynthesis. For decades, there have been efforts to improve catalysts for fuel cell and electrolyzer processes (i.e., hydrogen oxidation, oxygen reduction, hydrogen evolution, and oxygen evolution) with an effort to minimize the use of precious metals through the transition from precious metal blacks, to precious metal nanoparticles supported on nonprecious metal supports, to core−shell nanoparticles. In recent years, this focus on lowering the precious metal content has expanded to attempting to eliminate the precious metals, such as the development of manganese oxide films for the oxygen evolution reaction ([10.1021/acsnanoscienceau/3c00002\)](https://pubs.acs.org/doi/10.1021/acsnanoscienceau.3c00002). Also, a recent large effort in the field of electrocatalysis has been in developing stable and sustainable electrocatalysts for challenging transformations. For instance, researchers have developed metal chalcogenide materials for carbon dioxide reduction to fuels and nitrogen reduction to ammonia [\(10.1021/acsmaterial](https://pubs.acs.org/doi/10.1021/acsmaterialsau.1c00006)[sau.1c00006](https://pubs.acs.org/doi/10.1021/acsmaterialsau.1c00006)). Although metal nanoparticles are still the most popular electrocatalysts, there have been renewed efforts to develop stable and highly active single-atom electrocatalysts ([10.1021/acsmaterialsau.1c00041\)](https://pubs.acs.org/doi/10.1021/acsmaterialsau.1c00041), while others are focusing on intermetallic nanoarchitectures ([10.1021/acsnanoscien](https://pubs.acs.org/doi/10.1021/acsnanoscienceau.2c00045)[ceau.2c00045](https://pubs.acs.org/doi/10.1021/acsnanoscienceau.2c00045)). Some of these electrocatalysts have also been utilized for organic electrosynthesis, e.g., the reduction of substituted nitrobenzenes to anilines using polyoxometallate mediation ([10.1021/acsorginorgau.2c00047\)](https://pubs.acs.org/doi/10.1021/acsorginorgau.2c00047), and for biosen-

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sors for neurotransmitters ([10.1021/acsnanoscien](https://pubs.acs.org/doi/10.1021/acsnanoscienceau.2c00039)[ceau.2c00039](https://pubs.acs.org/doi/10.1021/acsnanoscienceau.2c00039)). Molecular electrocatalysts have also become very popular for reactions from hydrogen evolution [\(10.1021/](https://pubs.acs.org/doi/10.1021/acsorginorgau.1c00011) [acsorginorgau.1c00011](https://pubs.acs.org/doi/10.1021/acsorginorgau.1c00011)) to cross-coupling reactions.

Similarly to electrocatalysts, photocatalysts can be heterogeneous, homogeneous, or biological and there has been a lot of effort in water splitting, but recent efforts in photocatalysis have similarly focused on the photosynthesis of fuels and other value-added products, including the polymerization of polymers [\(10.1021/acspolymersau.1c00014\)](https://pubs.acs.org/doi/10.1021/acspolymersau.1c00014). The design and synthesis of heterogeneous photocatalysts have been popular, including $Cu₃NBS₄$ and $Cu₃NbSe₄$ sulvanite nanomaterials $(10.1021/acsnanoscienceau.2c00021)$ $(10.1021/acsnanoscienceau.2c00021)$ $(10.1021/acsnanoscienceau.2c00021)$, MoS₂ quantum dots as simultaneous catalysts and photosensitizers ([10.1021/acsorgi](https://pubs.acs.org/doi/10.1021/acsorginorgau.1c00040)[norgau.1c00040\)](https://pubs.acs.org/doi/10.1021/acsorginorgau.1c00040), $WO₃$ photoanodes $(10.1021/ac sphysche$ [mau.1c00004](https://pubs.acs.org/doi/10.1021/acsphyschemau.1c00004)), CdS/BiVO4 hybrid catalysts ([10.1021/ac](https://pubs.acs.org/doi/10.1021/acsphyschemau.1c00053)[sphyschemau.1c00053\)](https://pubs.acs.org/doi/10.1021/acsphyschemau.1c00053), graphene oxide hybrid photocatalytic materials [\(10.1021/acsmaterialsau.1c00022\)](https://pubs.acs.org/doi/10.1021/acsmaterialsau.1c00022), and sonophotocatalysts for wastewater treatment ([10.1021/acsnanoscien](https://pubs.acs.org/doi/10.1021/acsnanoscienceau.2c00058)[ceau.2c00058](https://pubs.acs.org/doi/10.1021/acsnanoscienceau.2c00058)). That said, homogeneous photocatalysts and photoredox catalysts have also gained popularity. For instance, porphyrins have been shown as photocatalysts for functionalizing biomolecules [\(10.1021/acsorginorgau.2c00025](https://pubs.acs.org/doi/full/10.1021/acsorginorgau.2c00025)). Iridium and noniridium catalysts have been developed for photoredox catalysis, including polyaza[7]helicenes as an alternative to iridium ([10.1021/acsorginorgau.2c00022](https://pubs.acs.org/doi/full/10.1021/acsorginorgau.2c00022)), and a cobalt-based polyoxometalate for oxygen evolving photocatalysis, with a concomitant push for sustainable iridium photoredox catalysts ([10.1021/acsorginorgau.2c00024](https://pubs.acs.org/doi/10.1021/acsorginorgau.2c00024)).

Enzymes and other biocatalysts have made significant advances in the past decade, both in techniques to engineer their properties, such as enzyme engineering and synthetic biology, and in next-generation characterization tools. *ACS Bio & Med Chem Au* published an exciting virtual [special](https://pubs.acs.org/page/abmcb8/vi/Radical-SAM?ref=vi_journalhome) issue in 2022 Celebrating 20 Years of Radical *S*-Adenosyl-L-methionine (SAM) Enzymology, including a contribution on using new crystal structures to understand and develop new functions ([10.1021/acsbiomedchemau.1c00051](https://pubs.acs.org/doi/full/10.1021/acsbiomedchemau.1c00051)) and another discussing the challenging tetrapyrrole substrates for radical SAM enzymes ([10.1021/acsbiomedchemau.1c00061](https://pubs.acs.org/doi/full/10.1021/acsbiomedchemau.1c00061)). This new virtual issue on contemporary catalysis discusses both the use of enzymes for synthesizing value-added products, and the breakdown or remediation of molecules and materials, including degrading polymeric micelles ([10.1021/acspolymer](https://pubs.acs.org/doi/10.1021/acspolymersau.2c00023)[sau.2c00023](https://pubs.acs.org/doi/10.1021/acspolymersau.2c00023)) and the biodegradation of organic contaminants ([10.1021/acsenvironau.2c00023\)](https://pubs.acs.org/doi/10.1021/acsenvironau.2c00023). Whole living organisms as biocatalysts (and, in this case, bioelectrocatalysts) have also been of recent interest because they are living organisms that can grow, reproduce, and continually regenerate their catalytic enzymes, including in applications for hydrogen production ([10.1021/acsenvironau.1c00021\)](https://pubs.acs.org/doi/10.1021/acsenvironau.1c00021). Finally, there has been a renewed focus on biohybrids combining biocatalysts with other catalytic materials (photocatalysts, electrocatalysts, etc.), including recent work combining PtSn nanoparticles with oxidoreductase enzymes for ethylene glycol fuel oxidation in a fuel cell [\(10.1021/acsmaterialsau.1c00029](https://pubs.acs.org/doi/full/10.1021/acsmaterialsau.1c00029)). Enzymes and microbes have also been used as bio(photo)electrocatalysts for a variety of applications, from measurement science, to conversion, to water remediation [\(10.1021/acsmeasures](https://pubs.acs.org/doi/10.1021/acsmeasuresciau.2c00042)[ciau.2c00042](https://pubs.acs.org/doi/10.1021/acsmeasuresciau.2c00042)).

Computational efforts in this field have been extensive in recent years for screening, including parametrization of homogeneous catalysts for organic synthesis ([10.1021/](https://pubs.acs.org/doi/full/10.1021/acsorginorgau.2c00050)

[acsorginorgau.2c00050](https://pubs.acs.org/doi/full/10.1021/acsorginorgau.2c00050)) and computational studies of alloy catalysts for nitrogen reduction ([10.1021/acsphysche](https://pubs.acs.org/doi/full/10.1021/acsphyschemau.1c00021)[mau.1c00021\)](https://pubs.acs.org/doi/full/10.1021/acsphyschemau.1c00021). Computational design and prediction are also popular, ranging from density functional theory calculations to molecular mechanics, with an ever-increasing focus on machine learning and artificial intelligence, e.g., to understand enzyme mechanisms ([10.1021/acsphyschemau.2c00005\)](https://pubs.acs.org/doi/full/10.1021/acsphyschemau.2c00005).

Recent efforts have also focused on developing new analytical tools for studying catalysis. These are frequently focused on in situ versus ex situ analysis, as well as trying to study heterogeneous catalysts and intermediates in more detail. This includes efforts to study the heterogeneity of electrocatalysts in situ using scanning electrochemical cell microscopy ([10.1021/acsmeasuresciau.2c00012\)](https://pubs.acs.org/doi/full/10.1021/acsmeasuresciau.2c00012), as well as in situ techniques for studying photocatalyst stability ([10.1021/](https://pubs.acs.org/doi/10.1021/acsmeasuresciau.1c00016) [acsmeasuresciau.1c00016](https://pubs.acs.org/doi/10.1021/acsmeasuresciau.1c00016)).

This virtual issue highlights the diversity of the field, covering just a subsection of the plethora of catalysts and their applications. But, more importantly, it highlights the need for better and more stable catalysts in all areas of sustainable chemistry, including (but not limited to) pharmaceutical synthesis, depolymerization, remediation, energy conversion, and biomedical applications. The *ACS Au* journals look forward to welcoming contributions in catalysis in the near future and being a part of new advances that emerge in the field in the coming decade.

Shelley [Minteer](https://pubs.acs.org/action/doSearch?field1=Contrib&text1="Shelley+Minteer"&field2=AllField&text2=&publication=&accessType=allContent&Earliest=&ref=pdf) @ orcid.org/0000-0002-5788-2249 [Stephanie](https://pubs.acs.org/action/doSearch?field1=Contrib&text1="Stephanie+L.+Brock"&field2=AllField&text2=&publication=&accessType=allContent&Earliest=&ref=pdf) L. Brock · orcid.org/0000-0002-0439-302X Géraldine [Masson](https://pubs.acs.org/action/doSearch?field1=Contrib&text1="Ge%CC%81raldine+Masson"&field2=AllField&text2=&publication=&accessType=allContent&Earliest=&ref=pdf) @orcid.org/0000-0003-2333-7047 [Raymond](https://pubs.acs.org/action/doSearch?field1=Contrib&text1="Raymond+E.+Schaak"&field2=AllField&text2=&publication=&accessType=allContent&Earliest=&ref=pdf) E. Schaak o orcid.org/0000-0002-7468-8181

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Notes

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