ACS Catalysis

Editorial

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Virtual Issue on Catalysis in Singapore

The chemical and pharmaceutical industries are major manufacturing sectors in Singapore and contribute greatly to the economy. Even though the economy is well developed, there is still a commitment to maintain a strong manufacturing base at around 20% of GDP. Together, chemicals and pharmaceuticals account for over 40% of manufacturing volume and almost 30% of the manufacturing contribution to the GDP. It is well recognized that innovation is key to future growth and sustainability in the industry, and catalysis is at the heart of innovation in manufacturing chemicals and pharmaceuticals. It is therefore no surprise that a vibrant catalysis research and development community exists in Singapore across several Agency for Science, Technology and Research (A*STAR) research institutes, universities, and research centers. Research areas of particular interest are the use of homogeneous, heterogeneous, and enzyme catalysts to convert lignocellulosic biomass to high-value chemicals and materials; developing nanocrystalline and nanoporous materials as heterogeneous catalysts; nanocomposites for energy storage and conversion; catalysts for metal air batteries; and novel catalysts and processes for more sustainable manufacture of pharmaceuticals and fine chemicals. These programs are supported by advanced chemometrics and analytical techniques and in situ reaction studies using synchrotron radiation.

The 3 reviews, 5 letters and 12 articles in this virtual special issue present a snapshot of the breadth and scope of this activity. The collection presents a broad spectrum of research, from new analytical techniques to new routes to novel materials, new materials as catalysts and catalyst supports, novel energy storage materials, enzyme catalysis, and computational catalysis.

The three reviews cover hydroboration, metal−organic frameworks with new catalytic functionality, and oxygen reduction reactions. The hydroboration review by Che and Kinjo illustrates recent advances in understanding the mechanism of transition and main group metal catalysts in making organoborane compounds. Zhang and Ying review the remarkable progress made over recent years in the development of main chain metal organic frameworks with unique properties as highly active and recyclable heterogeneous catalysts. Oxygen reduction reactions and catalysts are reviewed by Ge et al., with a particular focus on their use in zinc−air batteries and fuel cells in energy storage systems.

Three of the letters cover various aspects of reactions to generate complex organic compounds. Yang et al. present a study of the use of a cobalt catalyst, a diphosphine ligand and zinc for the intermolecular hydroacylation of olefins; Sim et al. describe the enantioselective hydroxylation of ketones using molecular oxygen and a phase transfer catalyst; and Dang et al. present the ruthenium-catalyzed methylation of amines. The other two letters are enzyme-focused. Xu et al. describe a computational study of aromatase-catalyzed estrogen formation, and Vahadi et al. present a simple method for the direct immobilization of an extracellular enzyme for the conversion of waste grease to biodiesel.

The 12 full articles cover a broad range of topics. Five are related to electrochemistry; Wang et al. show how palladium nanoparticles supported on a carbon support containing N atoms can give high selectivity in the electro-oxidation of glycerol; Ren et al. present the use of a copper oxide film for the electrochemical reduction of CO_2 to ethanol and ethylene; Zhao et al. also study copper oxide, but as a low-cost alternative to platinum in the electrolysis of water to produce hydrogen; Tan et al. also present hydrogen production by electrolysis, but using platinum nanoparticles; and Dutta et al. describe the use of a nickel−gold−platinum-on-graphene oxide catalyst for the oxidation of ethanol.

Three of the full articles relate to synthetic biology and enzyme systems. Go et al. describe how they have developed synthetic antimicrobial polyketides by combining multiple enzymes to produce a library of potential candidates. Ribiero et al. report a study of enzyme-catalyzed nitrile reductions using computational techniques to broaden the range of useable substrates, and Chuanprasit et al. use DFT-based computational techniques to suggest improvements to the performance of cytochrome P450 enzymes in oxidative biotransformations.

Continuing the theme of computational techniques, Roesch et al. describe the use of DFT-based computational methods to explain the action of transition metal complexes with redox-active ligands applied to alcohol oxidation.

Two articles report the use of catalysis in complex organic synthesis. Duan et al. use a heterogeneous catalyst formed by palladium supported on modified mesoporous silica to achieve high selectivity in oxidative Heck reactions, and Xie and Huynh use a ruthenium-*N*-heterocycle carbene catalyst to "tune" the selectivity of dehydrogenative amidations.

The remaining full article is by Xu et al. It describes mathematical approaches to elucidating reaction mechanisms from spectroscopic data with no a priori knowledge of the chemistry.

We hope the readership of *ACS Catalysis* will enjoy this Virtual Special Issue on Catalysis in Singapore (http://pubs.acs.org/page/accacs/vi/singapore). These contributions illustrate the breadth and depth of catalysis research in Singapore. There is a dynamic, highly active catalysis community covering a wide range of research interests and capabilities, and we look forward to even greater contributions in the future.

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