

*Editorial*

## Feature Papers to Celebrate the Landmarks of *Catalysts*

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Catalysis is a critical scientific field that underpins much of the world's chemical industry. For example, it is often quoted that catalysis plays a role in 90% of all industrial chemical products. This importance has led to numerous academic journals and specialized conferences on the subject, as practitioners seek outlets to publish their cutting-edge research on catalysis.

*Catalysts* started in 2011 with the goal of providing an open-source outlet for outstanding research on catalysis. In its first few years, *Catalysts* has enlisted the help of an active editorial board and hard-working guest editors to establish itself as a high-quality forum for catalysis papers. A primary focus has been to get *Catalysts* included in the major citation indices in order to provide its authors with the visibility and impact they desire. Recently, that goal was achieved, as *Catalysts* was selected for inclusion in Scopus and Science Citation Index Expanded (SCIE). In addition, *Catalysts* received its first impact factor in 2015. These are major milestones for the journal, and are worthy of celebration.

This issue is being published in recognition of these achievements. It is an opportunity to celebrate *Catalysts*' beginnings, and a way to look forward to its future. Nineteen articles from pre-eminent scholars in catalysis have been compiled in this special issue, representing a wide range of topics. This diversity is representative of the field of catalysis in general, as it touches so many areas of scholarship. In this special issue, you can find articles on catalyst synthesis [1–4], modeling of reaction kinetics on catalysts [5], polymerization [6], photocatalysts [7,8], oxidation catalysis [9], biomass conversion [10–14], electrochemistry [15], fuel cell catalysis [16], computational catalysis [17,18], and hydrogen production [19].

Highlights include:

1. Budhi and coworkers describe the synthesis of a unique material, titanium dioxide nanoclusters dispersed on cubic MCM-48, via a room temperature synthesis method [1]. They report that their procedure leads to highly dispersed TiO<sub>2</sub> particles with Ti<sup>4+</sup> ions mostly substituted in framework tetrahedral positions. The materials they synthesized were found to give 100% selectivity to

cyclohexene oxide in cyclohexane oxidation at room temperature with tert-butylhydroperoxide as the oxidant.

2. Shuh and coworkers used a mild hydrothermal synthesis procedure to synthesize bismuth molybdate catalysts for the selective oxidation of propylene [2]. Notably, they found that the pH used during synthesis impacted the catalytic performance of the material. A pH of 9 led to a less active catalyst than pH values of 6 or 7. The catalyst performance of the bismuth molybdate catalysts was closely linked with the bismuth molybdate phases present and the catalyst surface area, variables that were impacted by the synthesis procedure.
3. Brunner and coworkers prepared iron Fischer-Tropsch catalysts by using solvent-deficient precipitation, focusing on the impacts of different catalyst preparation steps [3]. They found that the key steps in catalyst synthesis were whether the precursor catalyst was washed, how the promoter was added, and the drying condition. The most active Fischer-Tropsch catalysts were produced from an unwashed catalyst via a one-step method with the drying step at 100 °C.
4. Soykal and coworkers publish a unique study where they evaluate whether the microgravity environment on the International Space Station impacted the physical and chemical properties of cerium oxide synthesized by a controlled-precipitation method [4]. They found that in microgravity the solutions do not sediment and movement of the free particles is significantly easier. Microgravity changed the crystallization behavior where oriented aggregation of particles had a more pronounced effect. The samples prepared in space were generally larger with lower surface area and a broader pore size distribution when compared to the control samples synthesized on Earth. The samples prepared in space had lower surface area, lower pore volume, and a broader pore size distribution in the range from 30–600 Angstroms when compared to the control sample synthesized on Earth. To best of our knowledge this is the first ceria synthesis study conducted in space which demonstrates the effect of microgravity, as well as showing that ceria nanorods can be prepared at ambient temperature and pressure.
5. Delgado and coworkers report on their work to develop a microkinetic model to describe the catalytic conversion of methane on nickel catalysts in oxidative and reforming conditions [5]. A 52 elementary-step surface reaction mechanism is described that includes reactions of 14 surface and six gas-phase species. This model is evaluated by comparison to experimental data obtained over nickel catalysts for various reaction conditions, and is used to predict the performance of a fixed bed reactor.
6. Haque and Nomura review the recent work to develop an acyclic diene metathesis polymerization process that allows the synthesis of defect-free conjugated polymers with well-defined chain ends [6]. One of the most exciting implications of this work is that the polymer that results from this process can further be functionalized to produce materials suitable for use as organic electronics. For instance, the authors demonstrate that the polymer can be treated by molybdenum-alkylidene complexes followed by addition of various aldehydes. Their results suggest that this polymerization method is attractive for synthesizing star conjugated polymers.
7. Chan and coworkers contribute to the state-of-the-art knowledge on photocatalytic processes by using NIR-Raman spectroscopy to monitor the photocatalytic epoxidation of cyclohexene over V-Ti/MCM-41 catalysts [7]. Using the *in situ* Raman spectroscopy to monitor characteristic bands, the authors were able to show, for the first time, that cyclohexene was directly

photo-epoxidized to 1,2-epoxycyclohexane by t-BuOOH. They also found that both Ti and V were active in photo-epoxidation, and suggested that the two metals could work in concert to give enhanced reaction efficiency.

8. Borges and coworkers investigated photocatalysis for the removal of emerging contaminants from wastewater effluent [8]. The authors studied the reaction of paracetamol as a model contaminant model in both a stirred photoreactor and a packed bed photoreactor with a TiO<sub>2</sub> photocatalyst. The authors demonstrated high photocatalytic activities and suggested that a packed bed reactor system is an effective method for removing emerging pollutants.
9. Jing and coworkers describe how supported (NH<sub>4</sub>)<sub>3</sub>HPMo<sub>0.11</sub>VO<sub>40</sub> catalysts change over time during the selective oxidation of isobutane by using a variety of characterization techniques [9]. Notably, they found that the thermal stability and reducibility of the Keggin units were enhanced by supporting 40% of the active phase on Cs<sub>3</sub>PMO<sub>12</sub>O<sub>40</sub>. They described the molecular processes responsible for structural changes in these catalysts. For example, the authors describe the decomposition of ammonium cations that lead to formation of vacancies that can favor cationic exchanges between vanadium from the active phase and cesium from the support.
10. Santillan-Jimenez and coworkers investigated molybdenum carbide supported on different carbon supports (activated carbon, carbon nanofiber, and carbon nanotubes) for the hydrodeoxygenation of guaiacol [10]. The authors found that all three catalysts produced catechol and phenol as the main products in hydrodeoxygenation of guaiacol, suggesting that guaiacol was converted to phenol by sequential demethylation and hydrodeoxygenation. They showed that use of carbon nanofibers as the support was generally superior for selective production of phenol.
11. Choi and coworkers investigated molybdenum carbides for low-temperature hydroprocessing of acetic acid [11]. In particular, the authors investigated the structural changes in the molybdenum carbides that result from exposure to hot aqueous environments. They found that bulk Mo carbides are maintained during aging in hot liquid water, but that some of the carbidic Mo sites were converted to oxide sites. Furthermore, they demonstrate that significant structural changes result from these reaction conditions, with changes in surface area and pore volume.
12. Guo and coworkers review the state-of-the-art in the use of B-site metal promoted La<sub>1-x</sub>Sr<sub>x</sub>Co<sub>1-y</sub>Fe<sub>y</sub>O<sub>3-σ</sub> perovskite oxides as cathodes for solid oxide fuel cells [16]. This review describes the impact of promoting perovskite oxides with Pd, Pt, Ag, Cu, Zn, and Ni, focusing on different synthetic methods and the effects of metal promotion on cathodic performance. A major contribution of the article is a discussion of the combined effects of the oxygen dissociation rate and the interfacial oxygen transfer rate between the metal and cathode phases.
13. Gurukcu, de Bruin, and Reek use computational methods to explore the mechanism of the allylic amination reaction between allyl alcohols and amines on a phosphoramidite palladium/1,3-diethylurea co-catalyst system [17]. This contribution uses DFT calculations to suggest that hydrogen bonding between the urea moiety and the hydroxyl group of the alcohol is key to facilitate the C-O oxidative addition step, which is the rate-limiting step in the reaction mechanism.
14. Pastor-Perez and coworkers explore the performance of a carbon-supported Ni-CeO<sub>2</sub> catalyst with a conventional Ni/CeO<sub>2</sub> bulk catalyst in the water-gas shift reaction [19]. They find that the carbon-supported catalyst is more active than the bulk catalyst due to its oxygen storage capacity.

This study could lead to a new generation of Ni-ceria catalysts for hydrogen production via water–gas shift that have a reduced amount of ceria.

15. Alegre and coworkers contribute to the field of electrochemistry by studying the electro-oxidation of methanol on highly mesoporous carbon xerogel and Vulcan carbon black [15]. Their objective is to understand how the preparation procedure impacts catalytic performance. The authors show that the carbon xerogel gave higher catalytic activities towards CO and CH<sub>3</sub>OH oxidation than the Vulcan support, mainly because of the higher mesoporosity of the carbon xerogel that allowed more facile diffusion of reactants within the catalyst.
16. Chan-Thaw and coworkers investigate AuPd nanoparticles for the selective oxidation of raw glycerol [12]. The impact of the support is investigated, and the authors demonstrate that activated carbon and nitrogen-functionalized carbon nanofibers gave the best catalytic results. The authors also note that glycerol obtained from the transesterification of rapeseed oil led to strong deactivation, in contrast with the results when pure glycerol was used.
17. Fajin and coworkers describe the use of the generalized-gradient approximation of the density functional theory to explore multicomponent catalysts for Fischer-Tropsch synthesis [18]. The authors describe how this modeling technique allows them to separate the influence of different parameters in the global catalytic performance. A major conclusion of the article is that computational studies can now compete with modern experimental techniques because of the efficient computer codes that have been developed for use on powerful computers that allow realistic molecular systems to be simulated.
18. Vasiliadou and Lemonidou investigated the catalytic glycerol hydrodeoxygenation with ethanol as a hydrogen donor [13]. With this novel concept, the hydrogen necessary for hydrodeoxygenation is provided in the same reactor by ethanol reforming. The authors investigated Pt, Ni, and Cu catalysts, and found that Pt/Fe<sub>2</sub>O<sub>3</sub>-Al<sub>2</sub>O<sub>3</sub> gave high selectivity to 1,2-propanediol. They also showed that milder reaction conditions should be applied to maximize 1,2-propanediol yield.
19. Giang and coworkers investigated the catalytic valorization of Vietnamese rice straw [14]. They propose that aqueous phase reforming of steam exploded rice straw hydrolysate and condensate could be used to produce platform chemicals. The authors show that tungstated zirconia catalysts could convert glucose to 5-hydroxymethylfurfural (HMF). They suggest that Lewis acid and/or base sites on the support catalyze glucose dehydration to fructose, which can then be dehydrated to HMF over Brønsted acidic tungsten oxide clusters.

I think practitioners in catalysis will find this Special Issue highly relevant and interesting. I want to thank all of the authors for their contributions, and the editorial staff at *Catalysts*, particularly Mary Fan, Senior Assistant Editor for their efforts. I hope you enjoy this Special Issue to commemorate the landmarks that *Catalysts* has achieved.

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