ACS Catalysis

Editorial

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ACS Catalysis Appoints Takashi Ooi as Associate Editor and Posts Virtual Special Issue on Theory and Computation in Catalysis

As a comprehensive catalysis journal, *ACS Catalysis* has always sought to have a diverse editorial team that represents the global breadth of catalysis research. While the editorial advisory board comprehensively covers all areas of catalysis and includes organic, inorganic, and physical chemists as well as chemical engineers, the team of associate editors, because of its smaller size, has not been as broadly composed. Owing to the strength of submissions on the subject of catalytic methods in organic synthesis, the addition of an organic chemist to the editorial team is strongly warranted. To this end, we are pleased to announce the appointment of Prof. Takashi Ooi, of Nagoya University, as a new Associate Editor who will focus his efforts on catalysis in organic synthesis. Ooi will bring his broad experience in asymmetric catalysis and chemical synthesis to the editorial team, partnering with associate editor and inorganic chemist T. Brent Gunnoe to adjudicate the majority of the papers submitted in molecular catalysis. Prof. Ooi's addition to the journal also expands the geographic breadth of the editorial team, with associate editors representing China, Japan, France, Italy, and the United States.

In parallel with the appointment of Prof. Ooi, we are pleased to release a new virtual special issue (VSI) on "Theory and Computation in Catalysis" (http://pubs.acs.org/page/accacs/vi/theory-computation.html). Catalysis, whether it be molecular, bio, or heterogeneous, requires understanding of elementary steps at the molecular scale. In the past decade, computational catalysis has emerged as a key scientific field providing strong insights to experimentalists on the general concepts driving catalytic reactions and on design principles for novel or improved catalysts. In all of its domains, catalysis directs similar questions to the computational chemist: What is the nature of the active site? How can we better interpret the results of spectroscopic methods? What is the detailed reaction mechanism? What are the factors controlling the selectivity of the reaction? Can we understand or predict the reaction kinetics?

In computational catalysis, the frontiers among homogeneous, bio, and heterogeneous catalysis are very diffuse, and all domains rely on the basic bond-breaking and bond-forming processes of a precise ensemble of atoms. Of course, there are some specific challenges in each domain. The computational chemist in homogeneous catalysis gets headaches about solvent effects (although heterogeneous catalysis is not exempt from challenges associated with solvents). The expert in biocatalysis needs to treat the complex environment that the enzyme exerts on the active site, and the modeler in heterogeneous catalysis is bound to consider a solid surface or nanoparticle and to bridge the complexities of solid state chemistry and molecular reactivity. Beyond these few singularities of the domains, the common challenges are, however, more numerous for the modeler, with an overall goal of shedding light on reaction mechanisms and on kinetic behavior in catalysis.

Computational chemistry, hence, addresses all the topics of *ACS Catalysis*, provides unification principles and has become an indispensable tool for the catalytic scientist today. The VSI on "Theory and Computation in Catalysis" assembles 48 papers, with a distribution of 18, 7, and 23 on molecular, bio, and heterogeneous catalysis, respectively. We hope you find it an enjoyable collection of contributions.

Christopher W. Jones, Editor-in-Chief

Georgia Institute of Technology

Philippe Sautet, Associate Editor

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Notes

Views expressed in this editorial are those of the authors and not necessarily the views of the ACS.

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