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Defragmenting Catalysis

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Catalysis underlies numerous chemical technologies that benefit human life worldwide, and catalysis mediates a plethora of transformations essential to living organisms. Not surprisingly, major advances in catalytic science have been recognized by Nobel Prizes for over a century, with four catalysis-related Chemistry Nobel Prizes in just the past eleven years. Nevertheless, and curiously, catalysis today is not recognized as a coherent scientific discipline. Thus, catalysis taught to life-sciences students is far different in focus and content from that taught to chemistry and chemical-engineering students. Furthermore, the recent Nobel Laureates in catalysis are frequently referred to as "synthetic chemists". Many of the catalysis papers in *Angewandte Chemie* are likewise classified as "synthesis" papers. Of course, one may argue that, because catalysis is almost as disciplinarily broad as chemistry, biochemistry, chemical engineering, and materials science together, it is most efficient to think about it within the tractable domains of homogeneous and heterogeneous catalysis (or more specifically bio-, organo-, metal, electro-, photo-, and surface catalysis). Herein we argue the opposite: catalysis is a coherent field that would greatly benefit from better communication among researchers.

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The unfortunate compartmentalization of catalytic science has historical roots, reflecting the great technological importance of surface catalysis, the fact that organometallic chemistry is at the core of much solution catalysis, and the importance of organocatalysis in laboratory synthesis. It also reflects differences in language, educational background, and policies of agencies that fund only specific research areas. This compartmentalization is particularly manifest in large scientific meetings. At the 2012 American Chemical Society meeting in San Diego, the Presidential Symposium focusing on catalysis was inadvertently scheduled in conflict with that honoring the winner of the ACS Somorjai Award for Creative Research in Catalysis. The former was aimed at a broad audience, while the latter dealt with surface catalysis, making it difficult for attendees interested in catalysis broadly to benefit from both symposia. At the International Congress on Catalysis in Munich in July 2012, almost all the 2200 attendees attended the plenary lectures (dominated by surface catalysis), but in the specialized symposia the attendees self-segregated. General chemistry journals such as *Angewandte Chemie* publish a broad swath of catalysis-related papers but we suspect that most of the reviewers come from the respective subfields. The well-established specialized catalysis journals are niche journals, but because authors go where they will be read, the editors struggle to expand their scope beyond their traditional subfields. New catalysis journals such as *ChemCatChem*, soon followed by *ACS Catalysis* and *Catalysis Science & Technology*, are bucking the trend; we applaud these innovations and will wait to see how they affect the catalysis literature as a whole.

We are also encouraged by continuing attempts by various catalysis organizations to bring scientists from the subfields together. Biocatalysis and surface catalysis have much in common, but researchers in these subfields have rarely communicated or collaborated—until recent activities addressing the prospects for large-scale catalytic applications in biomass conversion. Although biocatalysis specialists typically advocate biocatalytic routes just as surface catalysis researchers advocate processes with solid inorganic catalysts, recent efforts are leading to process conceptions that take advantage of both subfields.

In years past, biocatalysis helped guide the development of surface catalysis, and vice versa. For example, the term "turnover frequency", used early in enzyme catalysis, was adopted years later for metal surface catalysis. Saturation kinetics on isolated biocatalytic sites (e.g., Michaelis–Menten kinetics) roughly translates into the same equations in surface catalysis (e.g., Langmuir–Hinshelwood kinetics). Such connections were recognized early by G.-M.

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Schwab in his classic book “Katalyse vom Standpunkt der chemischen Kinetik” (English translation by H. S. Taylor and R. Spence from 1937: “Catalysis from the Standpoint of Chemical Kinetics”), but the connections were difficult to draw, and recognition of the coherence may even have declined over the years. For example, a model accounting for the influence of intraparticle diffusion on rates of reaction in porous solid catalysts developed independently by Damköhler, Thiele, and Zeldowitsch, was rediscovered decades later without realization of the foundational work by researchers working on supported enzymes. Ironically, workers in catalysis broadly rely on powerful methods for elucidating complex, coupled reaction networks, but they do not seem to rely much on each other!

Jargon and nomenclature “du jour” have also fostered the fragmentation of catalytic science, with all subfields burdened by off-putting usage: consider *heterogeneous catalysis* (better: *surface catalysis* or *interfacial catalysis*); *heterogeneous catalyst* (*solid catalyst*—or more properly, a catalyst with nonuniform surface sites); *tandem catalysis* (essentially, *bifunctional catalysis*); *heterogenized homogeneous catalyst* (*supported molecular catalyst*); *operando spectroscopy* (*spectroscopy of working catalysts*); *carrier* (*support*); *substrate* (to some, *reactant*, to others, *support*). *Mechanism* currently has a less precise meaning in surface catalysis than in molecular catalysis. Reaction networks are misidentified as reaction mechanisms; reactions are misidentified as (elementary) steps. In all the subfields, the term *reaction rate* is often misused to represent some average rate. *Turnover frequencies* are not always based on reaction rates, but often (incorrectly) on some measure of average rate, and they are frequently confused with *turnover numbers* (or *numbers of turnovers*).

We assert that catalysis should be viewed as a coherent scientific field that requires defragmentation to maximize research progress in all catalytic fields and to attract the best young minds. There is great commonality in the reactants, which are often organic compounds; the catalytic centers, which often contain metal atoms; and the importance of the dictum that reactions often occur at unusual “privileged” structures. Steps as simple as proton or electron transfers link countless reactions. Structures and the kinetics of catalytic processes are unifying quantitative frameworks. Of overarching importance are equilibria and phase distributions affecting reactants, catalysts, and products; the accessibility of catalysts to reactants (mixing and transport phenomena); and separation of products from catalysts. Issues of catalyst deactivation, recycling, regeneration and replacement, and temperature gradients in reactors further unify catalytic science.

Countless examples illustrate the benefits of teaching catalysis as a unified field. Researchers in surface catalysis benefit from an understanding of mechanisms of organic and organometallic reactions in solution. Those investigating organic and organometallic reactions in solution can benefit from understanding the mechanisms of enzymatic and surface reactions. Those doing organometallic catalysis in solution can benefit from understanding ligand effects in reactions of supported catalysts elucidated in the absence of complicating solvents. Furthermore, everyone carrying out catalytic research can benefit from the surging advances in physical characterization methods. The understanding of extremely fast reactions generally requires the understanding of transport phenomena. The understanding of phase-transfer catalysts, supported liquid-phase catalysts, and polymer-supported molecular organic and organometallic catalysts requires a foundation in phase equilibria, transport phenomena, and interfacial phenomena. Catalytic applications of materials having extremely small pores and high internal surface areas, such as metal–organic frameworks (MOFs), require the understanding of transport phenomena. The understanding of electrocatalytic phenomena requires a foundation in surface catalysis.

Moreover, modern theory and computational chemistry are helping advance all areas of catalysis in both understanding the properties of known catalysts and guiding the design of new ones—zeolite catalysis is benefiting particularly because the crystallinity of zeolites implies uniform surface sites that can be modeled accurately. Shouldn’t everyone teaching catalysis be aware of the power of STM in imaging molecules that are moving, colliding, and reacting on surfaces? Is it not helpful for us all to visualize images of isolated metal atoms on solid surfaces that constitute nearly ideal catalytic sites—or full three-dimensional structures of enzymes that similarly define the catalytic sites and allow elucidation of subtle effects of their surroundings, such as accommodating transition states?

We hope that this Editorial will trigger suggestions about how to break down the barriers between the subdisciplines. Here are some thoughts to start with:

1. Encourage young researchers from the various subfields of catalysis across the globe to start collaborative networks and challenge them to present visions for the future of catalysis.
2. Fund fellowships specifically targeted to send postdoctoral students and faculty on sabbatical leaves in order to cross the subdisciplinary boundaries of catalysis.
3. Inspire team authorship of textbooks that integrate catalysis.
4. Encourage team teaching of catalysis courses to stimulate broad thinking among our students.
5. Encourage funding agencies to support multi-investigator catalytic research crossing subdisciplines, and with budgets sufficient to allow researchers time to gain in-depth knowledge that crosses disciplinary boundaries.
6. Encourage authors, reviewers, and editors to purge jargon and use simple, unifying terms.