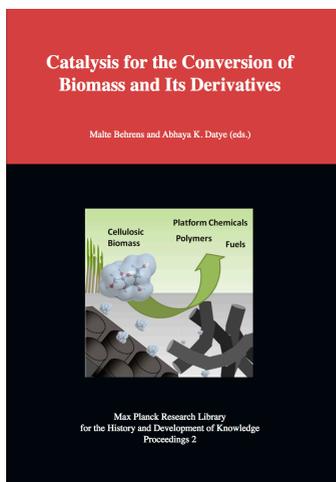


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Malte Behrens and Abhaya K. Datye:

Introduction



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Introduction

Opening Remarks

Fossil fuels such as coal, oil and natural gas currently provide over 75% of the world's energy supply needed to satisfy the great appetite for affordable and freely available energy of individuals and industries worldwide. Unfortunately, the growing global demand for fossil fuel resources comes at a time of rapidly diminishing reserves of non-renewable resources, causing widening concerns about a possible future scarcity of energy and the threat of rising oil prices. Furthermore, questions regarding the developing energy scenario cannot be separated from the discussion of evident changes in global climatic conditions by the increased combustion of fossil energy carriers and the large subsequent contribution to global CO₂ emissions.

In addition to the transportation sector and the energy-producing industries, another important user of fossil resources is the chemical industry, which relies extensively on petroleum for the production of valuable chemical intermediates in a wide variety of applications from polymeric materials to solvents and compounds for pharmaceuticals. There is a demand for renewable carbon-based feedstocks for chemical applications that are independent of fossil sources

The search for renewable alternatives for energy and chemicals is clearly a major societal need in every developed or developing country. Biomass, being a globally distributed resource, can serve as a valuable source for both energy and organic carbon. Due to its renewable nature, it is the only sustainable source of specific functional compounds for the chemical industry. A further advantage of the production of fuels from biomass is the potential to lower greenhouse gas emissions because the CO₂ released during energy conversion is recycled by the subsequent growth of biomass. The selective conversion of renewable biomass resources into tailor-made products is thus an important and attractive new area of research involving the fields of chemistry, biology and engineering.

Molecular manufacturing, i.e., the building of materials from the bottom up while retaining an atom-by-atom precision, has captured the fascination of researchers and the general public alike. However, achieving the same precision on a large scale remains a key challenge. Catalytic technology can carry out such molecular transformations in a precise manner to yield products—fuels, chemicals and other materials to serve the needs of society—in large-scale systems. It

relies on a chain of knowledge spanning such areas as the atomistic level of an elementary surface reaction, the materials science of catalytic particles and bench scale test reactors, and the chemical engineering world of reactors in industrial plants. Indeed, the success of the petrochemical industry can be attributed in part to an understanding of conversion processes and chemical mechanisms at a fundamental level such as metal-catalyzed hydrogenolysis, hydrogenation and oxidation reactions. Whereas a petrochemical refinery has reached its present state of efficiency by continuous improvement over the past 50 years, the “biorefinery” and the understanding and knowledge-based manipulation of the involved chemical reactions is still in its infancy. By utilizing new chemical, biological and mechanical technologies, such an envisaged biorefinery provides a means of transitioning to a more energy-efficient and environmentally sustainable chemical and energy economy. In an integrated biorefinery, the production of high-value chemicals will be coupled with the production of high-volume and low-value transportation fuels, leading to a profitable mix and supporting sustainable operations to meet rising energy demands. The biorefinery of the future will be analogous to the petrochemical refinery of the present: a highly integrated system of processes that are optimized for energy efficiency and resource utilization. New catalysts and catalytic processes must be developed to provide the flexibility needed for the biorefinery to adjust and optimize its performance to accommodate changes in feedstocks and market demands.

The development of the necessary technology has been identified as the greatest challenge to bridge the gap between the concept and the realization of a bio-based chemical industry. In the summer of 2010 a workshop to address the challenges in this growing area of research was organized in order to bring together leading academic and industrial experts in the fields of catalytic conversion, biomass growth, life cycle analysis and industrial applications. The workshop on “Molecular Engineering for the Conversion of Biomass-Derived Reactants to Fuels, Chemicals and Materials” was organized by the Fritz Haber Institute of the Max Planck Society and the Partnership for International Research and Education (PIRE) at Kloster Seeon in Bavaria, Germany (photo by Edward L. Kunkes).¹

¹More information can be found on <https://pire.unm.edu/>. The partner institutions, collaborators and principal investigators of this PIRE program are: University of New Mexico (Abhaya K. Datye, PI), University of Virginia (Robert J. Davis, co-PI and Matthew Neurock, co-PI), University of Wisconsin-Madison (James A. Dumesic, co-PI), Iowa State University (Brent Shanks, co-PI), Fritz-Haber-Institute der Max-Planck-Gesellschaft (Malte Behrens, Matthias Scheffler, collaborators, and Robert Schlögl, host Germany), Max Planck Institute of Colloids and Interfaces (Markus Antonietti, collaborator), Haldor Topsøe A/S (Stig Helveg, collaborator), Technical University of Denmark (Jens K. Nørskov, collaborator and Ib Chorkendorff, host Denmark), Twente University (Leon Leferts, collaborator), Åbo Akademi University (Dmitry Murzin, host Finland), Eindhoven University of Technology (Hans Niemantsverdriet, host Netherlands), Utrecht University (Harry Bitter, Krijn de Jong and Bert Weckhuysen, collaborators).



The objective of this international partnership is to enhance the collaboration between institutions in the United States and the European Union to elucidate the key factors controlling catalytic conversions of biomass-derived reactants, thereby providing a fundamental foundation for the design, development and operation of a biorefinery. The focus of this workshop was primarily pedagogical, assisting students and researchers in the field to clearly formulate some of the challenges and discuss possible paths to achieving a bio-based economy. The lectures presented at the workshop are compiled in this volume for a broader dissemination to the scientific community and interested laypersons.

This volume comprises 13 chapters and starts with the perspectives from industry and start-up companies, which are delivered by Friedrich Seitz and Leo Manzer, respectively. Before taking a deeper look into biomass chemistry, some relevant non-chemical aspects are treated, that define the boundary conditions of a large-scale use of biomass. Robert Anex reports on a life cycle perspective and Mark Stitt discusses aspects of plant growth for biomass production. The following chapter by Michael Ladisch, Eduardo Ximenes, Youngmi Kim and Nathan S. Mosier covers the fundamentals of biomass chemistry. Charles E. Wyman and Carol J. Wyman further focus on its aqueous phase processing. Analytical approaches for biomass conversion reactions are introduced by Dmitry Murzin and Bjarne Holmbom, and Amie Sluiter, Justin Sluiter and Edward J. Wolfrum in the following two chapters. The field of catalytic conversion of biomass is

then introduced by Robert J. Davis, and Elif I. Gürbüz and James A. Dumesic, who report on reaction engineering concepts and catalytic strategies, respectively. The development of suitable heterogeneous catalysts and the related challenges are covered in Brent H. Shank's chapter, while Thorsten vom Stein, Walter Leitner and Jürgen Klankermayer focus on the application of homogeneous catalysts for the conversion of biomass. Finally, the important deconstruction reactions of lingo-cellulose are treated in the chapter by Roberto Rinaldi and Jennifer Reece. In the second part of this introduction, short biographical sketches of the authors, the editors and their affiliations are listed to complement the scientific content of this book.

All lectures present introductory material designed to root the subject back into the respective disciplinary foundations as well as state-of-the-art results illuminating current knowledge. While a remote observer may be fascinated by the detail of understanding gained in some aspects of the treatment of the complex and non-uniform material called "biomass," the experts feel that the current understanding of catalysis, mainly devoted to increase the functionality of feedstock molecules for desired chemical reactivity, is still unsuitable to efficiently deal with the transformation of biomass. Here, the over-functionalized bio-molecule needs de-functionalization, being in strong competition with polymerization once it is activated by catalytic or stoichiometric reactions. A new paradigm of catalysis is needed that focuses on the selective activation of large reaction networks under conditions more favorable to precise kinetic control than those provided by present-day tools.

Also, the dimension of the challenge to develop test-tube chemistry into processes suitable to operate under economical constraints given by today's energy market became obvious. The discussions vividly reflected concerns about the large-scale viability of biomass as a resource for transportation fuels and highlighted the responsibility of science to also consider non-scientific aspects when developing new technologies that might interfere with fundamental requirements of human life such as biodiversity, food production or clean water resources.

The decision to make the teaching material of this course available in the present form was made because we believe that this emerging field of energy science requires input from many disciplines that are traditionally not in close contact with each other. The present text may thus be regarded as an annotated introduction into basic concepts and considerations relevant for biomass conversion research. The text is intended to familiarize researchers with questions and concepts of relevant neighboring fields without providing complete textbook reference or literature coverage. The book may be used as an introduction to those areas of knowledge and challenges required to master biomass transformation on a scale relevant for future energy applications.

We acknowledge the support of the PIRE program from the U.S. National Science Foundation Office of International Science and Education (OISE). Additional funding was provided by the Max Planck Society through a grant to the Fritz Haber Institute in Berlin. Besides the contributions from the authors of these lectures, we note that the students and post-docs participating in this workshop actively contributed to its content through their questions and discussion. In a novel format to stimulate exchange among participants, scientists from different teams and areas of research were selected and randomly assigned to groups of three. The tasks of these groups were to reflect on the lectures and formulate questions to each of the speakers. The discussions after dinner were primarily devoted to questions from students and post-docs. By the end of the workshop, every participant had asked a question or contributed to the discussion. The content of these after-dinner discussions is also incorporated in the lectures reproduced in this volume. The open-access format offered by the Max Planck Library for the History and Development of Knowledge allows us to make the contents freely accessible through the World Wide Web. We also express our gratitude to Beatrice Herrmann, Kai Surendorf and Antje Ota for their invaluable technical assistance. Without their expertise and continuous efforts the print-on-demand version and the online production of this book would not have been possible. We thank Beatrice Gabriel for the thorough and fast copy-editing of the manuscripts and Dorothea Damm for her help with organizational issues. Jürgen Renn is acknowledged for his continuous support of the project. The cover picture was designed by Sylvia Reiche.

Abhaya Datye, Malte Behrens and Robert Schlögl

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