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Preface

This special issue is an output of the research project titled 'Synthesis of Ecological High Quality Transportation Fuels', which has been promoted by a Research Promotion Committee in The Research for the Future Program of JSPS from fiscal 1998 to 2002. The chairman of the Research Promotion Committee of this Research Project was Emeritus Professor Yoshikazu Nishikawa (the President of Osaka Institute of Technology), and the leader of the Research Project was Professor Muneyoshi Yamada. The objective of the project is to develop next-generation catalysts to assure a compact productive process producing ecological high-quality transportation fuels from distributed untapped non-petroleum hydrocarbon resources (natural gas from dispersed remote gas field, coal bed methane, and biomass) via syngas.

Recently "highly efficient use of energy with low environmental impact" has become very important concept. From this point of view, diesel engine is very promising because its intrinsic thermal efficiency is higher than that of gasoline engine. However, its exhaust gas accounts for 75% of the automobile origin NO_x and almost 100% of the automobile origin PM. Therefore, development of ecological high-quality diesel fuel, which leads to reduce NO_x and PM in its exhaust gas, is very important to make the best use of the intrinsic high efficiency of diesel engine. Recently, it has become known that the tail gas from the combustion of DME or FT-oil in diesel engine contains much less PM and NO_x than that of the diesel fuel from petroleum (i.e. gas-oil). Therefore, by using DME or FT-oil instead of gas-oil as diesel fuel, the simultaneous reduction of CO₂, NO_x, PM, and SO_x is expected. Considering these new findings and the expectation, we have planned the following measures:

- 1. Catalytic formation of syngas from biomass: syngas production from distributed untapped non-petroleum hydrocarbon resources, such as small-scale natural gas fields, coal bed methane and biomass, is very important in this research project. Especially biomass conversion to syngas is very important from so-called "Carbon Neutral" point of view. This project has succeeded to develop a new catalytic system to convert biomass to syngas without producing tar and char.
- FT synthesis: the project aims to improve both catalytic activity and so-called Anderson-Schulz-Flory distribution for efficient production of diesel fuel. By using recently found mesoporous materials, such as MCM-41 and SBA-15, this project has succeeded to prepare

- Co/SBA-15 catalyst highly active for FT synthesis. And, this project has succeeded to develop new type of FT catalyst active for formation of iso-paraffins.
- 3. Methanol and DME synthesis: the project aims to develop a new catalytic system to produce methanol at a lower temperature, because lower temperatures are preferred from an equilibrium point of view. The project also aims to develop a single step process from syngas to DME with a hybrid catalyst system of methanol synthesis catalysts and solid acid catalysts. The project has succeeded to develop new type of methanol synthesis catalysts highly active at lower temperatures. It is not deactivated in the presence of CO₂ and water vapor. And, the project succeeded to develop highly active single step DME synthesis catalyst by using home made combinatorial catalysis technique.
- 4. Development of sulfur-tolerant catalysts to simplify or omit the desulfurization unit: sulfur compounds in syngas must be removed to less than ppm to prevent catalysts from sulfur poisoning at commercial processes. The project aims to develop sulfur-tolerant catalysts. The project has succeeded to find various kinds of sulfur-tolerant catalysts active for methanol synthesis and FT synthesis. The methanol synthesis activity of the newly found Pd sulfide and Rh sulfide is higher than the half of that of the conventional Cu/Zn catalyst. The former activity is kept even in the presence of 100 ppm H₂S.
- 5. Estimation and designing of active catalyst by using the computational chemistry: for efficient research, we have adopted an innovative molecular design technology, which combines combinatorial computational chemistry and a new accelerated quantum chemical molecular dynamics algorithm. The project has succeeded to develop an ultra-high speed computational program, 5000 times faster than the conventional one. This method has been successfully applied to find new catalyst active for methanol and Fischer–Tropsch syntheses.
- In situ observation of catalyst fine structure with EX-AFS, FT-IR, etc. and elucidation of surface chemistry based on the observation: the project has succeeded to observe meta-stable intermediate in methanol synthesis.
- 7. LCA analyses for synthetic fuels and clean energy cars.

The present research project has not only produced very important fruits as ecological high-quality transportation fuels but also brought large spin-off benefits to chemical industry and basic catalyst and surface chemistry. Since the process can treat various kinds of carbon resources, it is easily applicable in a hydrogen energy society and in a society ensuring sustainable development with biomass. This special issue has contained some of the outstanding results of the project.

Finally, on behalf of the research project team, we would like to express our thanks to the Research Promotion Committee of JSPS and Emeritus Professor Yoshikazu Nishikawa (the Chairman of the Committee and the President of Osaka Institute of Technology) for promoting our research project. We are grateful to Professor Kaoru Fujimoto (The University of Kitakyusyu) for encouraging our research project as the advisor. We are also grateful to Emeritus Professor Yuzo Sanada and Professor Masakatu Nomura for supporting our project as commentators. Our grateful thanks goes to everybody who contributed to this special issue.

Muneyoshi Yamada
Department of Applied Chemistry
Graduate School of Engineering, Tohoku University
Aoba 07, Aramaki, Aoba-ku, Sendai 980-8579, Japan
Corresponding author. Tel.: +81-22-217-7214
fax: +81-22-217-7293

E-mail address: yamada@erec.che.tohoku.ac.jp (M. Yamada)

Yasuo Ohtsuka

Research Center for Sustainable Materials Engineering Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Katahira Aoba-ku, Sendai 980-8577, Japan

Fax: +81-22-217-5655

E-mail address: ohtsukay@tagen.tohoku.ac.jp (Y. Ohtsuka)