Fri. Oct 28, 2022

Poser sess. room-A (P01-P08)

Poster presentation

[2a07-0900] Poster sess. A

9:00 AM - 3:00 PM Poser sess. room-A (P01-P08) (12G Conf. room)

[P01] Catalytic oligomerization of isobutyl alcohol to jet fuels over dealuminated zeolite Beta
○Xiaoyu Guo[1], Yingluo He[1], Guohui Yang[1], Noritatsu Tsubaki[1] (1. University of Toyama)

[P02] Effect of P addition on activity of Ru catalyst for C_2H_2 selective hydrogenation
○Mana Murakami[1], Yasuharu Kanda[1] (1. Muroran Institute of Technology)

[P03] Methylcyclohexane dehydrogenation activity of Ca added Pt catalyst
○Ayumu Kobayashi[1], Yasuharu Kanda[1] (1. Muroran institute of technology)

[P04] Gas-phase Oxidation of Benzene over Cu Catalyst Loaded on Molded MFI Type Zeolite
○Xindong Yin[1], Shuhei Miyamoto[1], Masaya Morimoto[1], Keita Taniya[1], Yuichi Ichihashi[1], Satoru Nishiyama[1] (1. Catalytic Reaction Engineering Group,Department of Chemical Science and Engineering, Graduate School of Engineering, Kobe University)

[P05] Chemical recycling of aliphatic polyesters by transesteirifcation using homogeneous Lews acd catalysts
○Youshu Jiang[1], Yohei Ogiwara[1], Kotohiro Nomura[1] (1. Tokyo Metropolitan University)

[P06] Synthesis of half-titanocene catalysts for efficient synthesis of cyclic olefin copolymers
○Taiga Fujioka[1], Jiahao Gao[1], Kotohiro Nomura[1] (1. Tokyo Metropolitan University)

[P07] Synthesis of New Bio-Based Polyolefins by Ethylene Copolymerization with Camphene by Nonbridged Half-Titanocene Catalysts
○Tomu Watanabe[1], Kotohiro Nomura[1] (1. Tokyo Metropolitan University)

[P08] Regioselective oligomerization of ω-siloxy-α-olefins using a zirconium complex : synthesis of novel ester-based lubricant precursors
○Kazuma Okada[1], Akihiko Ishii[1], Norio Nakata[1] (1. Department of Chemistry, Graduate School of Science and Engineering, Saitama University)

Poster sess. room-B (P09-P15)

Poster presentation

[2a08-0900] Poster sess. B

9:00 AM - 3:00 PM Poster sess. room-B (P09-P15) (12H Conf. room)

[P09] Mechanistic study of Ni_2P catalyzed dehydrogenative coupling of methane
Rattanawalee Rattanawan[1], Min Gao[1], Shoji Iguchi[2], Ichiro Yamanaka[2], ○Jun-ya Hasegawa[1] (1. Hokkaido University, 2. Tokyo Institute of Technology)

[P10] Machine Learning-Aided Catalyst Modification in Oxidative Coupling of Methane by Addition of Promoter Element
○Shun Nishimura[1], Junya Ohyama[2], Xinyue Li[1], Itsuki Miyazato[3], Toshiaki Taniike[1], Keisuke Takahashi[3] (1. JAIST, 2. Kumamoto University, 3. Hokkaido University)

[P11] Development of low-temperature methanol synthesis process from CO_2
○Ayaka Miura[1], Kenji Nakao[1], Noriyuki Yamane[1], Fei Chen[2], Noritatsu Tsubaki[2] (1. Nippon Steel Corp., 2. University of Toyama)

[P12] Gas-phase hydrogenation of CO_2 over supported iron-based catalysts.
○Misuzu Komuro[1], Miru Hirahara[1], Hitoshi Ogihara[1], Hideki Kurokawa[1] (1. Saitama University)

[P13] Mechanism of foaming phenomena during pre-heating in the liquid phase synthesis of bio-jet fuel form triglycerides
○Shimada Hikaru[1], Kenji Asami[1], Haruki Tani[2], Yayoi Murakami[3], Kaoru Fujimoto[3] (1. Asami Laboratory, The University of Kitakyushu, 2. Environment Energy Co., Ltd., 3. HiBD Research Institute, Inc.)

[P14] Optimization of reaction conditions with machine learning in woody biomass solvolysis using vegetable oil solvent
○Emi Fukutani[1], Mitsumasa Osada[1], Hiroshi Fukunaga[1], Nobuhide Takahashi[1], Iori Shimada[1] (1. Shinshu University)

[P15] Efficient prediction of jet fraction yield and optimal condition using machine learning in catalytic cracking of vegetable oils
○Yuzuki Katayama[1], Iori Shimada[1] (1. Shinshu University)

Poster presentation

[2a07-0900] Poster sess. A

Fri. Oct 28, 2022 9:00 AM - 3:00 PM Poser sess. room-A (P01-P08) (12G Conf. room)

[P01] Catalytic oligomerization of isobutyl alcohol to jet fuels over dealuminated zeolite Beta

○Xiaoyu Guo[1], Yingluo He[1], Guohui Yang[1], Noritatsu Tsubaki[1] (1. University of Toyama)

[P02] Effect of P addition on activity of Ru catalyst for C_2H_2 selective hydrogenation

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[P04] Gas-phase Oxidation of Benzene over Cu Catalyst Loaded on Molded MFI Type Zeolite

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[P05] Chemical recycling of aliphatic polyesters by transesteirifcation using homogeneous Lews acd catalysts

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[P06] Synthesis of half-titanocene catalysts for efficient synthesis of cyclic olefin copolymers

○Taiga Fujioka[1], Jiahao Gao[1], Kotohiro Nomura[1] (1. Tokyo Metropolitan University)

[P07] Synthesis of New Bio-Based Polyolefins by Ethylene Copolymerization with Camphene by Nonbridged Half-Titanocene Catalysts

○Tomu Watanabe[1], Kotohiro Nomura[1] (1. Tokyo Metropolitan University)

[P08] Regioselective oligomerization of ω-siloxy-α-olefins using a zirconium complex : synthesis of novel ester-based lubricant precursors

○Kazuma Okada[1], Akihiko Ishii[1], Norio Nakata[1] (1. Department of Chemistry, Graduate School of Science and Engineering, Saitama University)

(Fri. Oct 28, 2022 9:00 AM - 3:00 PM Poser sess. room-A (P01-P08))

[P01] Catalytic oligomerization of isobutyl alcohol to jet fuels over dealuminated zeolite Beta

○Xiaoyu Guo[1], Yingluo He[1], Guohui Yang[1], Noritatsu Tsubaki[1] （1. University of Toyama）

Keywords: Jet fuels, Isobutyl alcohol, Oligomerization

Various dealuminum methods of zeolite Beta to generate the jet fuels by converting isobutyl alcohol has been investigated in detail. And related factors of the zeolite catalyst were studied utilizing XRD, SEM, XRF, Nitrogen adsorption-desorption, NH_3-TPD, Py-FTIR, and ^{27}Al solid-state NMR. Removal of extra-framework aluminum or part of framework aluminum by hydrochloric acid dealumination, is able to improve the diffusion property of the products in the channel of zeolite Beta via increasing the ratio of Lewis/Brønsted. Consequently, isobutyl alcohol can be quantitatively oligomerized over dealuminated zeolite Beta with the selectivity of C_{8-16} exceeding 50% at a conversion of 98%.

(Fri. Oct 28, 2022 9:00 AM - 3:00 PM Poser sess. room-A (P01-P08))

[P02] Effect of P addition on activity of Ru catalyst for C_2H_2 selective hydrogenation

○Mana Murakami[1], Yasuharu Kanda[1] （1. Muroran Institute of Technology）

Keywords: Selective hydrogenation, Ruthenium phosphide, Acetylene

本研究では、P/Ru比が異なる非担持Ru-P触媒を用いてアセチレンの選択的水素化反応の活性種について検討した。XRD測定より、P添加したいずれの触媒でも水素還元後にRu_2Pが生成することを確認した。また、P/Ru比が1.2のRu-P触媒は、Ru触媒と比較して約20倍のTOFを示した。さらに、Ru-P触媒は高いアセチレン転化率においても、高いエチレン選択率を維持した。以上のことから、RuにPを添加することで、生成したRu_2Pが選択的水素化反応の活性種として機能することを明らかにした。

(Fri. Oct 28, 2022 9:00 AM - 3:00 PM Poser sess. room-A (P01-P08))

[P03] Methylcyclohexane dehydrogenation activity of Ca added Pt catalyst

○Ayumu Kobayashi[1], Yasuharu Kanda[1] （1. Muroran institute of technology）

Keywords: Dehydrogenation, Platinum, Calcium

本研究では，高性能なMCH脱水素触媒の開発のため，Pt/Al_2O_3触媒のMCH脱水素活性に与えるCaの添加効果について検討した．Caの添加により，触媒活性の低下が抑えられ，安定性が向上することが分かった．Ca添加Pt/Al_2O_3触媒のキャラクタリゼーションから，Caの添加によりPt粒子の凝集は確認されず，Ptは負に帯電することが明らかとなった．これより，Ptが電子豊富になることで，活性の安定性に影響を与えていると考えた．

(Fri. Oct 28, 2022 9:00 AM - 3:00 PM Poser sess. room-A (P01-P08))

[P04] Gas-phase Oxidation of Benzene over Cu Catalyst Loaded on Molded MFI Type Zeolite

○Xindong Yin[1], Shuhei Miyamoto[1], Masaya Morimoto[1], Keita Taniya[1], Yuichi Ichihashi[1], Satoru Nishiyama[1]
（1. Catalytic Reaction Engineering Group,Department of Chemical Science and Engineering, Graduate School of Engineering, Kobe University）
Keywords: Cu zeolite, Molded zeolite, Phenol synthesis

本研究では、銅を担持したMFI型ゼオライト成形体触媒においてベンゼンの気相酸化反応を検討してきた。成形体であるバインダレスゼオライトにイオン交換法で銅を担持した触媒は従来の粉末状のCu/HZSM-5触媒と同等のフェノール収率が観察されたことが分かった。気相原料の供給線速度及び触媒との接触時間を変化させることで供給原料の成形体内部への拡散について検討した。結果、触媒粒子境膜での物質拡散は十分な線速度の時には十分に速いことが示唆された。

(Fri. Oct 28, 2022 9:00 AM - 3:00 PM Poser sess. room-A (P01-P08))

[P05] Chemical recycling of aliphatic polyesters by transesteirifcation using homogeneous Lews acd catalysts

○Youshu Jiang[1], Yohei Ogiwara[1], Kotohiro Nomura[1]（1. Tokyo Metropolitan University）
Keywords: molecular catalysts, depolymerization, chemical recycling of polyester

In this presentation, depolymerization of aliphatic polyesters such as poly(ethylene adipate), poly(butylene adipate) etc. by transesterification with alcohols using homogeneous Lewis acid catalysts will be presented. In particular, the reaction by titanium catalysts afforded corresponding monomers in exclusive yields, and the detailed results will be presented in the symposium.

(Fri. Oct 28, 2022 9:00 AM - 3:00 PM Poser sess. room-A (P01-P08))

[P06] Synthesis of half-titanocene catalysts for efficient synthesis of cyclic olefin copolymers

○Taiga Fujioka[1], Jiahao Gao[1], Kotohiro Nomura[1]（1. Tokyo Metropolitan University）
Keywords: molecular catalysts, polymerization, cyclic olefin copolymers

環状オレフィン系共重合体、特に透明性や耐熱性に優れるエチレンとノルボルネンやテトラシクロドデセンとの共重合体の効率合成に有効なアニオン性支持配位子を有するハーフチタノセン触媒の合成に取り組んだ。特にシクロペンタジエニル配位子上の置換基の異なる各種ケチミド配位錯体、$Cp'TiCl_2(N=C^tBu)$、パラ位に異なる置換基を有するフェノキシ配位錯体、$Cp'TiCl_2(O-2,6-^iPr_2-4-RC_6H_2)$、の合成と目的反応への配位子効果を検討した結果を紹介する。

(Fri. Oct 28, 2022 9:00 AM - 3:00 PM Poser sess. room-A (P01-P08))

[P07] Synthesis of New Bio-Based Polyolefins by Ethylene Copolymerization with Camphene by Nonbridged Half-Titanocene Catalysts

○Tomu Watanabe[1], Kotohiro Nomura[1]（1. Tokyo Metropolitan University）
Keywords: Bio-Based Polyolefins, Polymerization, Titanocene Catalysts

最近当研究室では、ハーフチタノセン触媒によるエチレンとリモネンやピネンなどのバイオベースモノマーとの共重合を報告している。この種の原料のほとんどが2置換オレフィンや嵩高い環状オレフィンで、配位重合による合成例は本報告に限定される。本発表では、エチレンと精油から得られる環式モノテルペンであるカンフェンとの共重合を検討したので、ポスターで結果の詳細を報告する。

(Fri. Oct 28, 2022 9:00 AM - 3:00 PM Poser sess. room-A (P01-P08))

[P08] Regioselective oligomerization of ω-siloxy-α-olefins using a zirconium complex : synthesis of novel ester-based lubricant precursors

○Kazuma Okada[1], Akihiko Ishii[1], Norio Nakata[1] （1. Department of Chemistry, Graduate School of Science and Engineering, Saitama University ）

Keywords: oligomerization, zirconium complex, ester-based lubricant precursors

It is well known that ester-based lubricants are one of the useful synthetic lubricants having high flame retardancy and biodegradability. We have succeeded in the regioselective oligomerization of various α-olefins using Zr(IV) complexes supported by [OSSO]-type ligands. Herein, we present the synthesis of novel branched diesters, as ester-based lubricant precursors, by the oligomerization of ω-siloxy-α-olefins with the Zr(IV) complex.

Poster presentation

[2a08-0900] Poster sess. B

Fri. Oct 28, 2022 9:00 AM - 3:00 PM Poster sess. room-B (P09-P15) (12H Conf. room)

[P09] Mechanistic study of Ni_2P catalyzed dehydrogenative coupling of methane

Rattanawalee Rattanawan[1], Min Gao[1], Shoji Iguchi[2], Ichiro Yamanaka[2], ○Jun-ya Hasegawa[1] (1. Hokkaido University, 2. Tokyo Institute of Technology)

[P10] Machine Learning-Aided Catalyst Modification in Oxidative Coupling of Methane by Addition of Promoter Element

○Shun Nishimura[1], Junya Ohyama[2], Xinyue Li[1], Itsuki Miyazato[3], Toshiaki Taniike[1], Keisuke Takahashi[3] (1. JAIST, 2. Kumamoto University, 3. Hokkaido University)

[P11] Development of low-temperature methanol synthesis process from CO_2

○Ayaka Miura[1], Kenji Nakao[1], Noriyuki Yamane[1], Fei Chen[2], Noritatsu Tsubaki[2] (1. Nippon Steel Corp., 2. University of Toyama)

[P12] Gas-phase hydrogenation of CO_2 over supported iron-based catalysts.

○Misuzu Komuro[1], Miru Hirahara[1], Hitoshi Ogihara[1], Hideki Kurokawa[1] (1. Saitama University)

[P13] Mechanism of foaming phenomena during pre-heating in the liquid phase synthesis of bio-jet fuel form triglycerides

○Shimada Hikaru[1], Kenji Asami[1], Haruki Tani[2], Yayoi Murakami[3], Kaoru Fujimoto[3] (1. Asami Laboratory, The University of Kitakyushu, 2. Environment Energy Co., Ltd., 3. HiBD Research Institute, Inc.)

[P14] Optimization of reaction conditions with machine learning in woody biomass solvolysis using vegetable oil solvent

○Emi Fukutani[1], Mitsumasa Osada[1], Hiroshi Fukunaga[1], Nobuhide Takahashi[1], Iori Shimada[1] (1. Shinshu University)

[P15] Efficient prediction of jet fraction yield and optimal condition using machine learning in catalytic cracking of vegetable oils

○Yuzuki Katayama[1], Iori Shimada[1] (1. Shinshu University)

(Fri. Oct 28, 2022 9:00 AM - 3:00 PM Poster sess. room-B (P09-P15))

[P09] Mechanistic study of Ni$_2$P catalyzed dehydrogenative coupling of methane

Rattanawalee Rattanawan[1], Min Gao[1], Shoji Iguchi[2], Ichiro Yamanaka[2], ○Jun-ya Hasegawa[1] （1. Hokkaido University, 2. Tokyo Institute of Technology）

Keywords: Ni2P, dehydrogenative coupling of methane, density functional theory calculation

Ni$_2$P catalyst has been reported to convert methane to ethane by dehydrogenative coupling. In this study, the reaction mechanism was analyzed using density functional theory calculations. The results show that (1) the C-H dissociation of methane tends to occur on the P atom on the Ni hollow site, (2) the rate-limiting process is methyl radical desorption to the gas phase, (3) ethane formation by the Eley-Rideal mechanism, and (4)coke formation may be accelerated by the loss of P atoms on the hollow site.

(Fri. Oct 28, 2022 9:00 AM - 3:00 PM Poster sess. room-B (P09-P15))

[P10] Machine Learning-Aided Catalyst Modification in Oxidative Coupling of Methane by Addition of Promoter Element

○Shun Nishimura[1], Junya Ohyama[2], Xinyue Li[1], Itsuki Miyazato[3], Toshiaki Taniike[1], Keisuke Takahashi[3] （1. JAIST, 2. Kumamoto University, 3. Hokkaido University）

Keywords: Machine Learning, OCM catalyst, Additive element

メタンの酸化的カップリング（OCM）反応に関するランダムスクリーニング実験データの傾向を基に高活性・高選択性を実現する触媒開発のためのターゲット設定を行い、機械学習によるデータ拡張から必要な触媒開発の要素を抽出した。高選択性を示した３元素担持OCM触媒へ、高転化率の共通の要素となるマンガン（Mn）を第４元素として添加し、そのOCM触媒活性を評価した。その結果、NaMnW/SiO2と同程度の収率・選択性を有するLiFeBa-Mn/La2O3とLiBaLa-Mn/La2O3を得た。

(Fri. Oct 28, 2022 9:00 AM - 3:00 PM Poster sess. room-B (P09-P15))

[P11] Development of low-temperature methanol synthesis process from CO$_2$

○Ayaka Miura[1], Kenji Nakao[1], Noriyuki Yamane[1], Fei Chen[2], Noritatsu Tsubaki[2] （1. Nippon Steel Corp., 2. University of Toyama）

Keywords: carbon dioxide, methanol, carbon dioxide capture and utilization

当社では、CO$_2$からメタノールを合成する触媒プロセスの開発について、富山大学と取り組んでいる。本系では、系中に予めアルコールを添加することで平衡上有利な低温で反応が進行することに特徴があり、Cu/ZnO系触媒を用いている。本報告では、触媒組成の最適化や、アルコールの添加の有無で生産性を比較した結果を報告する。

(Fri. Oct 28, 2022 9:00 AM - 3:00 PM Poster sess. room-B (P09-P15))

[P12] Gas-phase hydrogenation of CO$_2$ over supported iron-based

catalysts.

○Misuzu Komuro[1], Miru Hirahara[1], Hitoshi Ogihara[1], Hideki Kurokawa[1]　(1. Saitama University)

Keywords: Supported iron catalyst, carbon dioxide hydrogenation, methane formation

Gas-phase hydrogenation of CO_2 to form lower hydrocarbons was performed over supported iron-based catalysts using a fixed-bed flow reactor. Effects of adding a second element (alkaline metal and transition metal) to the supported iron catalyst on catalytic activity and selectivity were investigated. At 300 ℃ an alumina-supported iron catalyst afforded CO as the main product with a small amount of CH_4. The addition of alkaline metal to the iron catalyst improved the catalytic activity, but the formation of CH_4 was suppressed.

(Fri. Oct 28, 2022 9:00 AM - 3:00 PM Poster sess. room-B (P09-P15))

[P13] Mechanism of foaming phenomena during pre-heating in the liquid phase synthesis of bio-jet fuel form triglycerides

○Shimada Hikaru[1], Kenji Asami[1], Haruki Tani[2], Yayoi Murakami[3], Kaoru Fujimoto[3]　(1. Asami Laboratory, The University of Kitakyushu, 2. Environment Energy Co., Ltd., 3. HiBD Research Institute, Inc.)

Keywords: HiBD, Liquid phase synthesis, Foaming phenomena

演者らは動植物性油脂から脱炭酸分解により高品質の炭化水素系バイオディーゼル燃料を得るプロセスの開発を行っている。これまでに、ハイドロタルサイト系触媒を用い、液相で反応を行うことにより、高収率でディーゼル燃料(HiBD)を得ることに成功しており、この技術を応用して廃食油からジェット燃料を製造するHiJETプロセスの開発を進めている。しかし、液相合成においては、初期の昇温過程で発泡現象が起こり、運転に悪影響を及ぼすことが分かった。そこで本研究ではこの現象の解明を試みた。

(Fri. Oct 28, 2022 9:00 AM - 3:00 PM Poster sess. room-B (P09-P15))

[P14] Optimization of reaction conditions with machine learning in woody biomass solvolysis using vegetable oil solvent

○Emi Fukutani[1], Mitsumasa Osada[1], Hiroshi Fukunaga[1], Nobuhide Takahashi[1], Iori Shimada[1]　(1. Shinshu University)

Keywords: solvolysis, vegetable oil, machine learning

本研究は植物油を用いた加溶媒分解によってバイオ燃料を製造し、船舶燃料に適応することを目標とする。目標達成のために、まず特徴の異なる三種類の植物油（カシューナッツ殻液、ヒマワリ油、パーム油）を用いて実験を行い、そのデータから機械学習を用いて液体収率と粘度を予測するモデルを構築する。さらにそのモデルから次の実験推奨点を導出し、実際に実験・検証、モデルの再構築を繰り返すことで最適な液体燃料製造を目指す。

(Fri. Oct 28, 2022 9:00 AM - 3:00 PM Poster sess. room-B (P09-P15))

[P15] Efficient prediction of jet fraction yield and optimal condition using machine learning in catalytic cracking of vegetable oils

○Yuzuki Katayama[1], Iori Shimada[1] （1. Shinshu University）

植物油の接触分解において、機械学習を用いることで新規触媒を用いた際のジェット留分収率予測及び最適条件探索の効率化を目的とした。モデル構築には大量のデータが必要となることに加えて、触媒を変更するごとにも大量のデータが必要となる。しかし、大量のデータ取得には労力を要する。この課題を、データ量が豊富である旧触媒データを活用することで、新規触媒に対応したモデルを少数データで構築することを目指した。