

# Unveiling Hidden Catalysts for the Oxidative Coupling of Methane based on Combining Machine Learning with Literature Data



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The front cover artwork for Issue 15/2018 is provided by National Institute for Materials Science; ICAT, Hokkaido University, Japan Advanced Institute of Science and Technology, and Nagoya University (all in Japan) as part of CREST: Catalysts Informatics Project. The image shows machine learning as a tool for catalyst design based on experimental catalysis data. See the Full Paper itself at <https://doi.org/10.1002/cctc.201800310>.

## How did the collaboration on this project start?

This collaboration was initiated as a part of the CREST project "Innovative Catalysts and Creation Technologies for the Utilization of Diverse Natural Carbon Resources", supervised by Professor Wataru Ueda and funded by Japan Science and Technology Agency. Comprised of leading researchers with expertise in experiment, computation, and data science, this project proposes the use of catalyst informatics in order to tackle methane conversion. The team is particularly eager to revolutionize the catalysis field through this approach.

## What aspects of this project do you find most exciting?

Challenges within catalyst design originate from the complexity of catalytic activities. Machine learning, however, offers a plausible solution. In particular, data science can be viewed as a game changer as catalyst data can be treated within multi-dimensional space. Hidden trends and periodicities are then unveiled and descriptors for determining catalytic reactions can be uncovered using machine learning and catalyst data. This project therefore demonstrates a revolutionary way of designing catalysts using data science.

## What future opportunities do you see?

With rapid advancement of high-throughput experiments and computation, collection of catalyst data can be achieved within a relatively short period of time. This marriage of data collection and data science has great potential in aiding the catalyst design process within the field of catalysis.

## What is in your opinion an upcoming research theme likely to become one of the 'hot topics' in the near future?

Implementation of data science is key to discovering novel catalysts or optimizing the performance of existing catalysts. The

movement of "X" science to "X" informatics, as seen in the case of bioinformatics, is beginning within catalysis. Thus, the fusion of catalysts and data science will play an important role in the near future.

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