

OGURA LAB.

Frontiers in Elements Circulation Society


 Research Center for Sustainable Materials Energy Integration
 Department of Materials and Environmental Science

Catalyst/Catalysis

Department of Chemical System Engineering, Graduate School of Engineering

<https://www.ogulab.iis.u-tokyo.ac.jp>

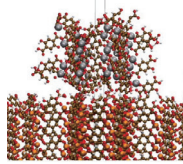
Design of solid catalysis using porous materials

Solid catalysts can cause “reactions that are difficult to occur” and are essential materials for achieving carbon neutrality. M. Ogura lab is designing solid catalysts, particularly using ordered porous materials (such as zeolites and metal-organic frameworks (MOFs)) whose structures are defined at the atomic level. These materials are recognized for their high catalytic activity and can be easily modeled using computational science. Recently, we successfully developed a catalyst for producing city gas from air (CO_2 hydrogenation catalyst) and a catalyst for the decomposition of greenhouse gases (methane combustion catalyst) by the prediction of the structure and activity of the catalysts through computational science.

- CO_2 capture/hydrogenation catalyst prepared from MOFs**

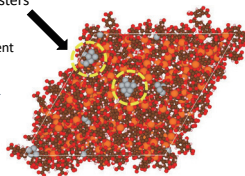
Ni-MOF-74 on Mg-MOF-74

Ni clusters

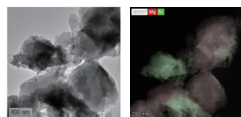


Before

Thermal treatment simulation

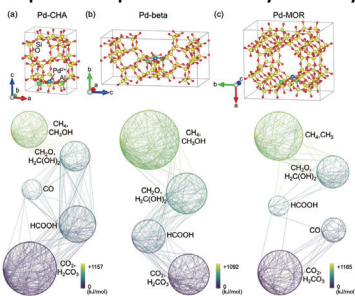


After



Confirmed by experiments

- Computational prediction of catalytic activity for methane combustion catalysis**

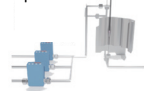


Exploring complete reaction maps

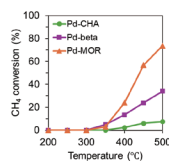
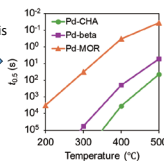
Computation



Experiment



Kinetic analysis



Predicting the catalytic activities

