Methodology for developing high-performance automotive catalysts and secondary batteries

Research Project Outline for 2nd Phase（FY2016–2018）

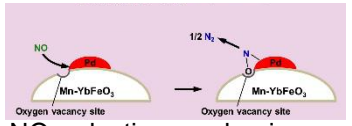
PGM reduction in automotive catalysts and high-performance sodium batteries

◎Understanding the effects of supports in catalytic reactions and searching for novel catalyst supports

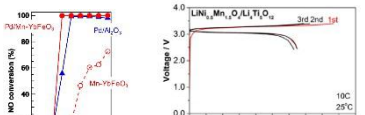
◎Development of sodium batteries with highly concentrated electrolytes

◎Long-time simulation and in-situ observation of chemical processes

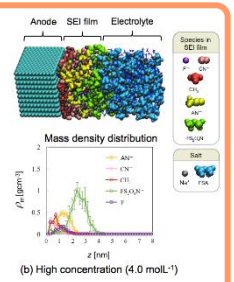
→**Proposing prototypes of PGM-reduced three-way catalysts and high-performance sodium battery systems and elucidating the reaction mechanisms to develop novel catalyst and battery materials**



NO reduction mechanism



Aqueous electrolytes



Simulation

Research Results (FY2016–2018)

◆ Fire-extinguishing organic electrolytes for safe batteries

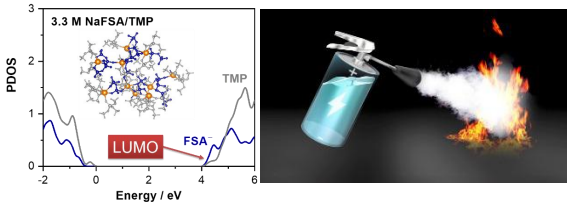
✓Ultimately safe concentrated electrolytes with high-voltage resistance

✓Long cycle life achieved by salt-derived passivation resulting from peculiar frontier orbital characters

✓Unique coordination structure revealed through experiments and simulations

A new electrolyte design strategy toward high-energy-density, large-scale, long-life, and safe rechargeable batteries

J. Wang, Y. Yamada, K. Sodeyama, E. Watanabe, K. Takada, Y. Tateyama, A. Yamada, Nat. Energy 2018, 3, 22-29. **JP2017-215587**



Peculiar LUMO character results in functional anion-derived passivation to achieve fire-extinguishing battery electrolytes.

◆Mn-modified hexagonal $YbFeO_3$ – a three-way catalyst

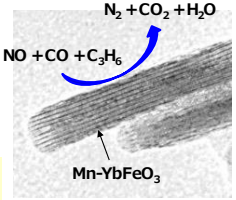
✓NO reduction by oxygen vacancy. An MvK-type NO reduction mechanism based on theoretical predictions

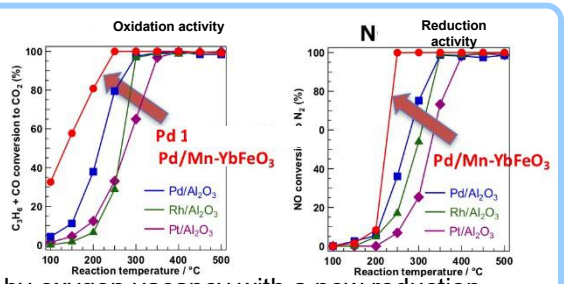
✓Pd is a promoter that functions as supply gates of NO, resulting in a lower NO reduction temperature

A new type of MvK mechanism for NO reduction

S. Hosokawa, R. Tada, T. Shibano, S. Matsumoto, K. Teramura, T. Tanaka, Catal. Sci. Technol. 2016, 6, 7868-7874.

PCT/JP2016/057771





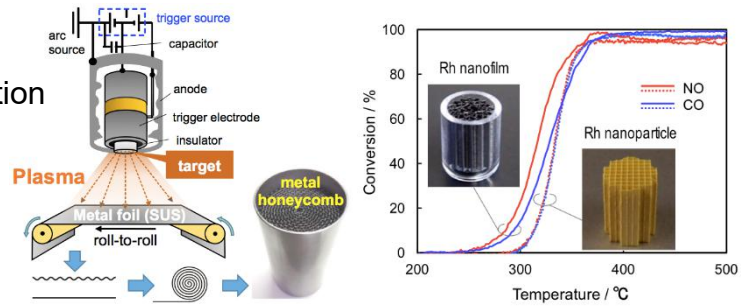
NO reduction by oxygen vacancy with a new reduction mechanism, enhancing low temperature activity compared with Al_2O_3-supported PGM catalysts and reducing the amount of catalyst to 1/10.

◆High TOF Rh nanofilm catalyst – novel TWC

✓Novel preparation of Rh nanofilm catalyst using arc plasma deposition
✓Very high TOF for NO reduction
✓1/3 lower Rh loading compared with Rh powder catalyst

Demonstration of the dependence of efficient NO reduction on Rh crystal surface

S. Misumi, H. Yoshida, S. Hinokuma, T. Sato, M. Machida, Sci. Rep. 2016, 6, 29737. **JP2015-166264**



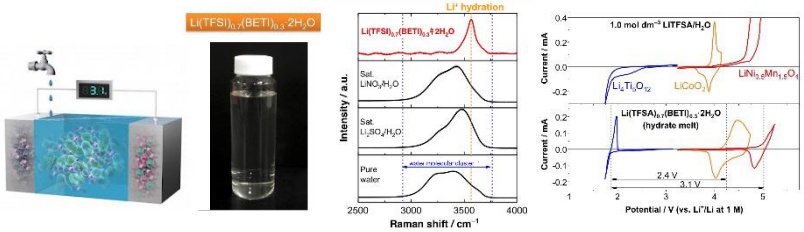
Metal honeycomb catalyst fabricated from Rh nanofilm on SUS foil using arc plasma deposition shows high activity for NO reduction with 1/3 lower Rh loading.

◆3.1 V aqueous batteries with novel hydrate-melt electrolyte

✓Aqueous electrolytes with > 3 V potential window
✓Unusual coordination state of water molecules
✓Safe, high-voltage, high-rate, and inexpensive batteries

A new class of aqueous electrolyte toward safe and high-performance batteries

Y. Yamada, K. Usui, K. Sodeyama, S. Ko, Y. Tateyama, A. Yamada, Nat. Energy 2016, 1, 16129. **PCT/JP2016/000167**



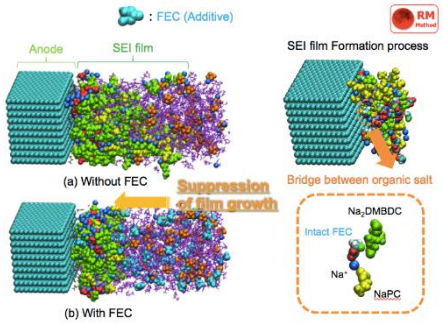
No hydrogen bond is observed in hydrate-melt. All water molecules are coordinated to Li^+ ions, which was confirmed by simulation. The voltage window was extended to realize high-voltage aqueous batteries.

◆Long-time simulation of SEI film formation by Red Moon method

✓Long-time simulation through a combination of the MC and MD methods.
✓Efficiently improves repeated cycle properties for precisely reproducing formation of SEI films. Also applicable to catalytic reactions.

Long-time simulation of SEI film formation

N. Takenaka, H. Sakai, Y. Suzuki, P. Uppula, M. Nagaoka, JPCC 2015, 119, 18046-18055.
N. Takenaka, T. Fujie, A. Bouibes, Y. Yamada, A. Yamada, M. Nagaoka, JPCC, 2018, 122, 2564-2571.



Simulation of SEI film formation by Red Moon method, which reproduced the difference in reactions with and without additives.