Elements Strategy Initiative for Catalysts and Batteries　　Director: Tsunehiro Tanaka (Kyoto University)

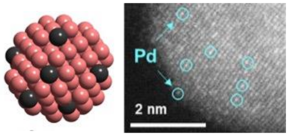
Methodology for developing high-performance automotive catalysts and secondary batteries

Research Project Outline for 3rd Phase (FY2018-2021)

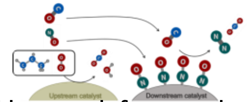
PGM reduction in automotive catalysts and high-performance sodium batteries

◎Developments of noble-metal-free catalyst systems based on reaction mechanisms.
◎Elucidation of metal-support interaction and design of high-performance catalysts.
◎Practical and rational developments of sodium ion batteries.
◎Searching novel electrolytes with safety and high-performance.

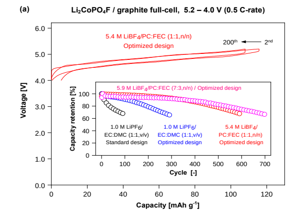
→Developing technologies for PGM-reduced three-way catalysts and high-performance sodium battery systems and elucidating the reaction mechanisms to develop novel catalyst and battery materials.



Cu_9Pd_1 single−atom catalyst



Noble−metal−free catalysts with tandem configuration



High voltage full cell with superconcented electrolyte

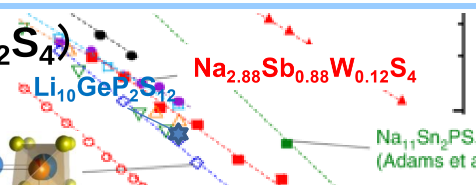
Research Results (FY2019)

◆ Na solid electrolyte superior to Li systems（$Na_{2.88}Sb_{0.88}W_{0.12}S_4$）

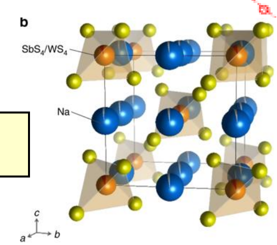
✓Formation of Na vacancies by substitution of Sb^{5+} in Na_3SbS_4 with W^{6+}
✓150 times increase in conductivity compared to Na_3SbS_4
✓High stability: suppression of H_2S generation even at high humidity, indicating the possibility of total solid Na batteries

32 mS cm^{-1} by introduction of Na vacancy at room temperature

A. Hayashi, N. Masuzawa, S. Yubuchi, F. Tsuji, C. Hoteyama, M. Tatsumisago, et al., Nature Commun. 10, 2019, 10, 5277.



Comparable to β−alumina at 500℃



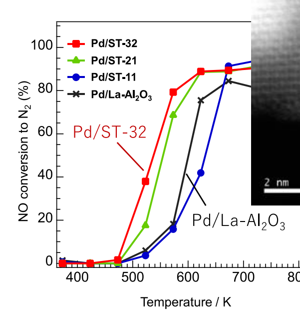
Structure of $Na_{2.88}Sb_{0.88}W_{0.12}S_4$
1−D Na conduction path (blue)

◆ Interaction between catalysis supports with high anchoring effect and metals in $Pd/Sr_3Ti_2O_7$

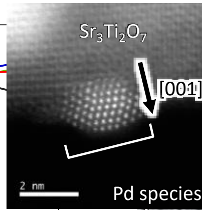
✓$Pd/Sr_3Ti_2O_7$: three-way catalyst with high thermal stability superior to benchmark catalysts
✓Pd atom is epitaxially supported due to metal-support interaction through oxygen atom (anchoring effect). Constant particle size ～2 nm during aging.

High activity after aging at 1000 ℃ due to high anchoring effect

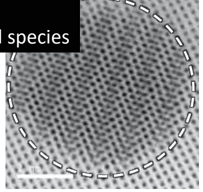
S. Hosokawa, C. Watanabe, T. Tanabe, H. Asakura, K. Teramura, T. Tanaka, To be published in Appl. Catal. B



High activity of NO reduction



dark field



bright field

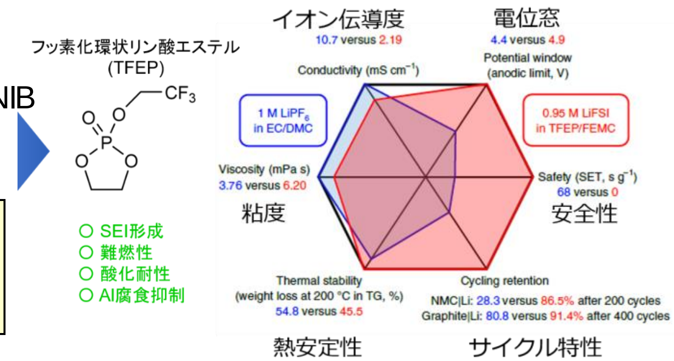
Pd atom is epitaxially supported on lattice plane
Stripes due to mismatch in atomic distances

◆TFEP: novel solvent for electrolyte with safety and high-performance

✓Rational design and synthesis of solvent molecules applicable to LIB and NIB
✓SEI formation, flame retardance, oxidation resistance applicable to design of batteries with safety, high-voltage, and long-life.

> Rational design of solvent molecules with high-performance:
> SEI formation; five-membered ring, oxidation resistance; F(fluorine), flame retardance; P(phosphorus)

Q. Zheng, Y. Yamada, R. Shang, S. Ko, Y. Lee, K. Kim, E. Nakamura, A. Yamada, Nature Energy., 2020, 5, 291-298.



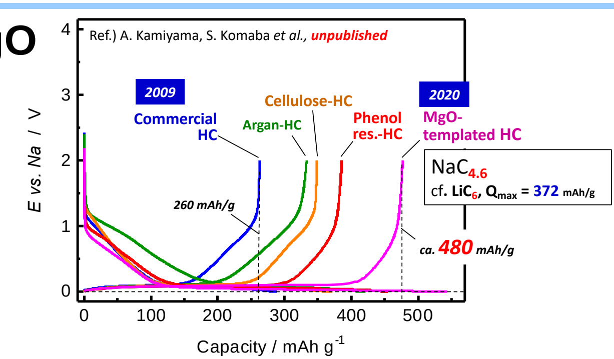
Excellent properties of TFEP solvent as electrolyte

◆ Synthesis of hard carbon of high capacity using MgO

✓New synthesis method of hard carbon with micropores using magnesium gluconate/glucose as precursors
✓Ratio of carbon stored in sodium: $NaC_{4.6}$, 480 mA h g^{-1}.

> Successful synthesis of hard carbon with micropores of high capacity（480 mA h g^{-1}）

A. Kamiyama, K. Kubota, S. Komaba, et al.,presented in 6th International Conference on Sodium Batteries, Naperville, USA 2019 November



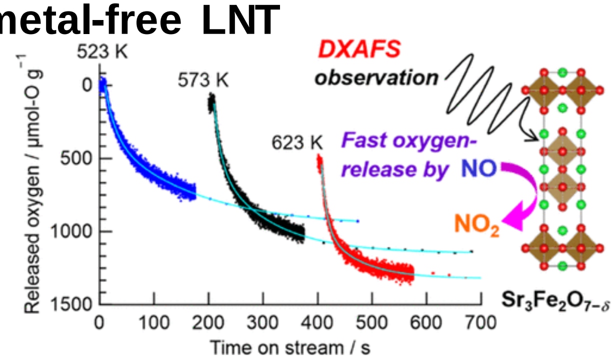
Two-fold increase in capacity of hard carbon in 8 years

◆ NO reduction by lattice oxygen in $Sr_3Fe_2O_7$: noble-metal-free LNT

✓Development of Pt-free LNT superior to $Pt/Ba/Al_2O_3$
✓Layered perovskite $Sr_3Fe_2O_7$ oxidizes NO in SrFe perovskite layer and stores NO_2 in SrO rock salt layer, showing dual function materials.
✓Rate determining step of NO reduction is diffusion process of lattice oxygen

> Elucidation of mechanisms of NO reduction in NOx stored $Sr_3Fe_2O_7$ catalyst

K. Tamai, S. Hosokawa, K. Ohnishi, C. Watanabe, K. Kato, H. Okamoto, H. Asakura, K. Teramura, ACS Catal. 2020, 10, 2528-2537



Dynamics of NO reduction by lattice oxygen