

## Principles and Their Applications Created by ESICB, Kyoto University

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Elements Strategy Initiative for Catalysts and Batteries (ESICB) has two distinct targets in elements strategy as found in its name. One is the reduction of the use of platinum group metal elements (PGM) and/or the replacement of PGM to base metals in automotive catalysts by enhancement of catalytic activity. The other is the creation of high-performance secondary batteries without critical elements like lithium, cobalt, etc.

(1) 'Three-way-catalyst (TWC)' works for the simultaneous removal of the residual hydrocarbons (HC) and the CO produced by incomplete combustion, by oxidation and nitrogen oxides (NO) by reduction from exhaust gas from automobile engine. The active component of TWC is platinum group metals (PGM). Most of the consumption of PGM is the use in TWC and hence reduction of PGM use and/or replacement of PGM to base metals is one of the urgent problems to be solved.

So far, it has been thought that reduction of NO takes place on the surface of PGM. Therefore keeping high dispersion of PGM on the support to guarantee the high specific surface area is the key to the reduction of the use of PGM. Our theoretical consideration and experimental study of single site catalysis shows that CO oxidation proceeds not only on a PGM atom but with a peripheral surface lattice oxygen, i.e., by Mars van Krevelen (MvK) mechanism. In MvK mechanism, CO is oxidized by lattice oxygen to form the oxygen vacancy and the vacancy is re-oxidized by an oxygen molecules. We proposed the possibility that the oxygen vacancy would be re-oxidized by the NO molecules.

We used the metal oxides like Mn-*h*-YbFeO<sub>3</sub> and Sr<sub>3</sub>Fe<sub>2</sub>O<sub>7</sub> and reduced them to produce oxygen vacancies. And then NO gas was flowed to the samples and we found the formation of N<sub>2</sub> gas. By the MvK mechanism by NO molecules, the TWC catalytic activity was enhanced resulting in the reduction of PGM use.

(2) Our study started with the aim of development of the materials with high energy density by replacement of Li to Na in lithium ion batteries. Because the number of candidate electrode materials of Na-containing compounds is much larger than those of Li-containing compounds due to the difference of ionic radii between Li and Na, we have developed many positive and negative electrode materials for Na ion batteries so far. Above all, alluaudite material consisting of Na, Fe and sulfate ions for a positive electrode and MXene consisting of Na, Ti carbide sheet for a negative electrode are noteworthy. Alluaudite sulfate shows higher voltage than 3 V comparable to LIB and high rate for charge/discharge and diffusion rate of Na ions are very high estimated from theoretical calculation. Na incorporation into MXene negative electrode is not due to formation of chemical bond by electron transfer but due to the adsorption like charge accumulation in a capacitor. From the view of the safety, we have developed ionic liquid as electrolytes. Relating to ionic liquids, we firstly developed super-concentrated electrolytes; while concentration of conventional electrolytes is 1 M, that of newly developed electrolytes are higher than 4 M. In the super-concentrated electrolytes, the simulation shows that all the solvent molecules are coordinated to Na/Li ions and interestingly activity of solvent is close to zero, indicating no vapor. If the solvent are water molecules, the system would be free from potential window and could deal with high voltage electrodes. This electrolyte can be applied to the battery cell of not only nonflammable but also extinguishing.

### Bibliography

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