



# Analysis of transition metal single atom catalyst for electrochemical CO<sub>2</sub> reduction

Park Gi-Dong<sup>1</sup>, Suchada Sirisomboonchai<sup>1</sup>, Koyo Norinaga<sup>1</sup>

<sup>1</sup>Department of Chemical Systems Engineering, Graduate School of Engineering, Nagoya University

キーワード : Electrochemical CO<sub>2</sub> reduction, Single atom catalyst

## 1. 背景と研究目的

Single-atom catalysts (SACs) have a unique structure composed of small reaction sites and a well-defined linkage surface. Owing to their unique electronic configuration, isolated metal atoms constitute excellent catalytic sites<sup>[1]</sup>. The geometric/electronic structure of the metal center of SACs critically impacts the catalytic performance and reaction pathway that is determined by the adsorption/ desorption of reactants and intermediate species and energy barriers for each reaction step. The local coordination environment can serve a crucial role in regulating the electronic properties of the metal center. Thus, the introduction of heteroatoms into carbon matrix was tried to enhance the electrochemical reaction kinetics. Herein, we verify the influence of heteroatoms doping.

## 2. 実験内容

Ni SAC is well known for its high performance for electrochemical CO<sub>2</sub> reduction to CO. In here, we prepared the several types of SAC to modulating the electronic nature of Ni by doping hetero-transition metal such as Zn and Mn. The Ni-, Zn-, and Mn-phthalocyanine and foil was used as a reference materials.

## 3. 結果および考察

The absorption edge energy is positively correlated with the oxidation state. As depicted in Ni K-edge XANES spectra (Fig. 1), compared to Ni Pc and Ni foil, the detected absorption edge energy of the prepared SACs indicate that Ni sites have an oxidation state between 0 and +2. Furthermore, the different energy results of prepared SACs revealed the electronic interaction between Ni and doped heteroatoms. The feature I indicated that the local coordination structure of Ni sites in Ni-N-C was highly disordered and defective. The weakness of feature II in the prepared SACs indicated the structural asymmetry of Ni sites. The intensity ratio of feature III to IV represented the significant displacement of the Ni sites; its increase further reflected the existence of structural asymmetry.

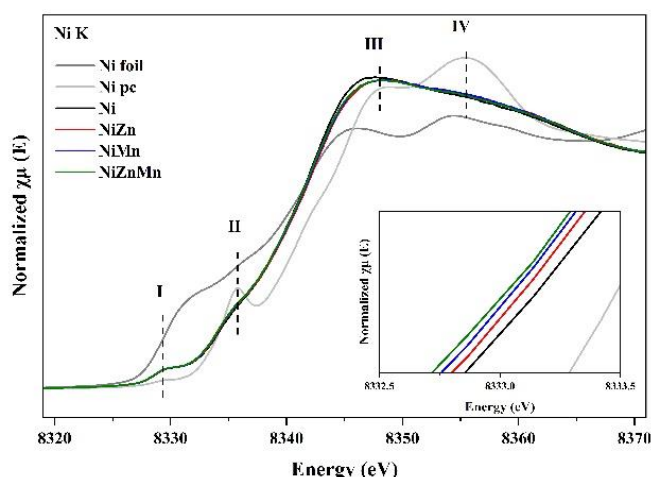


Fig. 1 Ni K-edge XANES spectra

## 4. 参考文献

1. GD. Park, S. Sirisomboonchai, K. Norinaga, ChemSusChem **2023**, 16, e202300530