論文 / 著書情報
Article / Book Information

題目(和文)	
Title(English)	Discovery of subnanoparticles for multi-electron transfer reaction
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出典(和文)	学位:博士(工学), 学位授与機関:東京工業大学, 報告番号:甲第12210号, 授与年月日:2022年9月22日, 学位の種別:課程博士, 審査員:山元 公寿,荒井 創,山口 猛央,和田 裕之,今岡 享稔
Citation(English)	Degree:Doctor (Engineering), Conferring organization: Tokyo Institute of Technology, Report number:甲第12210号, Conferred date:2022/9/22, Degree Type:Course doctor, Examiner:,,,,
学位種別(和文)	博士論文
Category(English)	Doctoral Thesis
種別(和文)	要約
Type(English)	Outline

（博士課程）

論文の要約

系・コース：応用化学系応用化学コース	申請学位：　博士（工学）
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This thesis entitled “Discovery of subnanoparticles for multi-electron transfer reaction” consists of 5 chapters.

In the first chapter, the properties and research advances of SNPs (subnanoparticles) that distinguish from NPs (nanoparticles) were introduced. Moreover, the current status about catalysts applied in multielectrons transfer reaction (HER, ORR, OER and etc) and the current status of applying machine learning (ML) in chemistry were introduced. To discover SNPs with good catalytic performance was the aim of this thesis.

In the second chapter, comprehensive and systematically synthesis of SNPs and NPs were described. The optimization of synthetic conditions of APD (arc plasma deposition) were discussed Characterizations such as STEM, mapping, XPS about for confirmation synthesis of SNPs and NPs were described and summarized in details.

In the third chapter, systematical analysis and investigation about SNPs and NPs for HER was investigated. The results revealed that positive synergistic effect and negative synergistic effect were found in SNPs and NPs, respectively. The strongest positive synergistic effect was found in PtZr SNPs, quantification of bonds was performed on PtZr SNPs to investigate the mechanism of strongest positive synergistic effect on PtZr SNPs.

In the fourth chapter, ML (machine learning) was carried to confirm the hypothesis that ubiquitous homogeneous alloying of atoms in SNPs makes them more predictable than NPs, in which phase segregation is unpredictable. In addition, ML revealed that the key factors that distinguish SNPs and NPs were the different correlation of work function to HER activity between SNPs and NPs. Investigation about the mechanism of strong correlation of work function and HER was performed. Moreover, ML algorithm with high prediction accuracy was constructed to accelerated the discovery of SNPs for HER.

In the fifth chapter, ML was applied to confirm the hypothesis that subnanoscaling can lead to the multifunctionalization of catalysts. HER, ORR and OER were selected as the target reactions. ML revealed that the key factors that matter in discovery of multifunctional catalysts were work function in both SNPs and NPs. To accelerated the discovery of multifunctional SNPs, three ML

algorithms were constructed. The results revealed that 65 SNPs could be multifunctional catalysts among 575 combinations.