【Grant-in-Aid for Scientific Research (S)】

Broad Section E

Title of Project : Innovative Functions Originating from Unexploited Electronic States in Nanowire Metal Complexes

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Research Project Number : 19H05631 Researcher Number : 60167707

Keyword : Nanowire complex, Electronic property, Strongly correlated electron system, Coordination polymer

【Purpose and Background of the Research】

Discovery of new electronic states in solids often develops new functions and research fields. For instance, conductive organic polymers, superconducting copper oxides, carbon nanotubes and graphene have been widely investigated because of their unique electronic states. Thus, it is important to develop the materials which have multistability of electronic states.

One-dimensional (1D) electron system intrinsically provides various electronic states and characteristic electronic properties based on the strong correlation between electrons and lattice. Therefore, the 1D electron system is key to create a platform for exploring new electronic states and properties. In this research, we especially focus on quasi-1D halogen-bridged metal complexes (MX chains), which have high tunability and rich electronic properties derived from organic and inorganic components, respectively. We believe that the development of new electronic states in MX chains will give us the unprecedented innovative electronic functions.

【Research Methods】

[1] Creation of innovative electronic functions based on Pt(III) averaged valence state

MX chains have the bistability of electronic states (i.e. M(III) averaged valence (AV) state and M(II/IV) mixed valence (MV) state). Although Pt complexes are most promising for achieving the high functionalities, all Pt complexes reported so far form MV state. In this subject, the techniques which successfully stabilized AV state in Pd complexes will be applied to Pt complexes (e.g. attractive force between alkyl chains and multiple hydrogen-bond networks).

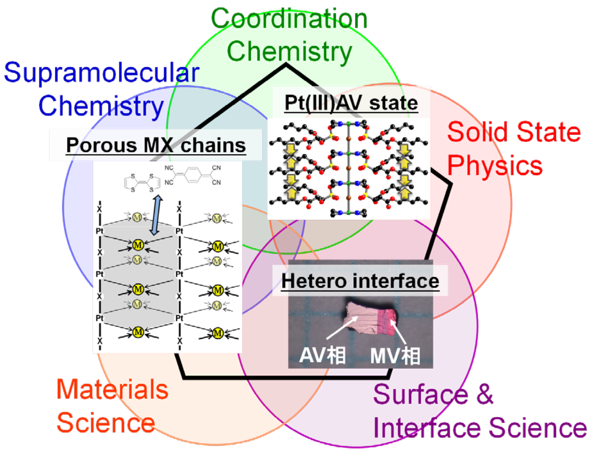
[2] Development of new electronic structures in nano and hetero interface

Heterojunction crystals and superstructures will be fabricated by epitaxial crystal growth from solution by using electrocrystallization. The electronic structure around the interface will be detected by STM and Raman spectroscopy. Moreover, we fabricate the heterojuction of p-type and n-type semiconducting MX chains to study the characteristics of the single-crystalline device.

[3] Modulating band filling by chemical doping in porous MX chains

In contrast to inorganic materials, it is quite difficult to achieve chemical doping in molecular crystals by ion substitution or defect, because the molecules have a certain size. To overcome this problem, we introduce porosity to MX chains and conduct carrier injection by the redox reaction with guest molecules.

【Expected Research Achievements and Scientific Significance】



In addition to the enhancement of gigantic third-order nonlinear optical susceptibility, various novel properties such as metallic conduction, diode characteristic, molecular-responsible switching will be developed. Moreover, the control of band filling should enhance the understanding of molecule-based materials with 1D electron system.

【Publications Relevant to the Project】

1) M. R. Mian, H. Iguchi, S. Takaishi, M. Yamashita et al., Multiple-Hydrogen-Bond Approach to Uncommon Pd(III) Oxidation State: A Pd−Br Chain with High Conductivity and Thermal Stability. *J. Am. Chem. Soc.* **139**, 6562–6565 (2017).

2) S. Kumagai, S. Takaishi, H. Iguchi, M. Yamashita, Charge-bistable Pd(III)/Pd(II,IV) coordination polymers: phase transitions and their applications to optical properties. *Dalton Trans.*, **44**, 8590–8599 (2015).

【Term of Project】 FY2019-2023

【Budget Allocation】 152,900 Thousand Yen

【Homepage Address and Other Contact Information】

http://coord.chem.tohoku.ac.jp/~sakutai/