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

Chemistry of Synergistic Interface Space for Trace Detection, Separation, Conversion of Toxic and Harmful Substances

Principal Investigator	Kyoto University, Institute for Advanced Study, Distinguished Professor KITAGAWA Susumu	Researcher Number:20140303
Project Information	Project Number : 22H05005 Keywords : PCP/MOF, hybrid materials, synergistic functions, trace detection/capture/conversion	Project Period (FY) : 2022-2026

Purpose and Background of the Research

●Outline of the Research

Our surroundings are full of toxic and harmful substances. Thus, it is important to explore methods of trace detection, separation, conversion of harmful substances. In general, hybridization is classified as a method of combining materials that complement each other's function to produce superior properties. As a representative example, cellular membranes incorporate proteins into the lipid bilayer to cooperatively and synergistically exhibit various functions. In this project, porous coordination polymers (PCPs) with spatial functions (such as capture, concentration, storage, and transport) and inorganic substrates with electron, phonon, photon transport capabilities are hybridized to generate highly functional hetero-interfaces. The goal of this project is to understand and control such " synergistic interface space" with the ability of trace detection, separation, conversion of harmful substances and to produce results that meet social demands (Figure 1).

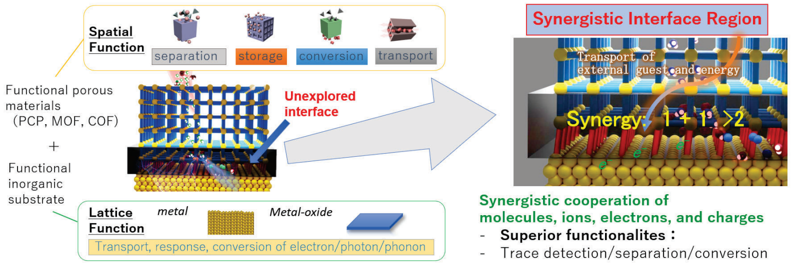

Figure 1. A schematic image of "Chemistry of Synergistic Interface Space"

●Research Background and Purpose

Previous work aimed to deepen the interface chemistry that integrate PCPs with different functionalities. The previous goal of the project was to establish the "chemistry of adaptable space", which responds to the external stimuli by generating and amplifying "flow" (JSPS Propos. No. 18H05262). Based on the results over the past few years, we have recognized a new goal for the further development of the PCP chemistry.

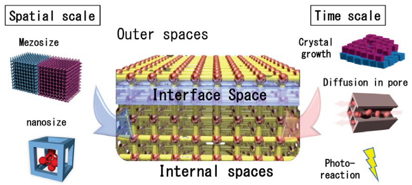

Figure 2. A schematic image of "Chemistry of Adaptable Space"

The integration between PCPs can enhance their spatial functions, but is insufficient to provide conversion functions. Inorganic materials, such as metal oxide (MO) must be integrated with PCPs to reinforce their lattice functions. In particular, the development of interface chemistry that creates continuous and synergistic interface between the regular atomic lattice structure of MO surface and the regular porous surface of PCPs is extremely important, and will undoubtedly bring about a major paradigm shift in the development of functional materials and devices in the future.

● Methods

The key issues in creating the synergistic interface space are the surface design of functional PCPs and the development of organic fusion methods between PCPs and hetero-materials. In other words, it is essential to develop interface-focused nanospace chemistry and their manipulation from a comprehensive viewpoint of size, scale, charge, and molecular motion. This research will improve upon the chemistry of porous materials pioneered by our group, and establish the following three pillars. This work will facilitate the creation of highly functional hybrid materials that can efficiently detect, separate, and decompose toxic and harmful substances.

(1) Organic hybridization and fusion of dynamic nanospaces and interface spaces
(2) Understanding dynamic phenomena using in-situ observation in dynamic nanospace and interface space
(3) Computational chemistry for comprehensive understanding of synergistic functions and design using data science

Expected Research Achievements

In this research project, we will address the following issues by creating a synergistic interface between PCPs with spatial functionalities and inorganic substrate materials with charge and electron transport properties.

● Highly sensitive detection

Currently, the limit of detection (LOD) of a well-trained olfactory dog is around several hundred parts per trillion (ppt). Although significant progress has been made in non-contact, real-time artificial sensors, the best sensors can only rival but cannot succeed the ppt sensing capabilities of animals. Thus, an outstanding scientific challenge is to create an artificial system that significantly exceeds the sensitivity, selectivity, and sensing speed of animal olfactory systems. In this project, PCP crystals with high affinity and selectivity for analytes will be grown on inorganic substrates. Concerted design of the synergistic interfaces that enable selective adsorption of the target molecules will dramatically improve the detection capability.

● Highly efficient decomposition and conversion of toxic substances

The air in living spaces often contains chemical substances that are harmful to humans and the ecosystem, such as volatile organic compounds (VOCs) originating from antiseptics, paints, and factory and car exhaust. It is desirable for developing devices that can efficiently decompose these harmful substances. To achieve that, the process of selectively capturing target substances is important. In this project, we will utilize the advanced capture and concentration function of PCP and integrate them with a conversion function (catalytic function by light, etc.) at the interface with MO as in the above non-contact sensor.

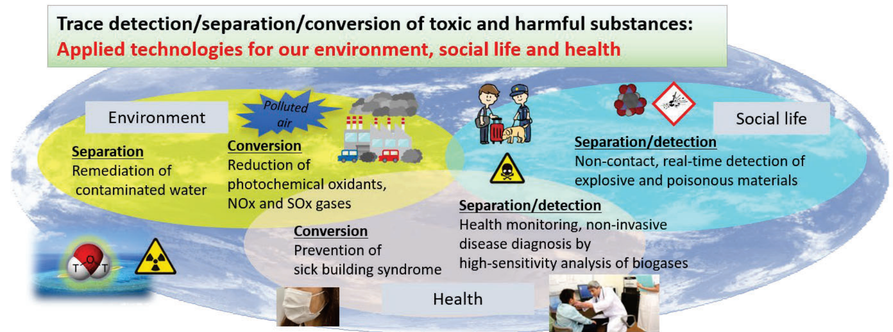

Figure 3. Potential social impact of this research

Homepage Address, etc.	iCeMS Kitagawa Laboratory HP: http://www.kitagawa.icems.kyoto-u.ac.jp/ Twitter: @KitagawaGroup