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

# Establishment of Academic Theory of Science of Water in Nanospace and Creative Development of Novel Self-Organized Nanostructured Membranes


| | |
|---|---|
| Principal Investigator | Shinshu University, Institute for Aqua Regeneration, Specially Appointed Professor<br>KATO Takashi Researcher Number : 70214377 |
| Project Information | Project Number : 25H00425 Project Period (FY) : 2025-2029<br>Keywords : Self-Organization, Water Treatment Membrane, Nanostructure, Hydrogen Bonding, Liquid Crystal |


## Purpose and Background of the Research

**●Outline of the research**

Water is essential for our lives and environment. Ensuring safe and high-quality water supply is an important global issue for sustainable society. Membranes have been used as important materials for obtaining high-quality water with lower energy consumption. However, the size and morphology of the pores in conventional membranes were not uniform. The purpose of the present study is development of high-performance water treatment membranes and creation of science of water in nanospace and new membrane science for separation based on self-organized nanostructured liquid-crystalline (LC) membranes forming uniform and ordered pores. We aim to achieve highly selective separation of useful substances and complete removal of harmful substances by using nanostructured LC membranes and amphiphilic self-organized polymers (Figure 1).

The structures of water molecules in the nanospace inside the pores of the membranes are revealed by advanced infrared spectroscopy, molecular dynamics simulations, and electrochemical measurements. New science of water treatment separation membranes is developed by studying the relationships between the properties of the water molecules and separation functions of the membranes.

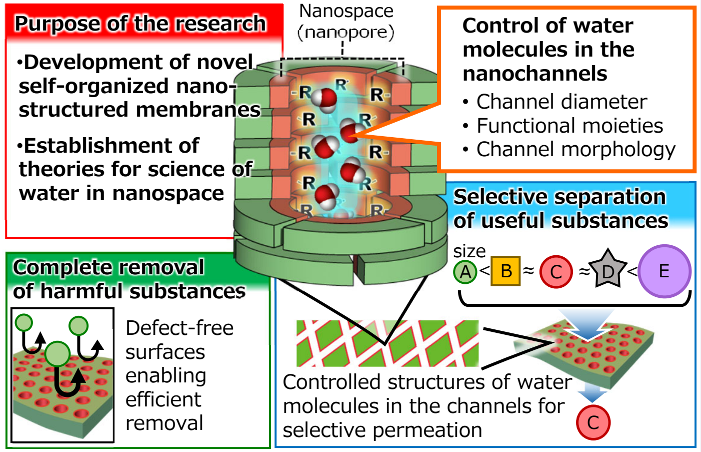



Figure 1. Overview of the present research.

**●Background and Purpose**

Use of membranes, which are thin films with small pores penetrating through both sides, is a facile method to remove unnecessary components from water (Figure 2). For example, the coffee extracts and grinded beans can be separated by using membranes (filter papers) because the pores of the membranes (10–100 μm) are smaller than the beans.

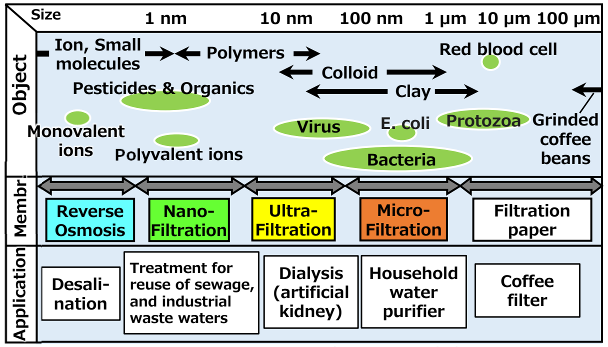



Figure 2. Water treatment membranes and their targets.

Separation of smaller substances from water is possible when the diameter of the pores is smaller. The pores with sub-10 nm allow removal of polymers, viruses, and bacteria (Figure 2). Moreover, the pores with sub-1 nm, which is comparable to sizes of molecules and ions, enable the rejection of salts (sodium and chloride ions) from water. This mechanism has led to the practical applications of reverse osmosis membranes, which converts seawater into drinking water. A key feature of our self-organized nanostructured LC membranes is the formation of uniform pore sizes and morphologies. Moreover, pinhole-free polymer membranes can be prepared by photopolymerization of monomers in the thin-film LC states with fluidic nature.

The principal investigator has shown that structures of water in nanostructured water treatment membranes are closely related to the separation functions (KAKENHI, "Aquatic Functional Materials", FY2019–FY2023).

In the present study, we aim to achieve highly selective separation of useful substances (valuable ions, nanoparticles, synthetic intermediates) and complete removal of harmful substances (harmful metal ions and organic molecules, PFAS, viruses) by development of self-organized nanostructured membranes and establishment of academic theory for science of water in nanospace and new nanomaterials science for water treatment.

## Expected Research Achievements

**● Development of Self-Organized Nanostructured Membranes Exhibiting New Separation Functions**

Nanostructured water treatment membranes having functional moieties inside the nanopores with uniform size and ordered morphology are developed by self-organization of LC molecules and amphiphilic polymers. Highly selective separation of useful substances and complete removal of harmful substances are attempted by considering not only sizes but also chemical properties and interactions with water (Figures 1 and 3). Molecular shape, types of functional moieties, and interactions of the compounds forming these membranes are designed with the help of molecular dynamics (MD) simulation, machine learning using computers, and electrochemical measurements with transistors.

**● Establishment of Academic Theory for Science of Water in Nanospace by Clarification of Structures and Properties of Water in Self-Organized Membranes**

The hydrogen bonding structures, energy states, and dynamic structures of water molecules in nanospace of the membranes are revealed by advanced measurements and MD simulation. These insights lead to establishment of science of water in nanospace of the membranes (Figures 1 and 3).

**●Creative Development of New Science for Separation in Nanospace**

New membrane science for separation in view of water are created by clarifying the relationship between the science of water in nanospace and separation functions of the self-organized nanostructured water treatment membranes (Figures 1 and 3).

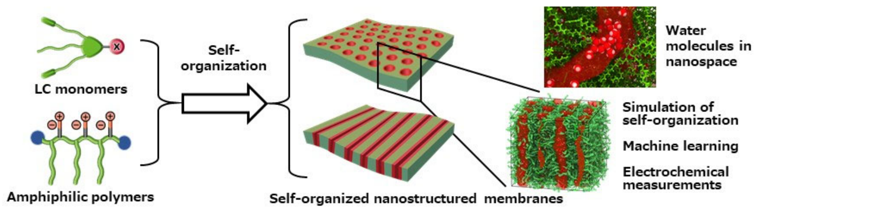



Figure 3. Formation and functionalization of self-organized nanostructured membranes and MD simulation.


| | |
|---|---|
| Homepage Address, etc. | https://researchmap.jp/Kato_UT?lang=en<br>https://kato.t.u-tokyo.ac.jp/index-e.html |