# 馬渕研究室 MABUCHI LAB

生体分子流動システム研究分野

*Biomolecular Flow Systems Laboratory*

# Visualizing the Molecular World

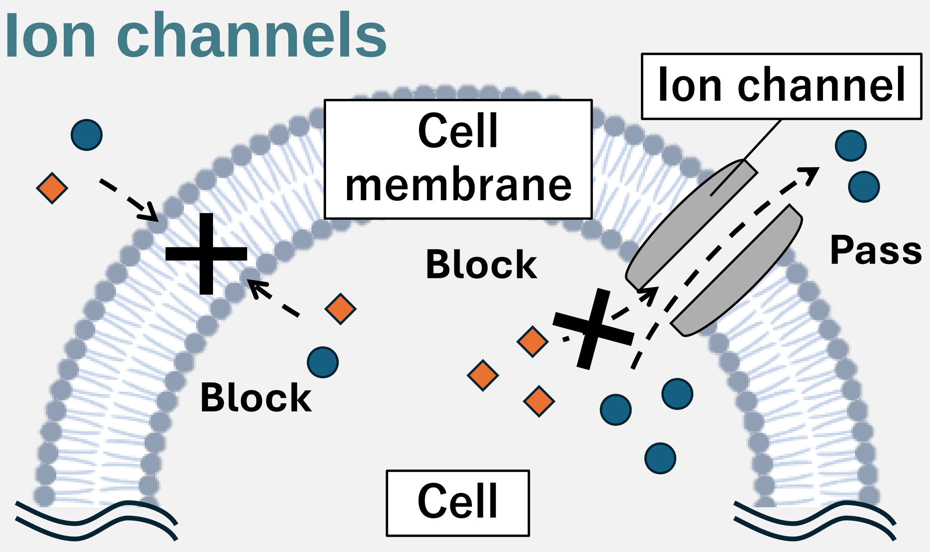
When small molecules, particularly ions, transport through complexly intertwined structures, what paths do they take and how fast can they move (conduct or diffuse)? Ion transport phenomena occurring in the nanoscale world play a crucial role in a wide range of fields, from biomolecules in life sciences to polymer materials in materials science.

We use theoretical approaches (e.g., molecular simulations) to elucidate these phenomena, which are difficult to observe in experiments, on challenging spatiotemporal scales. Our goal is to perform theoretical high-efficiency and high-functionality molecular design, and, in collaboration with experimental groups, we aim for broad applications ranging from engineering applications, such as constructing artificial cells and molecular systems, to medical applications, including drug discovery.

## $K^+$ selective transport by artificial DNA channel

Ion channels exist in the cell membrane and have the function of regulating ion transport. Artificial ion channels that mimic the function of ion channels and have applications in medicine and engineering are attracting attention. Therefore, we aim to design a mechanism to control ion transport by artificial DNA channels by modifying functional groups inside the artificial DNA channels and elucidating the transport mechanism.

### Ion channels




Mimics the transport function of ion channels

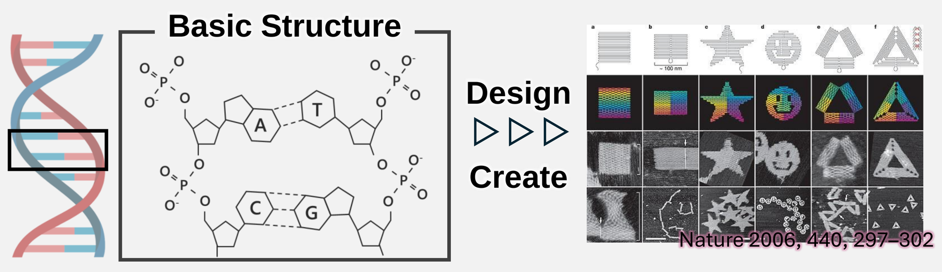
Design of Artificial Ion Channels

Medical Science — Engineering

Drug Delivery — Biosensor, Water Filtration

### DNA nanotechnology

Innovative molecular technology that uses sequence-specific molecular assembly and periodic structure of DNA to design and create nanoscale structures.

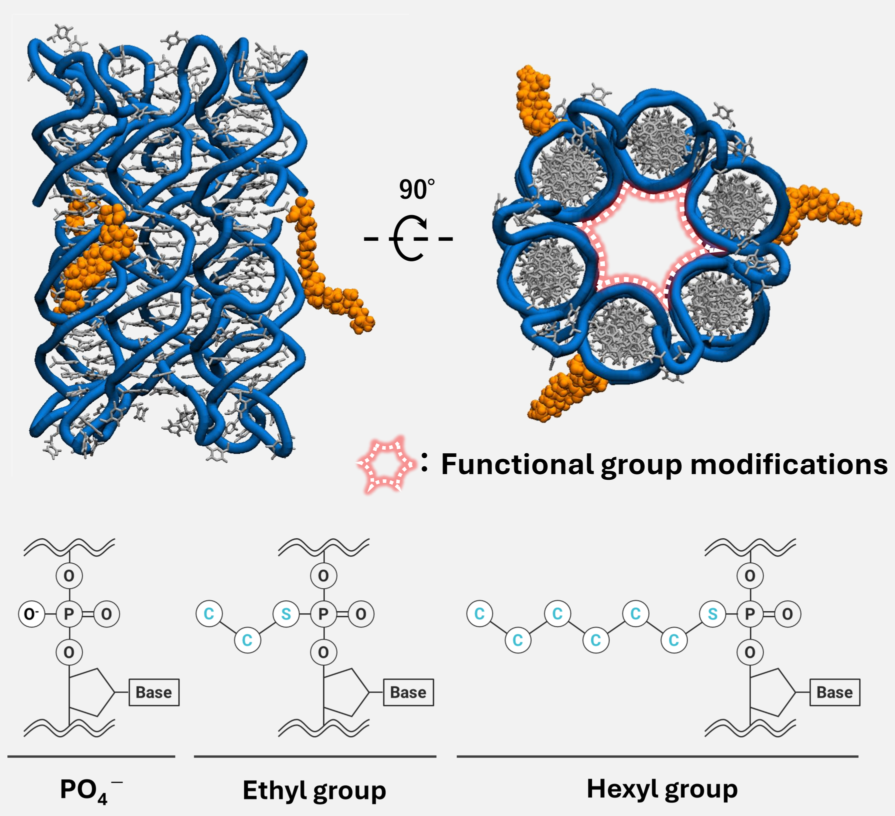


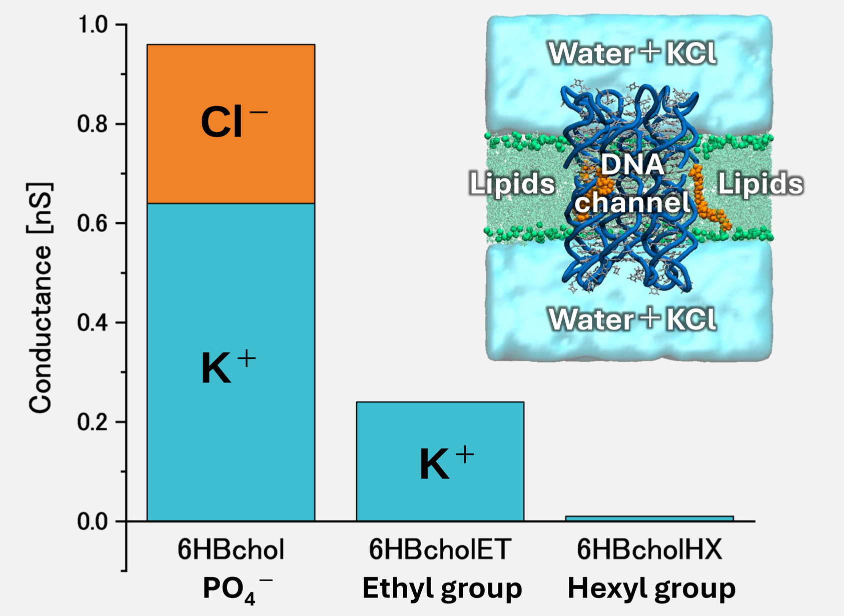

**Advantages**

- Single nucleotide design
- Modifications of other molecules

### Ion Transport Control by Artificial DNA Channel

Using artificial DNA channel, the effects of functional groups inside the channel on ion transport were investigated for the development of $K^+$ sensors.




**Results**

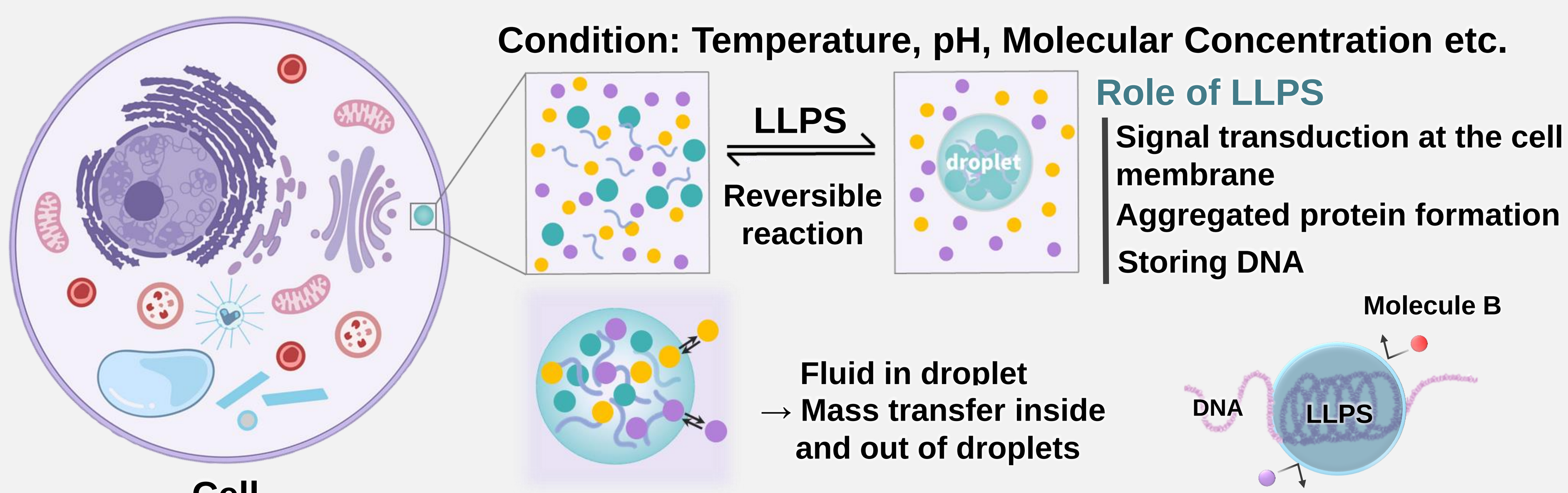
- Functional groups reduce transport
- Enables selective transport to K+

## Molecular uptake by liquid-liquid phase separation (LLPS)

Liquid-liquid phase separation (LLPS) is a phenomenon wherein biomolecules self-assemble under specific condition to form droplets, which holds potential applications in drug delivery. We aim to theoretically design artificial peptide molecules that can selectively uptake target molecules, using elastin-like polypeptides (ELP) as a base material to evaluate the uptake of small molecules into droplets.

### Liquid–liquid phase separation (LLPS)

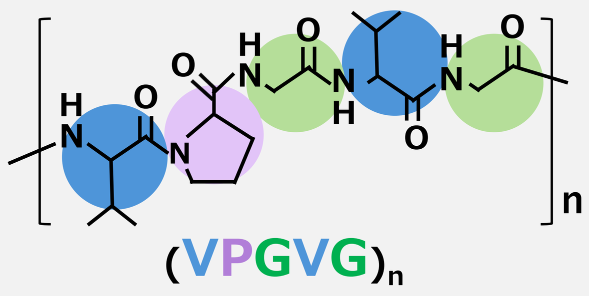
Condition: Temperature, pH, Molecular Concentration etc.




**Role of LLPS**

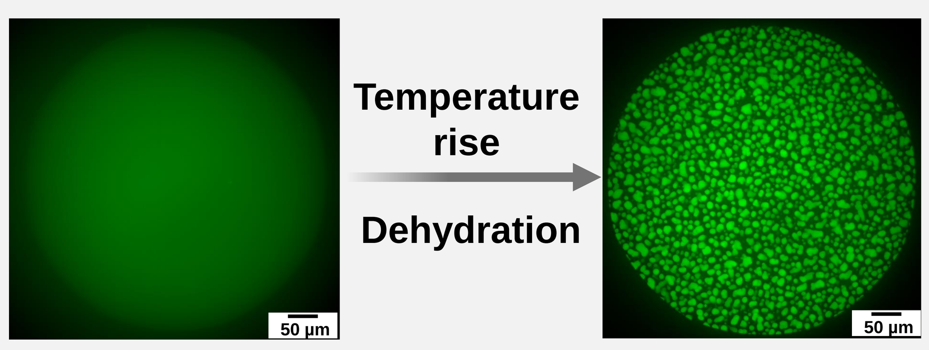
- Signal transduction at the cell membrane
- Aggregated protein formation
- Storing DNA

### Elastin-like polypeptides(ELPs)



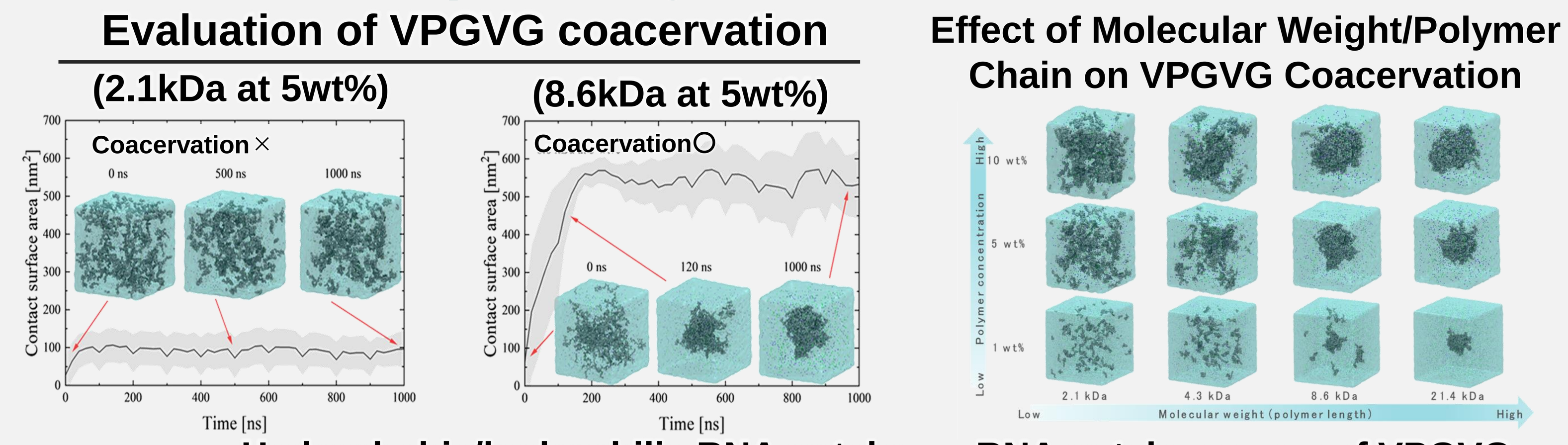

**ELP's property**

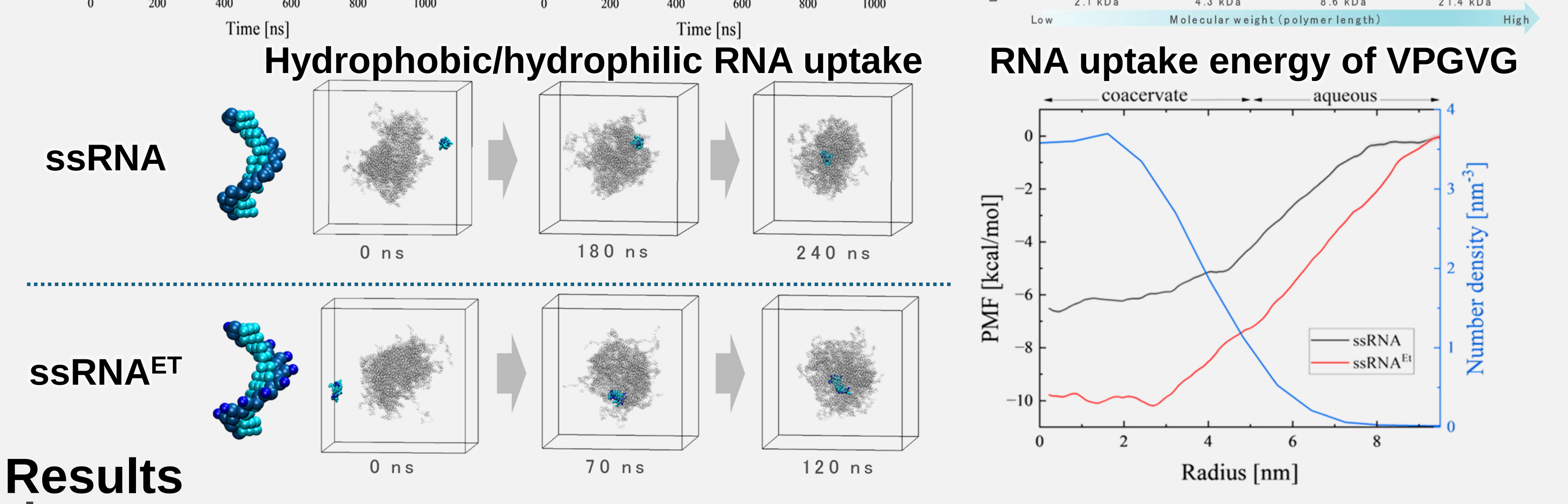
- LLPS induced by temperature rise
- Biocompatibility
- Relatively easy to prepare




V: Valine, P: Proline, G: Glycine, n: peptides length

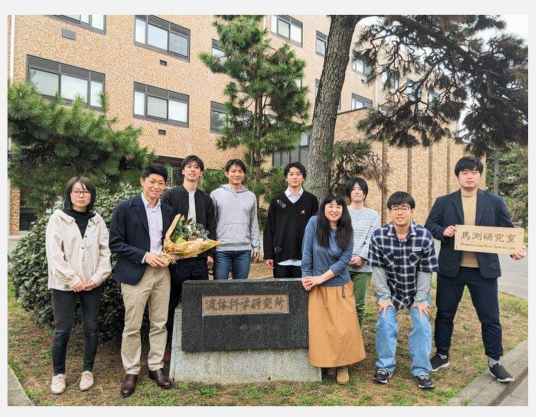
### Biomolecular uptake by VPGVG coacervate




**Results**

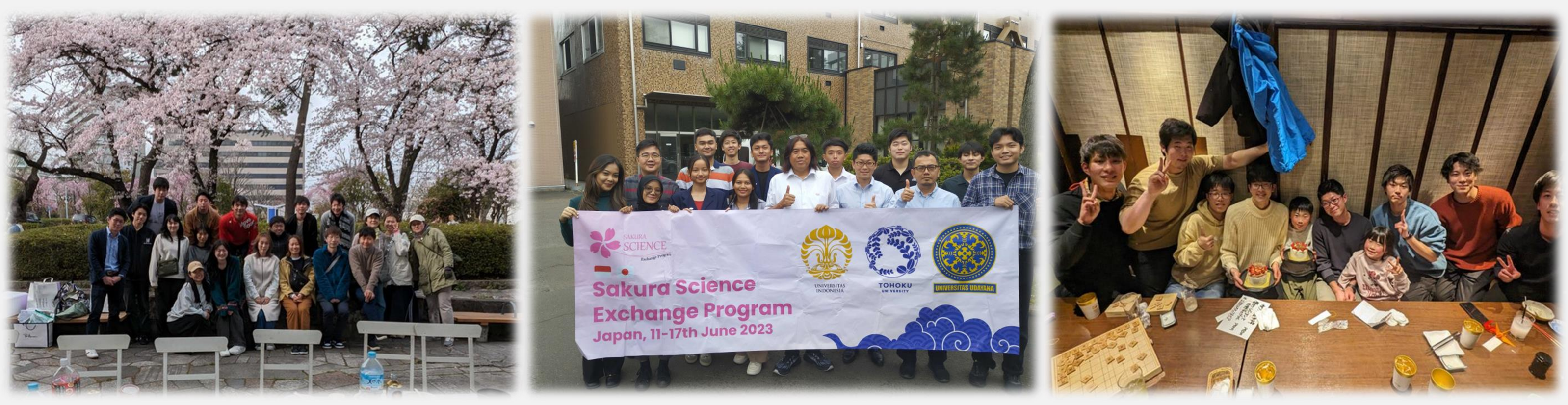
- The coacervation of VPGVG depends on molecular weight and polymer chain length.
- Hydrophobic $ssRNA^{ET}$ is more easily incorporated.




Associate Professor
Takuya MABUCHI


**Events**

- Exchange meeting with collaborators
- Cherry-blossom viewing
- Internship
- Recognition event



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