# Institute of Fluid Science
## KIKUGAWA GR / Molecular Composite Flow Laboratory

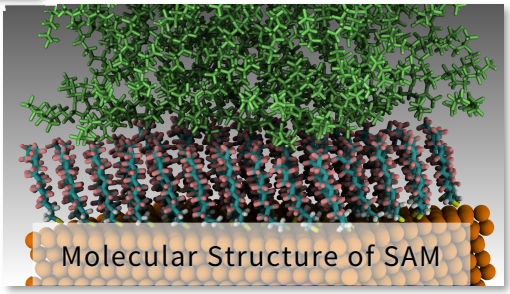
Finemechanics Course  Gota Kikugawa, Associate Professor

From nanoscale to macroscale, various thermal and fluid phenomena, to which composite molecular-scale physics gets engaged, are of critical importance in the wide range of engineering and industrial processes. By using large-scale numerical simulations such as the molecular dynamics method, we investigate heat and mass transfer phenomena in the thermal and fluid engineering from the microscopic viewpoint. Integrating numerical analysis methods which can cover multiscale physics, we aim to investigate thermal and fluid phenomena having multiscale aspects.

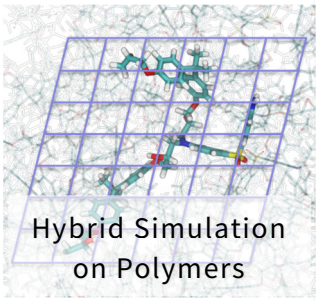
Keywords: Molecular dynamics, Thermal and fluid engineering, Heat and Mass transport, Surface modification, Multiscale analysis, Organic molecular film, Polymer, Machine learning, Materials informatics

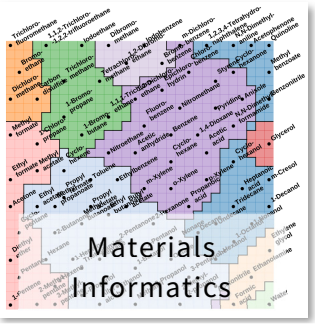
### Transport Phenomena of Organic Molecular Films

Novel surface modification techniques at the molecular level such as the self-assembled monolayer (SAM) have drawn attention as techniques to control the physical and chemical properties on solid surfaces. We investigate structure formation, interface affinity, and heat and mass transport characteristics of organic molecular films.


Molecular Structure of SAM

### Thermal and Fluid Properties of Polymeric Materials

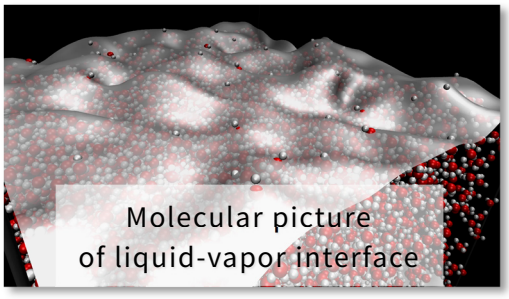

Hybrid Simulation on Polymers


Materials Informatics

As for development of polymeric materials, designing various properties by controlling the molecular-scale structure and phase separation is being required. Using integrated numerical analyses covering molecular-scale to macroscale phenomena and machine learning-aided informatics techniques, we aim to explore and design polymeric materials.

### Transport Phenomena in Confined Liquids

At the fluid and soft matter interfaces or inside the confined liquid in nanoscale structures, peculiar heat and mass transfer characteristics emerges. Our goal is an essential understanding of heterogeneous structure and corresponding transport phenomena at the molecular level and building of physical models which can bridge macroscopic thermal and fluid analyses.


Molecular picture of liquid-vapor interface

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