

# The Molecular Dynamics Simulation of Inclusion Complex Formation

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シクロデキストリンと高分子鎖において Coarse-grained model を用い、分子動力学シミュレーションを行うことで、擬ロタキサンや擬ポリロタキサンの形成メカニズム、及び包接化合物形成時における分子認識メカニズムを明らかにする。

## 1 Introduction

Recently, supramolecular assemblies have attracted attention because of their potentials for nanometer-sized functional materials. Cyclodextrins (CDs) are cyclic oligomers which be composed several glucose residues linked by  $\alpha$ -(1, 4) glycosidic bonds. It is well known that CDs form inclusion complexes (ICs) with various hydrophobic compounds. CDs are expected on development of new functional devices. In fact, many nanodevices, such as molecular shuttles [1] and insulated molecular wire [2], have been constructed by using the ICs of CD. In addition, slide-ring gel also has been synthesized [3]. The application range of CD is very widely. Therefore, it is important to recognize the formation mechanism of ICs at the molecular level in new material development. In this study, we clarify the mechanism of IC formation between CD and polymer chain and the molecular recognition by Molecular Dynamics (MD) simulations.

## 2 Simulation Method

The coarse grained models are used in these simulations. On the modeling of cyclodextrin, we take the following two properties of cyclodextrin into consideration. First, the hydrophobic and hydrophilic particles are arranged inside and outside of ring, respectively, in order to include the property in which the interior of CD is hydrophobic and the exterior is hydrophilic in aqueous solution. Second, the size of ring corresponds to  $\alpha$ -CD. About chain, we treat a single polymer chain with the hydrophobic particles. The interaction between the different kinds of particles is described by the soft-core potential, and the interaction between the same kinds of particles is described by the Lennard-Jones potential. The MD simulations are performed at the NVT-constant condition by using COGNAC in OCTA system [4].

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### 3 Results

#### 3.1 Simulations of the formations of pseudorotaxane and pseudopolyrotaxane

Initially, we performed the simulation from the initial state the ring and the chain separated in order to investigate the formation of pseudorotaxane. With time evolution, the pseudorotaxane was formed by the non-bonded energy decreasing. This result shows that the host-guest interaction plays important role for the formation of IC.



Figure 1: The simulation snapshot of pseudopolyrotaxane.

We also performed the simulation in the system with 40 rings and one chain to investigate the formation of pseudopolyrotaxane. The simulation snapshot obtained in the simulation is shown in Fig. 1. In formation of the pseudopolyrotaxane, the configuration of chain transforms from the random coil to the elongated state as the number of rings included in the IC is increased. The simulation results indicated that a few rings and a chain repeated the process of inclusion and dissociation after formation of a pseudopolyrotaxane with several rings.

#### 3.2 Molecular recognition at the formation of inclusion complexes

It is known that CDs recognize the chain length at the formation of ICs. The simulation was performed in the mixture system of short chains and long chains in order to investigate chain length recognition of CDs. At first, CDs form preferentially the ICs with short chains. However, with the time evolution, the number of ICs with long chains increases. Finally, we obtained the result that CDs formed only ICs with long chains. This result indicates that the ICs including short chains have not maintained their conformation for a long time and that they have dissociated quickly. On the other hand, although the formation of ICs including long chains takes time, it is difficult for the ICs including long chains to dissociate. Therefore, the chain length recognition is derived from the stability of IC.

### References

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