Theoretical, Computational and Data Science Studies on Structure Formation of Polymers

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In my presentation, I will talk about several research topics related to the characteristic structure formation and dynamics of polymer systems studied by using theoretical, computational and data science methods from the viewpoint of statistical-mechanical physics. Topics covered include the structure formation and rheological properties of associative polymers including self-sorting of amphiphilic polymers [1], the formation process of polyrotaxanes [2], the molecular mechanisms of baroplastics and so on.

[Associative Polymers] Hydrophobically modified water-soluble polymers (associative polymers) show characteristic properties due to the formation of various kinds of associated structures, such as intramolecular micelles, flower-type micelles, and physical gels. In the presentation, we will review recent developments in the study on the molecular origin of such structural and rheological properties by mainly using molecular dynamics simulations (Figure 1).

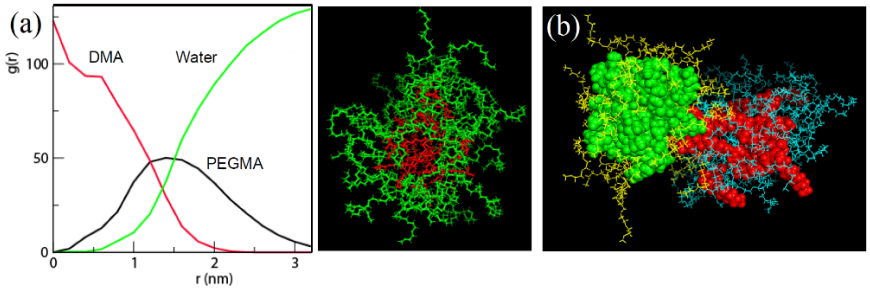

Figure 1(a) Number density profiles and a snapshot of intramolecular micelle of hydrophilic chains (PEGMA, green) with long hydrophobic side chains (DMA, red) by all-atom MD simulation. (b) Snapshot of a block copolymer of PEGMADMA (green) and PEGMA with short hydrophobic side chains (BMA, red).

[Polyrotaxanes] Cyclodextrin (CD) is capable of encapsulating various compounds in the hydrophobic space inside its ring structure, and this inclusion mechanism has been utilized in a wide range of applications, including drug transport, molecular recognition, and slide-ring gels. Polyrotaxanes have high filling ratio of CD that cannot be explained by a random inclusion process. To clarify the molecular mechanism behind this, we conducted research using statistical mechanical theory and molecular simulations, and found that hydrogen bonds between CDs play an important role in the formation of such inclusion complex (Figure 2) [2].

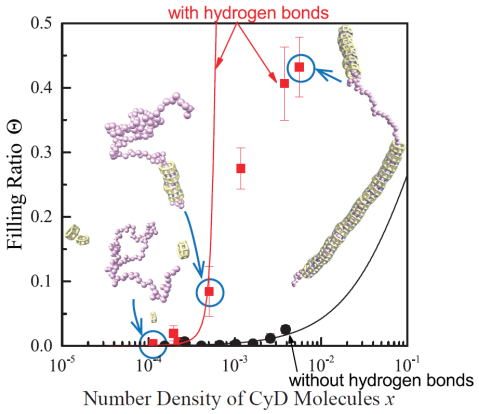

Figure 2 : The filling ratio in the presence (red) and absence (black) of hydrogen bonds. The symbols and solid lines show the results of the GCMC simulation and theoretical calculation, respectively. Pink spheres and cylinders indicate the polymer. Yellow cylinders and black lines indicate the CD molecules and the hydrogen bonds, respectively.

References

[1] Y.Hirai, T.Terashima, M.Takenaka, M.Sawamoto, *Macromolecules*., **49**, 5084-5091 (2016).

[2] T. Furuya, T. Koga, Polymer, 131, 193 (2017).

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