유기 형광분자의 나노 섬유상 자기집합구조 형성에 관한 근본적인 이해

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Fundamental Understanding of the Formation of Fibrillar Self-assembly Structure of Fluorescent Organic Molecules

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1. Introduction

One dimensional nanowire structure like nanotube and semi-conducting nanowires, have received much attentions because of its characteristic optical, electrical and mechanical properties. Up to now most studies are concentrated the nanowires based on inorganic or inorganic/metal hybrid[1-3].

We recently reported[4] fluorescent organic nanowire based on CN-TFMBE molecules (see Fig. 1), which have different molecular skeleton from other conventional self-assembly nanowires. In this study, we tried to explain the fundamental nature for the formation of the fibrillar self-assembly structure of those molecules using SAXS and multiscale computer simulation techniques. Especially, through the consideration of the relativity of individual energy components, the intermolecular interaction modes were monitored to explain the nature of self-assembly structure formation.

2. Materials

As shown in Fig. 1, CN-TFMBE and TF-DPST were used in this study for the comparison purpose.

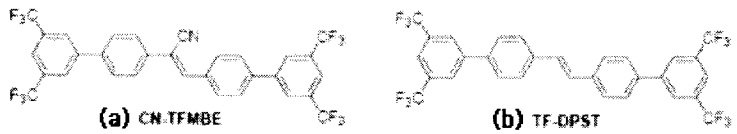

Fig. 1. Fluorescent organic molecules used in this study.

3. Methodology

3.1. Small Angle X-ray Scattering

CN-TFMBE sample was dissolved in 1,2-dichloroethane (0.8wt/vol%). A slide glass was dipped into the solution and dried. The dried slide glass was then subjected to

X-ray examination on a Nanostar (Bruker, Germany) equipped with High star 2D area detector, using Ni filtered Cu Kα radiation generated at 40kV and 35mA.

3.2. Multiscale Computer Simulation

In MS Modelling 4.0 (Accelrys, U.S.A.) Software package, Polymorph module was used for ab-initio structure determination, Discover module for force field based energy calculation and DMol3 module for quantum calculation.

4. Results and Discussion

It turned out that the introduction of CN group make the conjugated length shortened and the molecular plane distorted so that the molecules can not fully overlapped. The polarity was also found to be increased, implying that the electrostatic interaction increased so as to induce the closer molecular packing. This intermolecular interactions was found favorable to the formation of the head-to-tail self-assembly structure that leads to a fibrillar mophology.

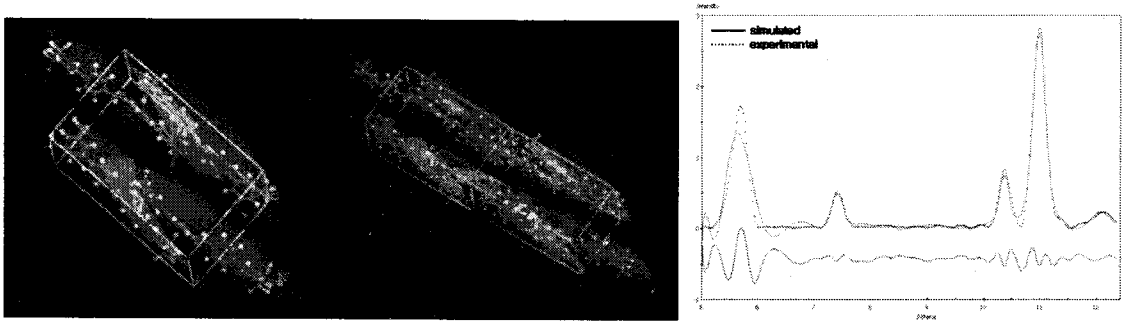

Fig. 2 Self-assembly structure and comparison between experimental and simulated SAXS data

5. References

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2. X Peng *et al.*, *Nature*, 2000, ***404***, 59
3. C. R. Martin *et al.*, *Nature*, 1994, ***266***, 1961
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