2B08

単一フォトクロミック分子ジアリールエテンに対する周囲の場の影響

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The photochromic molecule, diarylethene (Fig. 1), is considered to be a promising candidate for a molecular switch and memory.[1] Recently, the photochromic reactions of diarylethene derivatives[1] were detected at the single-molecule level by using a fluorescence technique.[2-5] The two isomers of the diarylethene, the open- and the closed-ring isomers, are distinguished by the on and off of the fluorescence from the attached fluorescent dye (Fig. 2). To obtain the time trace of the isomerizations, both the UV and visible lights are applied on the dye-attached diarylethenes in a polymer film. The experiment shows that the on/off of the fluorescence is considered to be affected by the surrounding

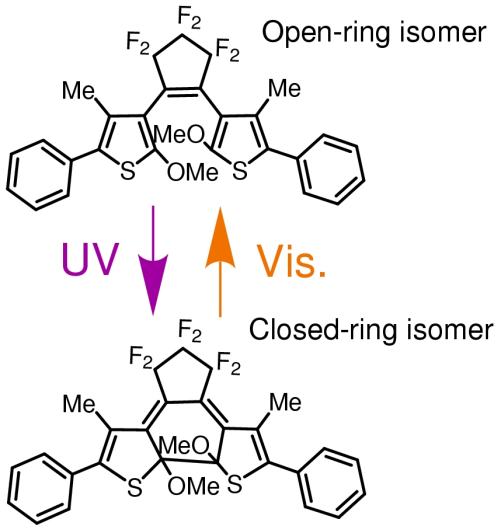

Fig.1 The open-ring isomer (upper panel) and the closed-ring isomer (lower panel) of the diarylethene derivative.

environment as well as the conformation of the diarylethene.

Here, we analyze the experimental results by models, quantum chemical calculations, and molecular dynamics calculations. The analysis requires the detailed understanding of the structure and the dynamics of the ground and excited states.[5,6] Unlike the previous computational studies on diarylethenes,[7-10] this system is further complicated due to the attachment of the fluorescent dye together with the surrounding polymers. Thus, we focus our study on the effect of the polymer on the diarylethenes.

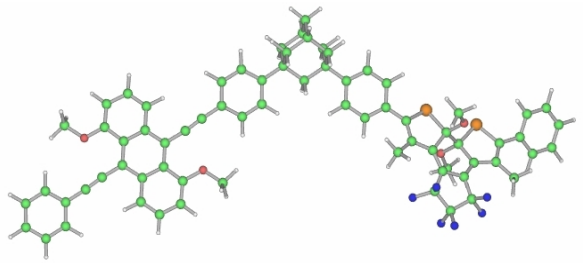

Fig. 2 The diarylethene is linked to fluorescent dye through adamantyl spacer.

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