Development of New Circularly Polarized Luminescent Materials; Use of Helical Macromoleculer Scaffold and the Prospects for the Utilization of Theoretical Calculation

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In recent years, more attention has been paid to chiral materials exhibiting circularly polarized luminescence (CPL) for the applications in chemical sensors, copy-safe printing, and three-dimensional displays. Increasing interest has focused on the switch of the handedness of CPL by external stimuli. However, reports on the full-color-tunable CPL materials with switchable handedness has been limited, because the mechanism of the switch of the CPL handedness was closely related to the structure of the luminophore.

Recently, we have reported that a poly(quinoxaline-2,3-diyl) (PQX) serves as a new helical macromolecular scaffold, which exhibits a solvent-dependent switch of its helical chirality.[1,2] Herein we report the incorporation of achiral luminophore units to the backbone of the PQX bearing chiral side chains for the color-tunable and handedness-switchable CPL.[3] PQXs bearing common chiral units containing (*S*)-2-butoxymethyl side chains and various 5,8-diarylqunoxalaine units (**1a–g**) were synthesized to investigate their optical properties (Fig. 1a). These polymers exhibited left-handed CPL in CHCl₃, although right-handed CPL was observed in 1,1,2-trichloroethane (1,1,2-TCE). We also report the prospects for the rational molecular design of CPL materials based on the theoretical calculations.



Figure 1. (a) Structures of **1a–g**. (b) Picture of **1a–g** in CHCl₃ or 1,1,2-TCE under UV-light (365 nm) irradiation.

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