

Two different π -electron distributions of Lumogen F Violet 570 crystals

조국현, 이시우, 이아라, 전태열¹, 이현휘¹, 문도현¹, 서일완², 이동렬², 김효정[†]

부산대학교; ¹포항공과대학교; ²승실대학교

(hyojkim@pusan.ac.kr[†])

Lumogen F Violet 570 (V570) has been applied to downshift film which can enhance the efficiency of solar cell. However, as the concentration of V570 increases, the ACQ phenomenon which decrease emission intensity occurs. In this study, two crystal phases of V570 were obtained using a tetrahydrofuran (THF) solvent and found that the crystals had optical properties that emit blue (454 nm) and green (513 nm) light. The structure of these two crystals was confirmed by x-ray analysis and it was confirmed that the mechanism having different fluorescence properties is related to the staking structure of V570 intermolecular naphtha group. According to the results of the DFT calculation, the green crystal structure is shared by the π electrons of the naphtha component in the LUMO molecular orbital. On the other hand, in the case of the blue structure, the intermolecular distance is similar to green, but the center distance of the intermolecular naphtha group is long. As a result, π electrons are not shared in the LUMO state. The V570 molecules have a green crystal structure in the thin film state and GIWAXS confirms that the (001) crystal plane is laminated in the predominant direction.