Theoretical study and optimization on cellulose derivatives intrinsic birefringence

이지윤, 곽상규[1,†]
울산과학기술원; [1]UNIST
(skkwak@unist.ac.kr†)

Cellulose as one of the most abundant materials on earth has emerged as a prominent protective film in display technology, owing to its low birefringence. An ever-growing demand on advance display technology drives the search of technique to control the birefringence of cellulose film. In this study we presented a comprehensive theoretical approach to find promising candidates among cellulose derivatives as display protective film. Density functional theory (DFT) calculation was used to calculate the absorption peak and intrinsic birefringence of the monomer of cellulose derivatives while altering the type, position, and conformation of substituent groups. Apart from substituent group effect, molecular dynamics (MD) simulation was employed to investigate the structural effects such as arrangement, order parameter, and conformation ratio of various substituent group. The presence of various conformation ratio and order parameter were taken into account by proposing a semi-empirical mixing rule approach. Based upon this theoretical approach we could suggest cellulose derivatives with acetyl group as a prominent candidate for protective film with negative birefringence.