

**Opto-mechanical behavior of Azobenzene-doped liquid crystalline polymer:**

**A molecular dynamics study**

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A photo-isomerization of azobenzene and its opto-mechanical effect on the photoactive liquid crystalline polymer is investigated via molecular dynamics (MD) simulation. In order to describe the cis-state of the azobenzene in classical MD model, an additional dihedral potential parameter of N=N bond is implemented into the fully condensed nematic polymer model. During the photo switching simulation, both the local conformational changes in the mesogen-contained microstate and the global photostrain of the bulk system are observed successfully with respect to the isomerization ratio in the molecular unit cell. For each relaxed model under photo-activated condition, a heating-up simulation is carried out sequentially, and the effective deformation of the material is characterized as a function of both temperature and isomerization ratio of the photoactive mesogen.

**Keywords:** Photo-isomerization, Liquid Crystalline Polymer, Photostrain, Molecular Dynamics

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