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[PL2] Plenary Talk 2

Multiscale modeling and realization of photo-responsive polymers

Chair: Alexey Lyulin(Technische Universiteit Eindhoven, The Netherlands)

2018年10月29日(月) 11:00 ~ 11:50 Room1

Maenghyo Cho

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Multiscale modeling and realization of photo-responsive polymers

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Liquid crystalline polymers which contain photochromic chromophores can show macroscopic mechanical deformation under light irradiations. The light-induced shape change of the photo-responsive polymers (PRPs) comes from the trans-to-cis, or cis-to-trans isomerization of the mesogens, and it can be utilized to the microscale opto-mechanical actuation device. However, it is difficult to analyze and precisely predict the deformation because the theoretical approach requires a comprehensive knowledge of broad, interdisciplinary physical regimes that range from photochemical reaction kinetics to manipulating continuum scale deformations. Here, we develop a new multiscale model which integrates light input conditions, mesogen alignment, and continuum polymer deformations through sequential multiscale framework combining the DFT(density functional theory), MD(molecular dynamics), and continuum FE(finite element) method. In addition, the multiscale approach is applied to design the photo-mechanical behavior of the PRP nanocomposites with the consideration of the opto-mechanical coupling effect and microscopic interaction between the PRP matrix and fillers. This integrated framework can help to design the PRP and its composites.