

Simulation of Organic Materials for Optical Properties

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Abstract

An optical response is one of the most important physical properties for light emitting materials such as polymer LEDs and display-related materials. The time-dependent density functional theory is expected to deal with the optical responses. We have been intensively studied and applied this theory to material design for several years. In this study, real-space and real-time calculation techniques are used for the electronic states instead of the conventional basis-expansion techniques. Our method seems more efficient since relatively small number of meshes is required for obtaining results with reasonable accuracy, which depends on an adjustable parameter, the total number of time steps. As the achievement in the application of Earth-Simulator, we report the analysis of emission spectra in the finite temperature and electronic structures

Keywords: Organic LED, Materials of Polymer LED, Optical Spectrum, Time-Dependent Density Functional Method