

# Development of High-efficiency Organic Light-emitting Materials

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## Abstract

Organic EL is undoubtedly expected for display-related and illuminating materials in the next generation. We have also been intensively developing light emitting materials for polymer LEDs, where optical spectra absorption and emission of materials are quite important properties. In the prediction technique for optical properties, the key is modeling of polymer and computational environment to be realized. We have been used time-dependent density functional theory, which provides fairly good accuracy as the prediction technique. In our study, real-space and real-time calculation techniques are applied to describe the electronic states instead of conventional basis-expansion techniques. This method ensures more efficiently in relatively small number of spatial meshes to obtain results with reasonable accuracy, which depends on an adjustable parameter, the total number of time steps. As our result from our modeling of polymer, which is a single chain, we have realized that a certain oligomer-length provides the electronic structure to be recognized as that of a polymer, and Earth Simulator provides the computational environment to realize the simulation of fairly large sizes. Analysis of the electronic structure around an emission site and the emission strength can be recognized as the achievement of our theme in 2007, which is, of course, based on the result in 2005 and 2006 about emission spectrum analysis in finite temperature and that of the electronic structure. In this paper, we report the analytical results of our polymer LED development including those in 2005 and 2006.

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