Development of High-efficiency Organic Light-emitting Materials

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Abstract

Organic EL display, as is self-emitting, has recently been developing to replace LCD in widely-used flat panel displays. Organic EL has a lot of advantages from the point of production cost and large scale display, because its device structure is quite simple. At present, the materials have been developing in rapid evolutions, and experimental production is now also being started in the market, which is expected to be grown in near future. This kind of material development is highly dependent on fairly accurate numerical calculations in recent computational environment. In particular, it is quite important to analyze spectra in emission/absorption processes. Development of time dependent density functional theory (TDDFT) provides us predictably emission spectra quite effectively. In our study, real-space and real-time calculation techniques are applied to describing the electronic states instead of conventional basis-expansion techniques. This method ensures more efficiently in a relatively small number of spatial mesh points to obtain results with reasonable accuracy, which depends on an adjustable parameter, the total number of time steps. Recent topics in the materials development is generally said to be the use of not only fluorescent but also phosphorous processes. Corresponding computational research needs to work for the wide variety of materials. As our theme in 2010, we have continued to improve our TDDFT code and have studied to look for optimum conditions on spatial mesh and time step for phosphorous materials. As the results, we have obtained fundamental spectra of phosphorous materials, although we have also found out an issue that our code gives small zero-field splitting of Xe atom compared with results of relativistic all-electron atomic calculation and experiments of atomic spectra.

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