

Abstract Submitted
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TDDFT Simulation of Organic EL Materials for Optical Properties¹ YASUNARI ZEMPO, Hosei University — Organic EL is expected to be a break-through for next-generation flat panel displays. There are lots of advantages from the point of production cost as a large scale display, because its device structure is quite simple. For the material development, it is quite important to analyze spectra in emission/absorption processes. It is of current interest for the emission efficiency to use not only fluorescent but also phosphorous processes. Time dependent density functional theory (TDDFT) has applied to study the optical responses of the conjugated polymers and complex molecules such as poly(9,9-dialkyl-fluorene) and Ir(PPY)₃. It provides us predictably emission spectra quite effectively. 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. The development and performance of our code, taking spin-orbit interactions into account, will be also discussed.

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