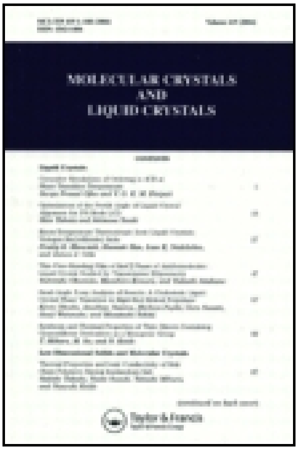

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Exciton Condensate in Model Dendrimers

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We calculate the time evolution of exciton density in a model dendrimer. Possible models with dendrimers for exciton condensates are proposed.

Keywords: exciton; Bose-Einstein condensate; dendrimer

INTRODUCTION

Active controls of electronic, magnetic and optical properties of materials by external variables such as electric and magnetic fields have attracted current interests not only because of a scientific importance but also in relation to technological applications. In previous paper [1], we have studied the photo-induced superconductivity for the copper oxides of $Bi_2Sr_2Ca_{1-x}Y_xCu_2O_8$ and have discussed the possibilities of the photo-induced superconductor in relation to the Little model of exciton mechanism.

Recently, the dendrimer supermolecules [2-9] having fractal structures with light capture antenna have been synthesized, and the design of the molecular structures and their optical properties have also been attractive in view of scientific interests and technological applications. After capture of light at the outer edges of the molecule, the generated excitons migrate along the legs of the molecular structures and carry energy obtained from incident light. Then, the excitons move to the center of the supermolecule to emit light by recombination of electrons and holes.

In this paper, we discuss the possibility of Bose-Einstein condensation (BEC) of excitons in a fractal system in relation to the dynamics of excitons and propose a model system, which consists of fractal antenna supermolecules. The exciton BEC has been investigated in a semiconductor quantum well structure as GaAs quantum well [10] or in Cu_2O [11]. The problem in realizing the exciton BEC is how high densities of excitons could be achieved experimentally by generating an effective pressure.

MODEL DENDRIMERS

Here, we consider dendrimers made up of a phenylacetylene repeat unit in a self-similar fashion around the core as shown in Fig.1. The dendrimers have a varying segment length that increases for higher generations. For simplicity, we focus on a model dendrimer shown in Fig.1(a). We consider a model Hamiltonian of the system as

$$H = \sum_{r,s=1}^{25}\left[h_{rs}^{HOMO} a_r^+ a_s + h_{rs}^{LUMO} b_r^+ b_s\right] - U\sum_{r=1}^{25} a_r^+ a_r b_r^+ b_r \; ,$$

where $a_r^+(a_r)$ and $b_r^+(b_r)$ are creation(annihilation) operators of hole and particle at r-th site, respectively. h_{rs}^{HOMO} and h_{rs}^{LUMO} indicate HOMO-HOMO and LUMO-LUMO transfer integrals between r-th and s-th sites, respectively. Note that $h_{rr}^{HOMO}(h_{rr}^{LUMO})$ means HOMO's(LUMO's) energy level. The second term corresponds to the Hubbard model with negative repulsion between hole and particle in the same site.

RESULTS AND DISCUSSIONS

In this study, we consider one exciton distributed at all sites. In this

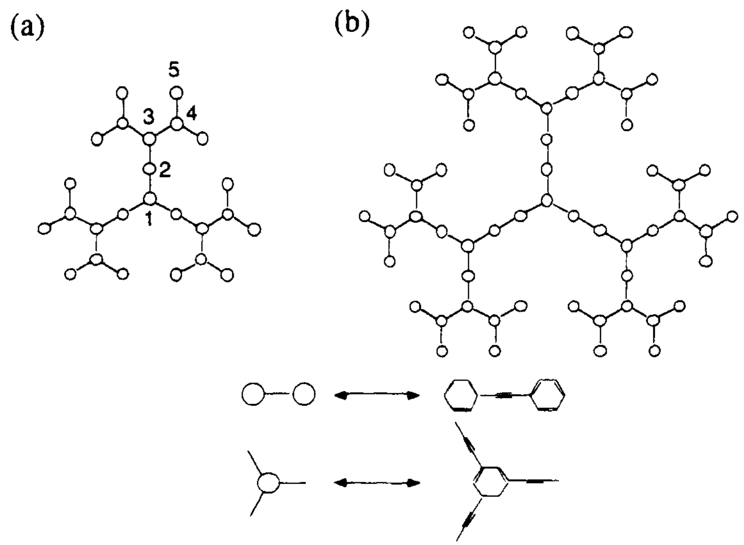

FIGURE 1. Model dendrimers.

calculation, all transfer integrals between nearest neighbor sites for each level are -1.0 (a.u.) and others are zero, and all energy gaps ΔE are 6.0 (a.u.) except for the energy gap ΔE_1 at the 1st site; $h_{rr}^{HOMO}=-h_{rr}^{LUMO}=-3.0$ (a.u.) (r=2,...,25) and $\Delta E_1=h_{11}^{LUMO}-h_{11}^{HOMO}$. Exciton density is shown in Fig.2. Figure 2(a) shows the time evolution of exciton densities at sites numbered in Fig.1(a) for $\Delta E_1/\Delta E=1$. From Fig. 2(b), we can find the more evident tendency of collecting excitons to the center than that shown in Fig.2(a), when $\Delta E_1/\Delta E<1$. The result implys that the HOMO-LUMO gap at the center, which is smaller than that at other sites, plays an important role for collecting excitons. On the other hand, when $\Delta E_1/\Delta E>1$, we can find that it is more difficult to collect excitons to the center as shown Fig.2(c).

Here, we propose models to realize the exciton Bose-Einstein condensate (BEC) by using the fractal systems. In general, the problem in realizing the exciton BEC is how high densities of excitons could be achieved experimentally by generating an effective pressure. Figure 3 il-

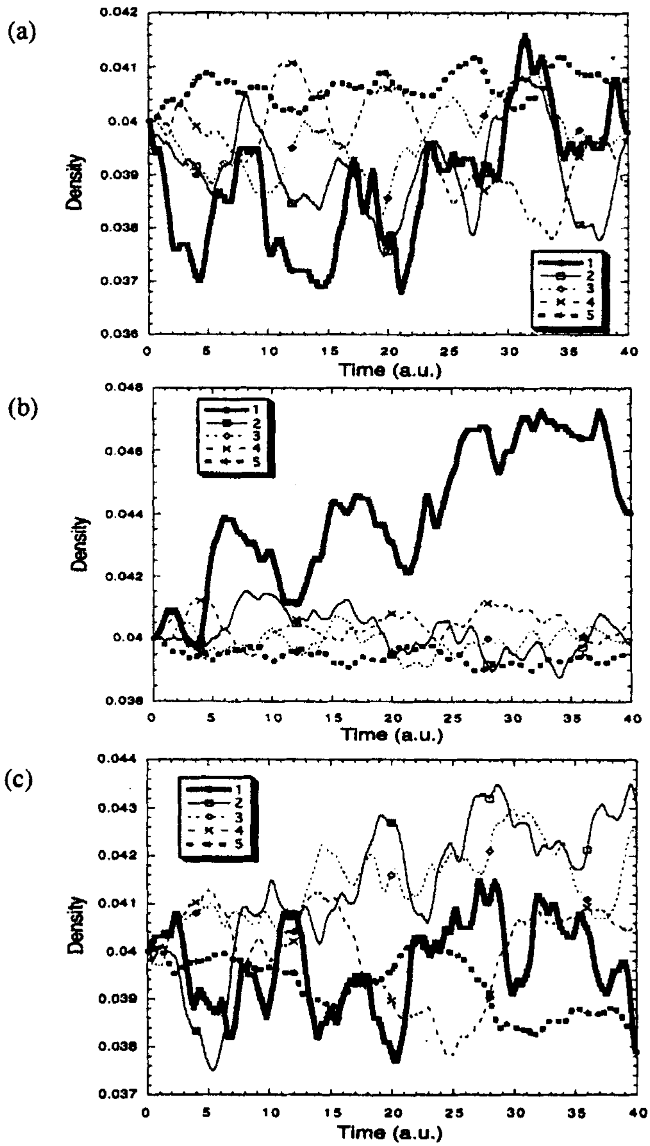

FIGURE 2. Time evolution of exciton density. (a) $\Delta E_l/\Delta E=1$. (b) $\Delta E_l/\Delta E=0.67$. (c) $\Delta E_l/\Delta E=1.33$.

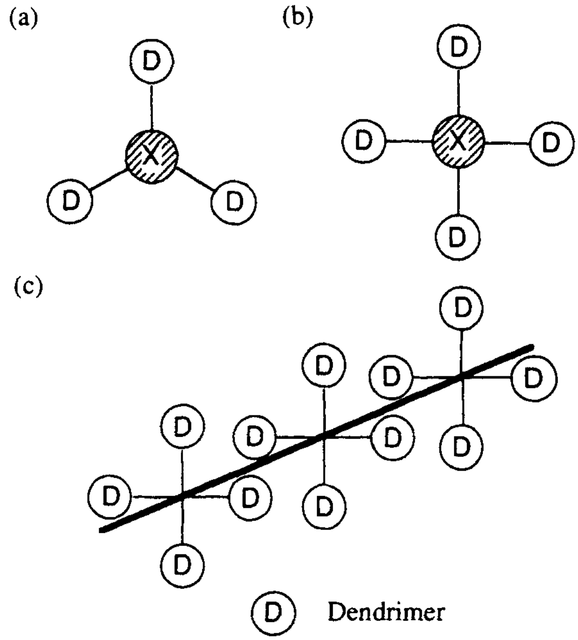

FIGURE 3. Possible models for exciton condensate. (a) and (b) X corresponds to a cluster or a crystal. (c) Polymer with dendrimers.

lustrates possible models for exciton condensate using dendrimers. From the above result, when HOMO-LUMO gaps of a cluster or a crystal X shown in Figs.3(a) and (b) is smaller than that of each site in dendrimers, excitons migrate to the center X. Here, we assume that when the excitons move to the center after illumination, the recombination of electrons and holes is forbidden. This means that the high density of excitons is appeared at the center. We can expect that the high density of excitons may yields the exciton BEC. In similar, for a polymer shown in Fig.3(c), if the band gap is smaller than the HOMO-LUMO gap of each site in dendrimers, the exciton condensate may be observed. When the polymer is a Kondo insulator, the exciton condensate will become p-wave BEC. In the Anderson lattice model for a mixed-valent system, the d-f hybridization can possess a *p*-wave symmetry[12].

In conclusion, the present results suggest that HOMO-LUMO gap at the center is important to migrate excitons. We can expect to realize the Bose-Einstein condensation of excitons at the center in systems with dendrimers.

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