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Electronic Structures of the Tube–like Fullerene Dimers $(C_{60+10n})_2$

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Electronic Structures of the Tube–like Fullerene Dimers $(C_{60+10n})_2$[#]

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Abstract

Motivation. In the fullerene C_{60} polymers, the polymerization reaction can be described as a [2+2] cycloaddition across parallel 6,6–ring fusion bonds in neighboring C_{60} molecules. The bonds are known to be active in addition reactions due to their high double bond character. The fullerene C_{70} with the D_{5h} symmetry also has such active 6,6–ring fusion bonds nearby the poles of the molecule, and it have been shown that a [2+2] cycloaddition cap–to–cap C_{70}–dimer is synthesized. The fullerene C_{70} with the D_{5h} symmetry is the smallest member of a group named the tube–like fullerene C_{60+10n} (n = 1, 2, …) consisting of the bisected caps of C_{60} and a single–wall cylinder. According to the Pauling bond order analysis, the C_{60+10n} has the active 6,6–ring fusion bonds and the [2+2] cycloaddition dimer similar to the cap–to–cap C_{70}–dimer is expected. Here we consider the electronic structures of the cap–to–cap dimers $(C_{60+10n})_2$. Analyzing the MOs nearby the HOMO–LUMO gaps, the mutual relations between MOs of the dimer and of the monomer are shown.

Method. MO calculations are made in the semiempirical CNDO/S approximation. The geometries optimized with Gaussian 03 at the AM1 level are used.

Results. The HOMO–LUMO gap energy of the $(C_{60+10n})_2$ shows a periodic n–dependence quite similar to that of the C_{60+10n}. The gap value calculated on the $(C_{60+10n})_2$ is almost the same to that on the C_{60+10n}, although the former is slightly less than the later. The HOMO (LUMO) of the dimer can be described in terms of the HOMOs (LUMOs) of the corresponding two monomers.

Conclusions. The MO properties of the C_{60+10n} are maintained in the [2+2] cycloaddition dimer $(C_{60+10n})_2$ nearby their HOMO–LUMO gap.

Keywords. Tube–like fullerene; dimer; [2+2] cycloaddition; HOMO–LUMO energy gap; semiempirical MO method.

1 INTRODUCTION

Since a report by Rao *et al.* [1] on photoinduced polymerization in thin solid C_{60} films there have been many reports on fullerene polymers obtained by applying high pressure and temperature [2–7]. The polymer structure depends on the condition of pressure and temperature: Linear chain

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structures are obtained at a relatively moderate condition [4], while two–dimensional networks are formed at a more intense condition [5]. For both structures, the polymerization reaction can be described as a [2+2] cycloaddition across parallel 6,6–ring fusion bonds in neighboring C_{60} molecules. The smallest polymer is the C_{60}–dimer, which has been proposed as an initial intermediate in the polymerization process [8]. The C_{60}–dimer itself can be synthesized by several methods [8–10]. Experimental data [11,12] suggested that not the 5,6–ring fusion bonds but the 6,6–ring fusion bonds participated in the [2+2] cycloaddition in the dimer. The 6,6–ring fusion bonds considered as the double bonds are the reactive centers not only for C_{60} dimerization but also for oxidation and many other reactions [13]. Several groups theoretically investigated some properties of the C_{60}–dimer and the polymer [14–18].

The polymerization of C_{70} fullerene by applying high pressure and temperature has been also attempted [19–22]. Lebedkin *et al.* [22] showed that a [2+2] cycloaddition cap–to–cap C_{70}–dimer with the C_{2h} symmetry (isomer I in Figure 1) was synthesized in high yield. In this isomer, 6,6–ring fusion bonds first closest to the poles of C_{70} participate in the cycloaddition. The authors also theoretically investigated a [2+2] cycloaddition C_{70}–dimer and found energetically favorable isomers shown in Figure 1.

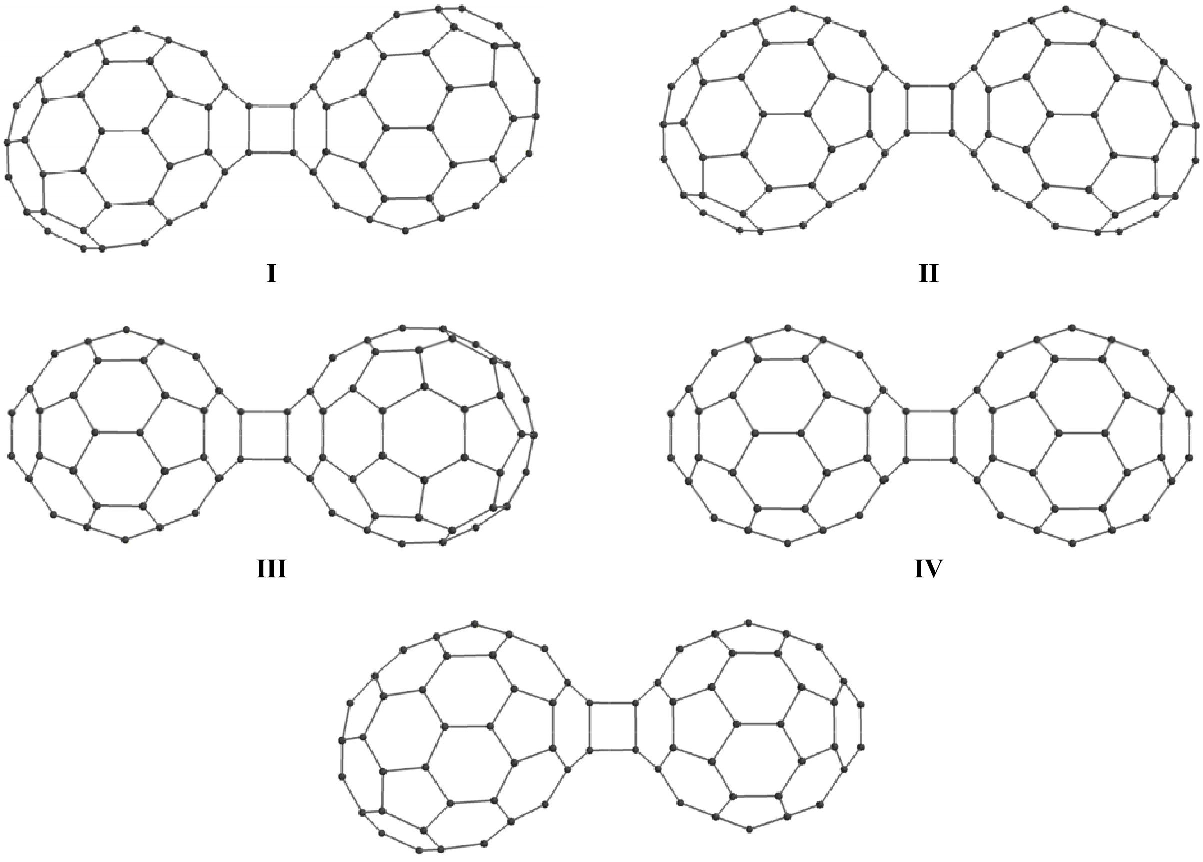

Figure 1. Energetically favorable isomers for the [2+2] cycloaddition C_{70}–dimers. Isomers **I**, **II**, **III**, **IV** and **V** hold the C_{2h}, C_{2v}, C_{2h}, C_{2v}, and C_1 symmetries, respectively.

According to their estimation due to semi–empirical PM3 calculations, the energy differences between the five isomers are small (about <0.5 kJ/mol), and other isomers of [2+2] cycloaddition are energetically unfavorable (>70 kJ/mol). In these energetically favorable isomers, 6,6–ring fusion bonds first and secondarily closest to the poles of C_{70} participate in the cycloadditions. These bonds of C_{70} are known to be active in addition reactions [23,24].

The fullerene C_{70} with the D_{5h} symmetry is the smallest member of a group named the tube–like fullerene C_{60+10n} consisting of the bisected caps of C_{60} and a single–wall cylinder. According to *ab initio* [25] and semiempirical [26] calculations, a periodic *n*–dependence was seen in the HOMO–LUMO energy gap of the C_{60+10n}. Analyzing with the Pauling bond order (PBO) [27], we attributed the origin of the periodicity to the pseudo π–conjugation formed on each layer of the *cyclo*–pentaphenylene structure in the cylindrical part [26]. In the PBO–analysis on the C_{60+10n} with $n = 1, 2, \ldots, 12$, we also noticed that 6,6–ring fusion bonds closest to the poles of the molecules possessed strong double–bond character. This indicates that [2+2] cycloaddition dimers similar to the cap–to–cap C_{70}–dimer [22] may be able to be formed for the C_{60+10n} with $n \geq 2$.

In this paper, we consider the electronic structures of the tube–like fullerene dimers $(C_{60+10n})_2$ ($n = 1, 2, \ldots$), taking notice of their *n*–dependence. Structures of the dimers are assumed to be similar to that of the cap–to–cap C_{70}–dimer with the C_{2h} symmetry (isomer **I** in Figure 1), which has been able to be synthesized in high yield [22]. The MO calculations on $(C_{60+10n})_2$ are made using the CNDO/S approximation [28,29] as was used in our previous calculations on the tube–like fullerenes [26,30]. We will show a periodic *n*–dependence in the HOMO–LUMO gap energy of the $(C_{60+10n})_2$. The mutual relations between MOs of the dimer $(C_{60+10n})_2$ and of the monomer C_{60+10n} will be also discussed especially for the HOMO–LUMO energy region.

2 METHODS

For each [2+2] cycloaddition cap–to–cap dimer $(C_{60+10n})_2$, a geometry similar to that of the cap–to–cap C_{70}–dimer with the C_{2h} symmetry (isomer **I** in Figure 1) is initially assumed. According to the geometry optimization with Gaussian 03 at the AM1 level, the $(C_{60+10n})_2$ ($n = 1, 2, \ldots, 12$) keep the cap–to–cap dimer structures with the C_{2h} symmetry. With the optimized geometries, we perform the CNDO/S calculations on the $(C_{60+10n})_2$. We also calculate the CNDO/S–MOs of the C_{60+10n}–monomer, and examine the mutual relations between MOs of the dimer and of the monomer.

3 RESULTS AND DISCUSSION

Figure 2 shows the HOMO–LUMO gap energies of the dimer $(C_{60+10n})_2$ ΔE_{D} (indicated by red line). The HOMO–LUMO gap energies of the monomer C_{60+10n} ΔE_{M} [26] (indicated by blue line) are also shown for comparison. There we notice that the ΔE_{D} periodically decreases with *n* and takes minimum values at $n = 2, 5, \ldots$ Note that the behavior of the ΔE_D is quite similar to that of the ΔE_M and that the ΔE_D value is almost the same to the ΔE_M one with the exception in the case of $n = 1$.

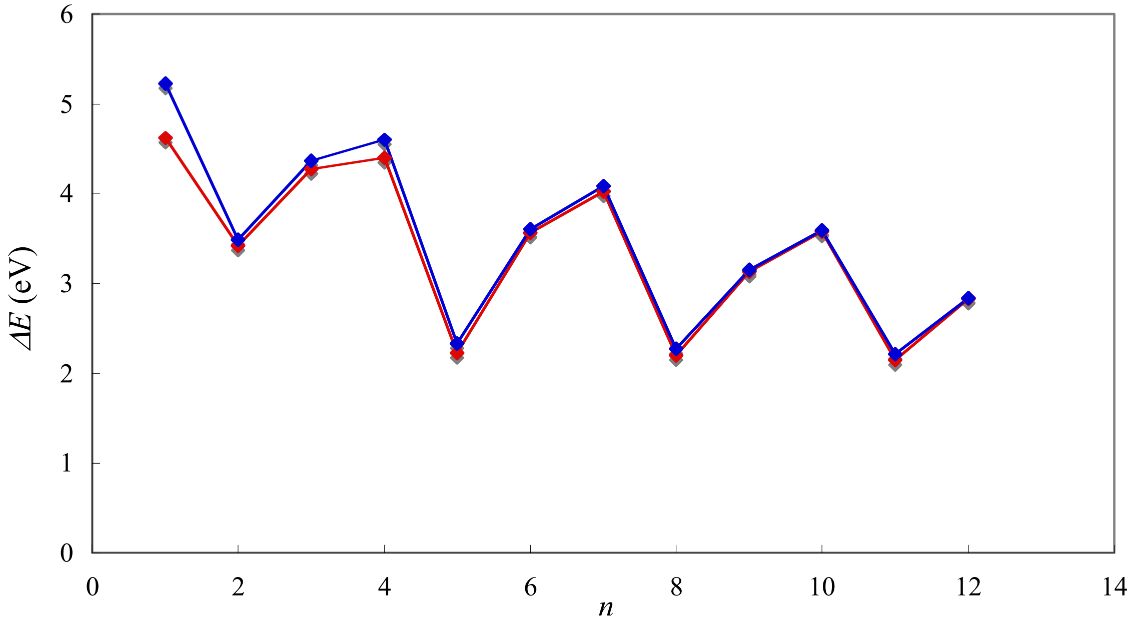

Figure 2. The HOMO–LUMO gap energies ΔE_D and ΔE_M vs. n, calculated with the CNDO/S approximation. The red and the blue lines indicate the ΔE_D and the ΔE_M, respectively.

Table 1. The contributions (%) of the *homo* and the *lumo* to the HOMO and HOMO–1 and to the LUMO and the LUMO+1, respectively. These MOs are obtained with the CNDO/S approximation.

n	HOMO–1	HOMO	LUMO	LUMO+1
1	72.8	78.2	63.2	54.5
2	97.0	94.5	92.4	91.1
3	99.0	99.0	89.1	90.7
4	95.8	96.9	65.5	92.7
5	96.8	97.3	97.2	98.3
6	99.6	99.6	95.8	95.9
7	99.5	99.5	92.9	98.6
8	97.8	98.2	98.9	99.3
9	99.7	99.7	97.5	97.7
10	99.7	99.7	97.3	97.4
11	98.2	98.5	99.2	99.4
12	97.8	98.3	97.4	97.7

The similarity between the ΔE_D and the ΔE_M may suggest that the natures of the HOMO and the LUMO of the (C_{60+10n})$_2$ reflect those of the C_{60+10n}. We therefore examine the mutual relations between MOs of the (C_{60+10n})$_2$ and of the C_{60+10n}. A partial MO $\left|\phi_k^\mathrm{D}\right\rangle$ at a unit C_{60+10n} part in the (C_{60+10n})$_2$ can be expanded in terms of MOs $\left|\phi_\ell^\mathrm{M}\right\rangle$ of the C_{60+10n}:

$$\left|\phi_k^\mathrm{D}\right\rangle = \sum_\ell \left|\phi_\ell^\mathrm{M}\right\rangle\left\langle\phi_\ell^\mathrm{M}\middle|\phi_k^\mathrm{D}\right\rangle,$$

where $\left\langle \phi_\ell^{\mathrm{M}} \middle| \phi_k^{\mathrm{D}} \right\rangle$ is the overlap between MOs $\left| \phi_k^{\mathrm{D}} \right\rangle$ and $\left| \phi_\ell^{\mathrm{M}} \right\rangle$. The degree of the contribution of $\left| \phi_\ell^{\mathrm{M}} \right\rangle$ to the whole MO of the $(C_{60+10n})_2$ is described as $2\left|\left\langle \phi_\ell^{\mathrm{M}} \middle| \phi_k^{\mathrm{D}} \right\rangle\right|^2$, because the shape of the partial MO at one part is the same as that at the other part except the sign. Table 1 shows the contributions of the HOMO and the LUMO of the monomer C_{60+10n} (denoted italic "*homo*" and "*lumo*", hereafter) to the HOMO and HOMO–1 of the $(C_{60+10n})_2$ and to the LUMO and the LUMO+1, respectively. The capital "HOMO" and "LUMO" are used for the dimer $(C_{60+10n})_2$, hereafter.

Note that the *homo* and the *lumo* dominantly contribute to the HOMO and the HOMO–1 and to the LUMO and the LUMO+1, respectively, with an exception in the case of $n = 1$. In Figure 3, the MO energy levels nearby the HOMO–LUMO gap is shown for the $n = 6$, *i.e.*, C_{120} and $(C_{120})_2$, as a typical example. The dotted lines indicate the mutual relation of the HOMO and the LUMO of the $(C_{120})_2$ with the MOs of the C_{120}.

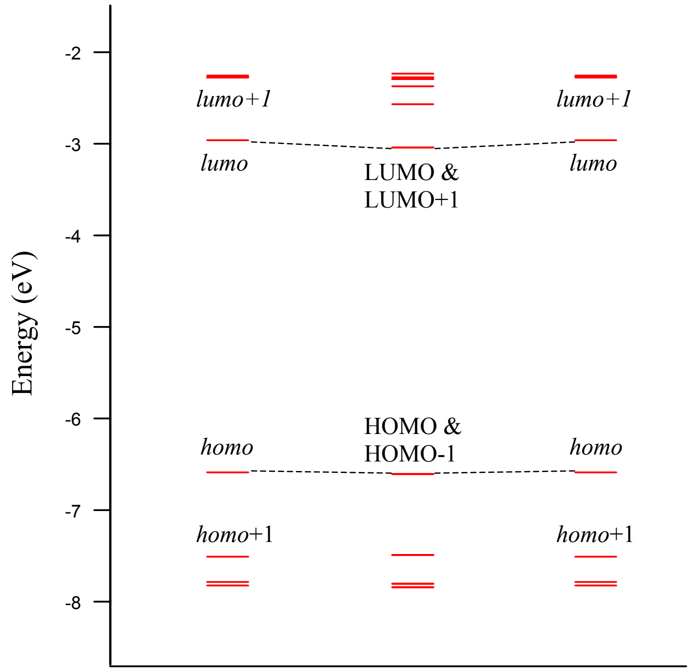

Figure 3. The mutual relation between MOs of the C_{120} and the $(C_{120})_2$.

For the C_{120}, the *homo* and the *homo*–1 belong to the irreducible representations (*irreps*) a_{1u} and a_{1g} of the D_{5d} symmetry, respectively. In the $(C_{120})_2$ of the C_{2h} structure, the interaction between these MOs is forbidden because the *homo* and the *homo–1* are anti–symmetric and symmetric with respect to the σ–operation, respectively. Thus, the *homo* orbitals of the two monomers dominantly contribute to the HOMO and the HOMO–1, both that are anti–symmetric MOs (belonging to the *irreps* a_2 and b_1 of the C_{2h} symmetry, respectively). The *lumo* and the *lumo*+1 belong to *irreps* a_{2u} and a_{2g} and their interaction also is forbidden. The anti–symmetric *lumo*+1 do not contribute to the symmetric LUMO and the LUMO+1 (belonging to *irreps* b_2 and a_1, respectively). Note that the energy differences between the HOMO and the HOMO–1 and between the LUMO and the LUMO+1 are very small. This indicates that the inter–unit interaction is weak.

The situation that the interactions between the *homo* and the *homo*–1 and between the *lumo* and the *lumo*+1 are forbidden is common to all members except the case of $n = 1$. Figure 4 shows the MO energy levels for the $n = 1$, *i.e.*, C_{70} and $(C_{70})_2$ nearby the HOMO–LUMO gap.

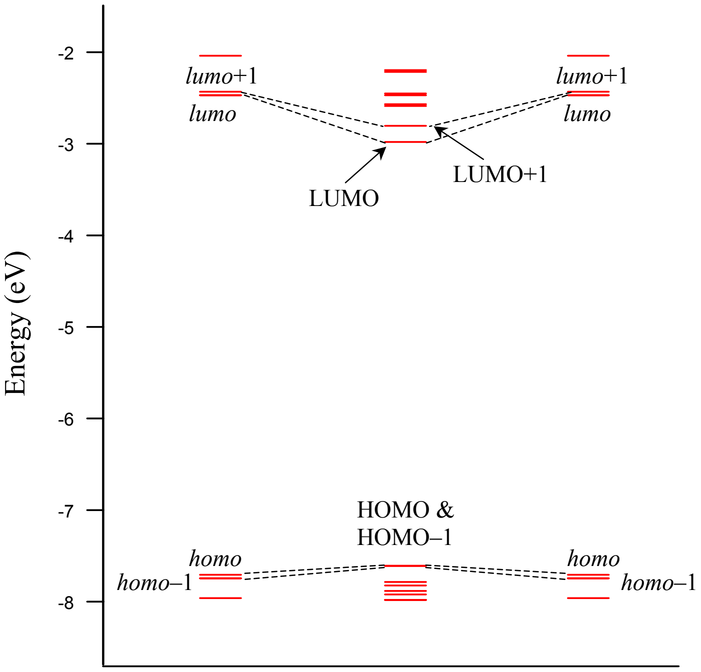

Figure 4. The mutual relation between MOs of the C_{70} and the $(C_{70})_2$.

For the C_{70} with the D_{5h} symmetry, the *homo*, the *homo*–1, the *lumo* and the *lumo*+1 belong to irreps a_2'', e_1'', e_1'' and a_1'', respectively. The *homo*–1 and the *lumo*+1 are energetically very close to the *homo* and to the *lumo*, respectively. The interactions between the *homo* and the *homo*–1 and between the *lumo* and the *lumo*+1 become allowed, because the structure of the C_{70}–unit in the $(C_{70})_2$ is slightly distorted. Due to these intra–unit interactions, the *homo*–1 and the *lumo*+1 also contribute to the HOMO and the HOMO–1, and the LUMO and the LUMO+1, respectively. Their contributions are: *homo*–1→ HOMO (17%), HOMO–1 (21%); *lumo*+1 → LUMO (27%), LUMO+1 (42%). It is supposed that the large decrease of the LUMO and the LUMO+1 energies are mainly due to the intra–unit interaction by the distortion of the C_{70}–unit. We have confirmed that the *lumo* and *lumo*+1 lower large when the distorted C_{70} geometry is used. Because of the decrease of the LUMO energy, the difference $\Delta E_\mathrm{M} - \Delta E_\mathrm{D}$ is large (about 0.6 eV). On the other hand, the differences of other members with $n \neq 1$ are relatively small: $\Delta E_\mathrm{M} - \Delta E_\mathrm{D} < 0.2$ eV.

Here we present a simple group–theoretical consideration on the optical property of the

$(C_{60+10n})_2$. In the case of the C_{60+10n} monomer, we have shown that the [*homo*→*lumo*] transition is forbidden and that the lowest transition–allowed state consists of the two singly–excited configurations, the [*homo*→*lumo*+1] and the [*homo*–1→*lumo*] [30]. On the other hand, for the $(C_{60+10n})_2$, the transitions corresponding to the [*homo*→*lumo*] transition become allowed. For instance, the HOMO, HOMO–1, LUMO and LUMO+1 of the $(C_{120})_2$, belong to *irreps* a_2, b_1, b_2 and a_1, respectively, and the [HOMO→LUMO] and the [HOMO–1→LUMO+1] transitions are optically allowed. According to our previous calculations on the C_{120}, the excitation energies of the lowest excited state due to [*homo*→*lumo*] is 1.28 eV [26]. Thus, it is expected that the lowest transition–allowed state of the $(C_{120})_2$ appears nearby 1.2 eV which is lower than the excitation energy 2.03 eV [29] of the lowest transition–allowed state of the C_{120}. The appearance of the new lowest transition–allowed state is common to all members without exception.

Finally, we consider the cases of other isomers of the [2+2] cycloaddition dimer $(C_{60+10n})_2$ (similar to $(C_{70})_2$ isomers **II**, **III**, **IV** and **V** in Figure 1), based on the CNDO/S calculations. For the all four isomers, we obtain the same results, *i.e.*, 1. The periodic *n*–dependence of the ΔE_D is quite similar to that of the ΔE_M. 2. For $n \neq 1$, the *homo* and the *lumo* dominantly contribute to the HOMO and the HOMO–1 and to the LUMO and the LUMO+1, respectively. Because the energy differences between the HOMO and the HOMO–1 and between the LUMO and the LUMO+1 are very small, it is expected that the inter–unit interaction is weak. 3. For $n = 1$, the *homo*–1 and the *limo*+1 also contribute to the HOMO and the HMO–1 and to the LUMO and the LUMO+1, respectively, through the intra–unit interaction induced by the distortion of the C_{70}–unit. 4. The transitions corresponding to the [*homo*→*lumo*] transition become optically allowed.

4 CONCLUSIONS

CNDO/S calculations were made on the [2+2] cycloaddition dimer $(C_{60+10n})_2$ ($n = 1, 2, \ldots, 12$) with C_{2h}–symmetry (similar structure to $(C_{70})_2$ isomer **I** in Figure 1). A periodic *n*–dependence was found in their HOMO–LUMO gap energies and its behavior was quite similar to that obtained for the monomer C_{60+10n}. The mutual relation between the MOs of the $(C_{60+10n})_2$ and those of the C_{60+10n} was shown. Generally, the *homo* and the *lumo* dominantly contribute to the HOMO and the HOMO–1 and to the LUMO and the LUMO+1, respectively. That is, the *homo* and the *lumo* of the C_{60+10n} are preserved in the $(C_{60+10n})_2$. For of the $(C_{70})_2$, however, the *homo*–1 and the *lumo*+1 also contribute to the HOMO and the HOMO–1 and to the LUMO and the LUMO+1, respectively. This is because the interactions between the *homo* and the *homo*–1 and between the *humo* and the *lumo*+1 are allowed and the *homo*–1 and the *lumo*+1 are energetically very close to the *homo* and the *lumo*, respectively. Examinations for other isomers similar to $(C_{70})_2$ isomer **II**, **III**, **IV** and **V** in Figure 1 give the same results mentioned above.

According to the group–theoretical consideration, the [*homo*→*lumo*] transition of the C_{60+10n} is optically forbidden. And we previously showed that the lowest allowed–transition of the C_{60+10n} was due to the [*homo*→*lumo*+1] and the [*homo*–1→*lumo*] transitions [30]. On the other hand, in the $(C_{60+10n})_2$, the transitions corresponding to the [*homo*→*lumo*] became optically allowed. For instance, the [HOMO→LUMO] and the [HOMO–1→LUMO+1] transitions of the $(C_{120})_2$ are allowed. Therefore, it is expected that the new spectral peak appears for the $(C_{60+10n})_2$ in the lower energy region compared with the energy of the lowest allowed–transition of the C_{60+10n}.

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5 REFERENCES

[1] A. M. Rao, P. Zhou, K. Wang, G. T. Hager, J. M. Holden, Y. Wang, W. Lee, X. Bi, P. C. Eklund, D. S. Cornet, M. A. Duncan, and I. J. Amster, *Science* **1993**, *259*, 955–957.
[2] Y. Iwasa, T. Arima, R. M. Fleming, T. Siegrist, O. Zhou, R. C. Haddon, L. J. Rothberg, K. B. Lyons, H. L. Carter Jr., A. F. Hebard, R. Tycko, G. Dabbagh, J. J. Krajewski, G. A. Thomas, and T. Yagi, *Science* **1994**, *264*, 1570–1572.
[3] M. Núñez–Regueiro, L. Marques, J–L. Hodeau, O. Béthoux, and M. Perroux, *Phys. Rev. Lett.* **1995**, *74*, 278–281.
[4] P.–A. Persson, U. Edlund, P. Jacobsson, D. Johnels, A. Soldatov, and B. Sundqvist, *Chem. Phys. Lett.* **1996**, *258*, 540–546.
[5] L. Marques, J–L. Hodeau, M. Núñez–Regueiro, and M. Perroux, *Phys. Rev. B* **1996**, *54*, R12633–R12636.
[6] A. M. Rao, P. C. Eklund, J–L. Hodeau, L. Marques, and M. Núñez–Regueiro, *Phys. Rev. B* **1997**, *55*, 4766–4773.
[7] S. Kawasaki, A. Yao, Y. Matsuoka, S. Komiyama, F. Okino, H. Touhara, and K. Suito, *Solid State Commun.* **2003**, *125*, 637–640.
[8] V. A. Davydov, L. S. Kashevarova, A. V. Rakhmanina, V. M. Senyavin, V. Agafonov, R. Ceolin, and H. Szwarc, *JETP Lett.* **1998**, *68*, 928–934.
[9] G.–W. Wang, K. Komatsu, Y. Murata, and M. Shiro, *Nature* **1997**, *387*, 583–586.
[10] Y. Iwasa, K. Tanoue, T. Mitani, A. Izuoka, T. Sugawara, and T. Yagi, *Chem. Commun.* **1998**, 1411–1412.
[11] V. C. Long, J. L. Musfeldt, K. Kamaras, G. B. Adams, J. B. Page, Y. Iwasa, and W. E. Mayo, *Phys. Rev. B* **2000**, *61*, 13191–13201.
[12] H. Tanaka and K. Takeuchi, *Japanese J. Appl. Phys.* **2004**, *43*, 4462–4463.
[13] R. Taylor (Ed.), *The Chemistry of Fullerenes*, World Scientific: River Edge, NJ, 1995.
[14] K. H. Lee, H. M. Eun, S. S. Park, Y. S. Suh, K.–W. Jung, S. M. Lee, H. Young, and E. Osawa, *J. Phys. Chem. B* **2000**, *104*, 7038–7042.
[15] J. M. Cabrera–Trujillo and J. Robles, *Phys. Rev. B* **2001**, *64*, 165408/1–16548/6.
[16] J. Ribas–Arino, A. Curioni, W. Andreoni, and J. J. Novoa, *J. Phys. Chem. A* **2005**, *109*, 4979–4982.
[17] Y. Kita, K. Wako, I. Okada, and M. Tachikawa, *J. Theor. Computional Chem.* **2005**, *4*, 49–58.
[18] T. A. Beu, *J. Optoelectron. and Adv. Materials*, **2006**, *8*, 177–180.
[19] Y. Iwasa, T. Furudate, T. Fukawa, T. Ozaki, T. Mitani, T. Yagi, and T. Arima, *Appl. Phys. A* **1997**, *64*, 251–256.
[20] M. Premila, C. S. Sundar, P. C. Sahu, A. Bharathi, Y. Hariharan, D. V. S. Muthu, and A. K. Sood, *Solid State Commun.* **1997**, *104*, 237–242.

[21] V. D. Blank, N. R. Serebryanaya, G. A. Dubitsky, S. G. Buga, V. N. Denisov, B. N. Mavrin, A. N. Ivlev, S. N. Sulyanov, and N. A. Lvova, *Phys. Lett. A* **1998**, *248*, 415–422.
[22] S. Lebedkin, W. E. Hull, A. Soldatov, B. Renker, and M. M. Kappes, *J. Phys. Chem. B* **2000**, *104*, 4101–4110.
[23] C. C. Henderson, C. M. Rohlfing, K. T. Gillen, P. A. Cahill, *Science* **1994**, *264*, 397–399.
[24] M. S. Meier, G.–W. Wang, R. C. Haddon, C. P. Brock, M. A. Lloyd, and J. Selegue, *J. Am. Chem. Soc.* **1998**, *120*, 2337–2342.
[25] J. Cioslowski, N. Rao, and D. Moncrieff, *J. Am. Chem. Soc.* **2002**, *124*, 8485–8489.
[26] Y. Nomura, H. Fujita, S. Narita, and T. Shibuya, *Chem. Phys. Lett.* **2003**, *375*, 72–75.
[27] L. Pauling, L. O. Brockway, and J. Y. Beach, *J. Am. Chem. Soc.* **1935**, *57*, 2705–2709.
[28] J. Del Bene, H. H. Jaffe, *J. Chem. Phys.* **1969**, *50*, 1126–1129.
[29] R. L. Ellis, G. Kuehnlenz, and H. H. Jaffe, *Theor. Chim. Acta* **1972**, *26*, 131–140.
[30] Y. Nomura, H. Fujita, S. Narita, T. Shibuya, *Internet Electron. J. Mol. Des.* **2004**, *3*, 29–36.

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