Chromophores as Elements of Structure for Pico Technology Optical Computers

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The transfer of the energy of optical excitation between the different chromophores of anthraquinone and perylene dyes has been controlled by their relative orientation. Such assemblies are basic components for optical computers on the picometer scale.

Key words: Optical Computing, Energy Transfer, Fluorescence

Introduction

Optical computing where the processing of electrical energy is replaced by light quanta is very attractive for future technologies [1 – 3]. The replacement of wires by optical pathways is of special interest because light can cross without interference and thus, the complex wiring of modern computers may be appreciably simplified. Moreover, optical computers can operate at very high rates because there are not the problems of electrical computers such as inductivities of wires and loading of parasitic capacitors. Chemical structures are required for the handling of light and this has to be done by suitable chromophores. Organic materials are preferred because of their chemical variability and uncritical recycling for mass production.

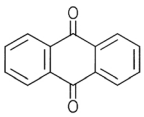
There are mainly three obstacles for the development of optical computers: firstly the preservation of the optical energy, secondly the low light-fastness of many active optical components and thirdly the comparably long wavelengths of light of about 0.5 μm. The former two problems can be solved by the application of highly light-fast fluorescence dyes where the fluorescence quantum yield is a measure of the preservation of light-energy; light fast fluorescent dyes with 100% fluorescence quantum yield are known [4].

The third problem sets a lower limit to the size of conventional optical components and hinders the construction of an optical computer on a molecular scale. However, the development of molecular optics would reduce the size of such components by a factor of 500.

Results and Discussion

The limitation of resolution by the wavelengths of light may be overcome by the transport of the energy of light instead of the emission and absorption of light quanta. This corresponds to the use of the alternating current ($\nu = 50$ Hz) with a problematic wavelength of some 6000 km ($\lambda = c \cdot \nu^{-1}$) where the electrical energy is handled on a human scale or even lower.

In analogy to such a transport of electrical energy an energy transfer between chromophores can replace the absorption and emission of light quanta in optical signal processing components. The transfer will proceed rapidly if the distance between the two chromophores lies within the Förster radius, that means between 2 and 3 nm for most combinations of similarly absorbing chromophores. On the other hand, this Förster radius would be the natural lower limit for the size of complex arrangements of switching components for handling energy transfer because going below this limit would spread energy over many chromophores without control; a solution of this limiting problem would be the prerequisite for the development of optical computers with very high densities of integration.



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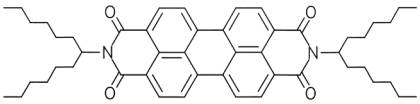

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We studied the energy transfer from an anthraquinone chromophore as an energy donor to a

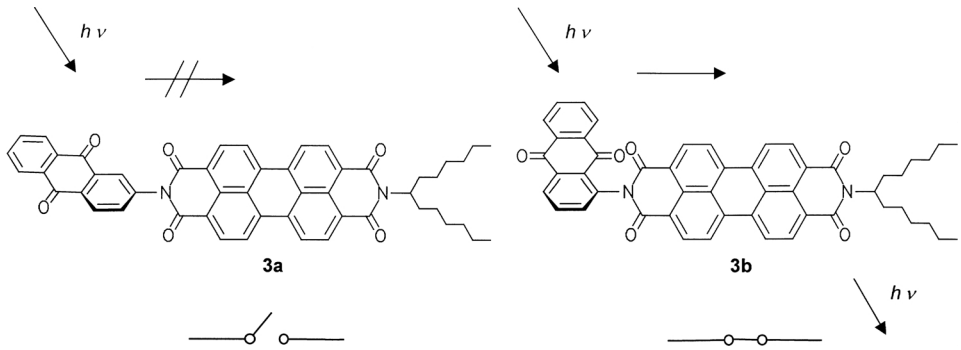

Fig. 1. Switch for energy transfer and analogies with presentations of electric circuits.

perylene bisimide chromophore as an acceptor. Anthraquinone (**1**) is non-fluorescent and only a fast energy transfer to the perylene bisimide unit (**2**) would preserve the energy of excitation; on the other hand, the perylene bisimide chromophore is highly fluorescent and can completely emit any transferred energy.

We have linked [5] the anthraquinone unit **1** closely to the perylene unit **2** by the synthesis of the bichromophoric dye **3a**; both chromophores in **3a** are electronically well isolated because there are nodes [6] at the nitrogen atoms of **2** both in the HOMO and the LUMO and both chromophores are placed nearly orthogonally by steric interactions, see Fig. 1. An indicator for the isolation of the two chromophores is the observation that the UV/vis absorption spectrum of **3a** in the region of long wavelengths is nearly congruent with the spectrum of **2**. A fluorescent quantum yield of more than 80% was found for **3a** if its perylene chromophore **2** was irradiated with light having wavelenghts greater than 450 nm, see Fig. 2. A sharp drop to fluorescent quantum yields of about 40% is found for shorter wavelengths where the anthraquinone chromophore **2** absorbs light; this quantum yield corresponds to the ratio of absorptivities of the two chromophores. One must therefore conclude that the energy transfer from **1** to **2** is not fast enough to compete with electronic deactivation in the anthraquinone unit and therefore cannot preserve the energy of excitation.

A completely different situation is obtained if the orientation of chromophore **1** is altered by 60° to give the positional isomer **3b**. The fluorescent quantum yield of **3b** remains high throughout the whole spectral region, see Fig. 2. One must therefore conclude that a very fast energy transfer from the **1** to **2** proceeds in **3b**. Thus, the efficiency of energy transfer is dependent of the orientation of the two chromophores.

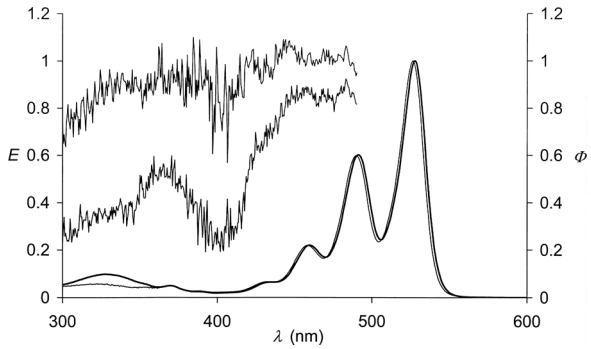

Fig. 2. UV/vis absorption spectra (E) of dye **3b** (thick line) compared with **2** (thin line) in chloroform; fluorescence quantum yield (Φ) of **3b** as a function of the wavelength of excitation (upper noisy line), and fluorescence quantum yield (Φ) of **3a** (lower noisy line); emission at 577 nm. The absorption spectra of **3a** and **3b** are very similar.

The energy transfer from **1** to **2** can be switched on by controlling the orientation of the two chromophores in suitable assemblies. This means that the flow of energy can be guided even at a molecular level and this is the prerequisite for the construction of components for computers at such small dimensions. The centres of gravity of the two chromophores are separated from each other by only 900 pm and the peripheries by only 140 pm and thus it could be demonstrated that such switches for energy transfer may be constructed in picometer dimensions. Other known fluorescence switches [1,7] quench the energy of excitation by some chemical influence and cause the loss of the energy of excitation, whereas the novel system can actively switch on the transport of the energy of excitation. Therefore, the transport of the energy of excitation can be directed to different pathways by controlling the orientation of the components.

Conclusion

The novel system opens the way for picometer technology. The concept will be also suitable for the construction of quantum computers on a picometer scale because single light quanta can be handled.

Experimental Section

Spectra

UV/vis spectra: OMEGA 20 from Bruins. The maximum absorbance was 0.80/1 cm at 528.0 nm for **3a** and 0.94/1 cm at 527.8 nm for **3b** in chloroform. Fluorescence quantum yields were determined with a totally corrected [4] Fluorescence Spectrometer 3000 from Perkin Elmer by irradiation at 490 nm and integration of the emission from 500 – 800 nm (detector: R928 from Hamamatsu). Excitation spectra were recorded with a totally corrected [8] LS50B spectrometer from Perkin Elmer and referred to the emission at 577 nm. The excitation spectra were normalized to the excitation at 490 nm and to the fluorescence quantum yield obtained by integration.

For synthesis, spectroscopic and physical data of compounds **3a**, **b**, see lit. [5].

Acknowledgements

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[1] B. L. Feringa (ed.): Molecular switches, Wiley-VCH, Weinheim (2001).
[2] F. L. Carter, (ed.): Molecular Electronic Devices, Proceedings of the First/Second International Workshop on Molecular Devices, Marcel Dekker, (1982/1984).
[3] F. M. Raymo, Adv. Mater. **14**, 401 – 414 (2002).
[4] H. Langhals, J. Karolin, L. B.-Å. Johansson, J. Chem. Soc., Faraday Trans. **94**, 2919 – 2922 (1998).
[5] H. Langhals, S. Saulich, Chem. Eur. J. **8**, 5630 – 5643 (2002).
[6] H. Langhals, S. Demmig, H. Huber, Spectrochim. Acta **44A**, 1189 – 1193 (1988).
[7] J. Walz, K. Ulrich, H. Port, H. C. Wolf, J. Wonner F. Effenberger, Chem. Phys. Lett. **213**, 321 – 324 (1993).
[8] S. Kalinin, M. Speckbacher, H. Langhals, L. B.-Å. Johansson, Phys. Chem. Chem. Phys. **3**, 172 – 174 (2001).