

Molecular logic gates.

Demeter Tzeli^{1,2*}

¹Department of Chemistry, National and Kapodistrian University of Athens, Panepistimiopolis Zografou, Athens 157 84, Greece

²Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Ave., Athens 116 35, Greece

Abstract

Molecular logic gates are devices that can perform Boolean logic operations. They have remarkable properties and they can gradually replace traditional silicon based electronic computers. They used or they can be used in disease diagnosis and treatment, in food safety, in metal detection, and as biosensors. They have many development prospects and potential.

Keywords: Molecular logic gates, Food safety, Metal detection, Biosensors.

Editorial

Over the past four decades, a lot of research has been conducted to investigate and to develop artificial receptors for species sensing and recognition, as well as to design molecular systems that can process information [1-28]. In general, molecules can respond to changes related to their environment, e.g., pH, temperature, light, solvent polarity, presence of other neutral or charged species, etc.; and then under certain conditions, the information could be processed, similar to electronic systems [3-7]. The “input” is the change of their environment, while the “output” is the measured property. These molecules are characterized as molecular logic gates (MLG) and they can demonstrate sequential advanced logic functions such as those used to make memory devices, storage and delay elements, and finite state machines. Firstly, this idea was demonstrated by de Silva in 1993 [1]. and very soon interdisciplinary research on this topic blossomed.

Very often, the property that it is used as an output is the absorption or emission spectra. In order a molecular system to be used as chemosensor or MLG, it is necessary to occur a reversible change; i.e., the MLG must be transformed between two forms by the absorption of electromagnetic radiation, where the two forms have different absorption or emission spectra. In plain language, this can be described as a reversible change of color upon exposure to light. The changes of their spectra are affected by photoinduced electron transfer (PET), electronic energy transfer (EET), internal charge transfer (ICT), proton transfer (PT), and photochromic processes (PC) [3]. Generally, most of the fluorescence chemosensors, molecular switches, and molecular logic gates are based on the “on-off” or “off-on” response of photoinduced electron transfer (PET). The molecular systems are designed according to the principles of modular PET, i.e., in a ‘fluorophore–

spacer–receptor’ or ‘fluorophore–spacer–receptor1–spacer–receptor2’ format where the fluorophore and receptor sites are purposely separated [3-6]. Furthermore, there is a fragment that can serve as an “antenna” for the absorption of photons and of using the photon energy to transform the molecular structure, as well as a fragment whose reactivity changes as a result of the structural transformation. The advantage of PET process is that it produces very sharp changes in the signal intensity, and it can be modulated in such a way as to generate significant changes in the emission spectra of molecules. The impact of PET on UV-vis absorption is often negligible and other phenomena, such as intramolecular charge transfer (ICT) could affect it. Finally, it should be noted that there are also fluorescent switches which are not built based on PET, but on other mechanisms, such as twisted intramolecular charge transfer [3,7-10].

MLG are defined as devices that make the input signals transform to specific output signals by Boolean logic operation. A “threshold” is introduced in logic gates that can distinguish two kinds of different states in a process. For example, different concentrations of analytes or the light radiation are taken as an input signal, and the generating of different fluorescence intensities are regarded as the output signals. In terms of input signals, the presence and absence of inputs are defined as “1” and “0”, respectively. If the value of the produced output intensity is higher than a specific threshold, the logic gates will have an output “1” or “TRUE”, while if it is lower, the output will be “0” or “FALSE”. Additionally, it worths to mention that MLG can be complexed, and the same molecular system can perform multiple logic operations. This was demonstrated for the first time by Baytekin and Akkaya [2]. who show that multiple logic behaviors can be resulted from a single system by changing the wavelength of excitation and/or detection. This remarkable property has been demonstrated in other MLG, see for instance [6,24].

*Corresponding to: Demeter Tzeli, Department of Chemistry, National and Kapodistrian University of Athens, Panepistimiopolis Zografou, Athens 157 84, Greece, E-mail: tzeli@chem.uoa.gr

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Finally, it should be noted that the progress of molecular logic gates is very impressive. Up to now, many experimental and computational articles have been published, where many promising candidates as MLG have been studied [1-13]. Additionally, many reviews have been written that report the new advancements on this topic, while they provide ideas and discuss possible future directions [14-28]. This research area is now firmly established. The next one or two decades many applications are expected to be developed in different research directions from medicine, for instance, intracellular and biomedical uses, [25] photodynamic therapy, [26] devices with autonomous therapeutic applications, [17] to material science [27] and information security, [19] for instance replacement of semiconductors in the IT industry which will overcome all issues occurring when semiconductors approach nano-dimensions; to environmental analysis, for instance water quality monitoring and heavy metal ion detection [28] and to food safety. To sum up, MLG have broad development prospects and huge development potential. Their study is an extremely active direction of research and it will remain active for the next decades.

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