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Molecular Information Processing: from Single Molecules to Supramolecular Systems and Interfaces – from Algorithms to Devices – Editorial Introduction

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Fast development of electronic computers with continuous progress [1] resulting in doubling their complexity every two years was formulated as the Moore's law in 1965 [2] (Figure 1.1). However, because of reaching physical limits for miniaturization of computing elements [3], the end of this exponential growth is expected soon. Economic [4] and fundamental physical problems (including limits placed on the miniaturization by quantum tunneling [5] and by the universal light speed [6]), which cannot be overcome in the frame of the existing paradigm, abolish all forms of future sophistication of computing systems. The inevitably expected limit to the development of the computer technology based on silicon electronics motivates various directions in unconventional computing [7] ranging from quantum computing [8], which aspires to achieve significant speedup over the conventional electronic computers for some problems, to biomolecular computing with a ''soup'' of biochemical reactions inspired by biology and usually represented by DNA-based computing [9].

Chemical computing, as a research subarea of unconventional computing, aims at using molecular or supramolecular systems to perform various computing operations that mimic processes typical of electronic computing devices [7]. Chemical reactions observed as changes of bulk material properties or structural reorganizations at the level of single molecules can be described in terms of information processing language, thus allowing for formulation of chemical processes as computing operations rather than traditional chemical transformations.

The idea of using chemical transformations for information processing originated from the concept of ''artificial life'' as early as in 1970s, when *artificial molecular machines* were inspired by chemistry and brought to computer science [10]. Theoretical background for implementing logic gates and finite-state machines based on chemical flow systems and bistable reactions was developed in 1980s and 1990s [11], including application of chemical computing to solving a hard-to-solve problem of propositional satisfiability [12]. However, the practical realization of the theoretical concepts came later when already known Belousov–Zhabotinsky chemical oscillating systems [13] (Figure 1.2) were applied for experimental design of logic gates [14]. Extensive research in the area of reaction-diffusion computing systems [15] resulted in the formulation of conceptually novel circuits performing

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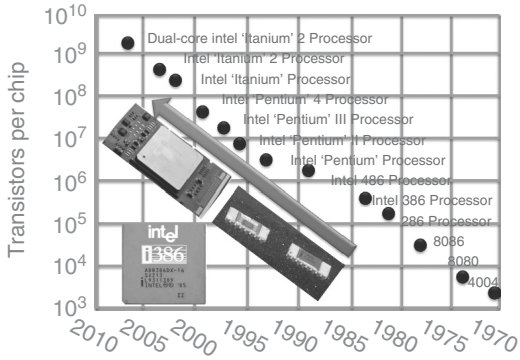

Figure 1.1 Moore's law demonstrating exponential growth of sophistication of electronic computing systems resulting in doubling of their complexity every two years.

Figure 1.2 Spiral waves in the Belousov–Zhabotinsky reaction – background for many chemical computing systems. (Adapted with permission from [13b]; Copyright (2006) National Academy of Sciences, USA.)

information processing with the use of subexcitable chemical media [16]. Developments in this area resulted not only in new chemical ''hardware'' for information processing but also in novel approaches to computing algorithms absolutely different from those presently used in silicon-based electronics. The major difference and advantage comparing with presently used electronic computers is the possibility of using 10^{23} molecules performing computations in parallel, thus resulting in great parallelization and acceleration of computing, which is not achievable in the present electronic paradigm. It should be noted that upon appropriate design, chemical systems can realize any kind of nonlinear behavior, which leads to the possibility to emulate any computational device needed for assembling information processing systems.

Information processing can be performed at the level of a single molecule or in a supramolecular complex. On the basis of early ideas to use molecules as logic gates [17], one of the first examples, a molecular AND gate, was reported in 1993 by de Silva *et al.* [18]. This novel research direction has been developed

rapidly from the formulation of single logic gates mimicking Boolean operations, including AND, OR, XOR, NOR, NAND, INHIB, XNOR, and so on, to small logic networks [19]. Combination of chemical logic gates in groups or networks resulted in simple computing devices performing basic arithmetic operations [20] such as half-adder/half-subtractor or full-adder/full-subtractor [21]. Sophisticated molecular design has resulted in reversible [22], reconfigurable [23], and resettable [24] logic gates for processing chemical information. Other chemical systems mimicking various components of digital electronic devices were designed, including molecular comparator [25], digital multiplexer/demultiplexer [26], encoder/decoder [27], keypad lock [28], as well as flip-flop and write/read/erase memory units [29].

Many of the chemical systems used for information processing were based on molecules or supramolecular ensembles that exist in different states. These states can switch reversibly from one to another upon application of various external physical or chemical inputs. Ingenious supramolecular ensembles operating as molecular machines with translocation of their parts upon external signals were designed and used to operate as chemical switchable elements performing logic operations. Rotaxane supramolecular complexes (Figure 1.3) designed by the group of Prof. Stoddart as early as 1990s [30] can be mentioned as examples of such signal-switchable systems – research that later received numerous extensions and applications [31].

Chemical systems can solve computing problems at the level of a single molecule resulting in nanoscaling of the computing units and allowing parallel computations performed by numerous molecules involved in various reactions. Chemical transformations in switchable molecular systems used for mimicking computing

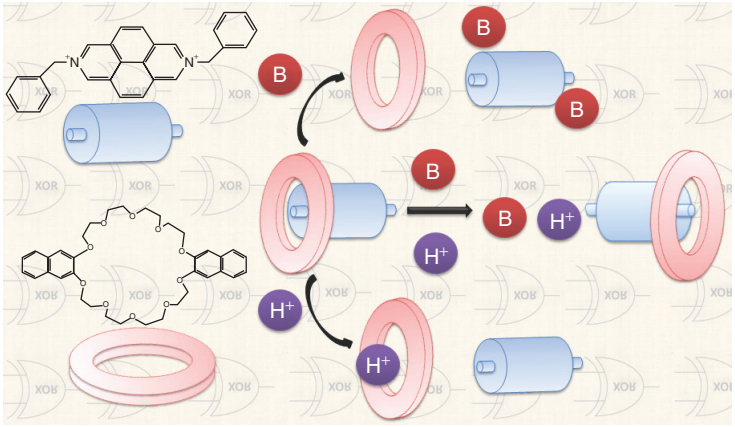

Figure 1.3 An example of a pseudorotaxane supramolecular complex activated by light, producing fluorescence only when the molecular hoop is released from the axle. The complex dissociates, thus resulting in fluorescence on application of an acid (H^+) or a base (B), while in the absence or presence of both chemical inputs the hoop remains in place and quenches the fluorescence. The system mimics the Boolean logic XOR (eXclusive OR), which is activated only in the presence of 0,1 or 1,0 input combinations, while being mute in the cases of 0,0 and 1,1 inputs.

operations can be based on redox changes, acid–base or chelating reactions, and isomerization processes [32]. The most representative research performed by the group of Prof. de Silva yielded various Boolean logic gates based on reconfiguration of switchable supramolecular complexes [33]. Chemical reactions in switchable systems have been induced by external physical signals, for example, light, magnetic field, or electrochemical potential, and by chemical signals, for example, pH changes or metal cation additions. Some of the studied switchable systems can respond to two kinds of physical or physical/chemical signals, for example, potential applied to an electrode and illumination, pH change and illumination, or ion addition and applied potential. The output signals generated by the chemical switchable systems are usually read by optical methods: UV–vis or fluorescence spectroscopies or by electrochemical means: current or potential generated at electrodes or in field-effect transistors. Association of chemical logic systems with electrode interfaces [34] or nanowires [35] resulted in electronic devices with implemented molecular logic performing on-chip data processing functions for lab-on-a-chip devices [36].

To some extent, the design of chemical "hardware" for information processing and future built-up of molecular computers depends on the success of molecular electronics [37] – the subarea of nanotechnology aiming at coupling of single molecules and nanoobjects for performing various electronic functions [38]. This approach resulted in numerous hybrid molecular-nanoobject systems performing various electronic functions potentially applicable to molecular computers. For example, nanowires made of conducting molecules [39] or templated by polymeric molecules [40] were designed for nanoelectronic applications (Figure 1.4) [41]. Single-molecule transistors and other functional molecular devices integrated with nanoscale electronic circuitries became possible (Figure 1.5). However, this approach copying the present conceptual design of electronic systems to the novel molecular architecture might be counterproductive for creating computers of next generation. A more effective way of assembling and operating molecular computing systems, aiming at massively parallel nonlinear computers mimicking human brain operation, requires absolutely novel approaches to the "hardware" and computing algorithms – their design is presently at a very preliminary stage. Novel

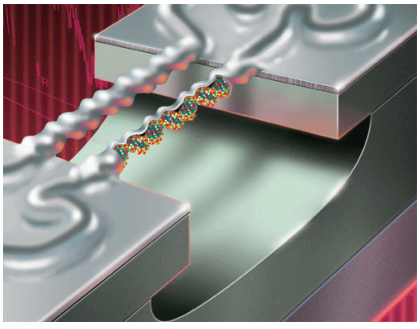

Figure 1.4 The artistic view of molecular-templated nanowires connecting microelectrodes. (Adapted from [40b] with permission; courtesy of Prof. Alexey Bezryadin.)

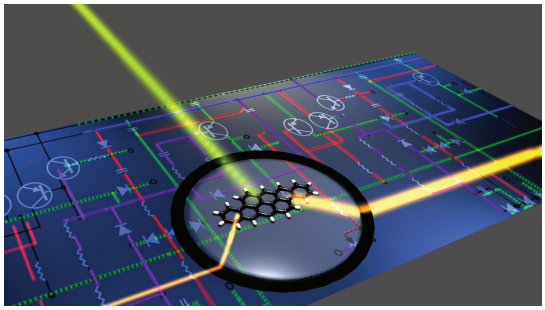

Figure 1.5 An artistic representation of a single-molecule optical transistor integrated into a nanocircuitry. (Adapted from *http://www.opfocus.org/index.php?topic=story&v=7&s=2*; courtesy of Prof. Vahid Sandoghdar.)

algorithms in information processing, particularly for hard-to-solve computational problems, are emerging in this study. Application of these algorithms with the use of chemical massively parallel computing might be much more efficient for solving hard-to-solve problems rather than the use of presently available supercomputers.

Before chemical computing becomes practically possible, many issues addressing the architecture and operation of molecular systems have to be addressed. Particularly important are the scaling up of the systems complexity and management of noise in chemical systems [42]. As an information processing network becomes larger and information is processed in greater quantities and at higher levels of complexity, noise inevitably builds up and can ultimately degrade the useful "signal," which is the intended result of the logic processing or computation. One then has to develop approaches to achieve what is known as "*fault-tolerant*" information processing that involves noise control and suppression. Chemical systems are much more prone to noise than electronic computer components. Their applications are in environments where the inputs (reactant chemicals' concentrations) and the "gate machinery" (other chemicals' concentrations) are all expected to fluctuate within at least a couple of percent of the range of values between the "digital" 0 and 1. Therefore, consideration of control of noise is required already in concatenating as few as two to three logic gates. While noise analysis in large chemical networks might be very complicated and requires heavy computational facilities [43], in single chemical gates and small networks noise analysis resulting in the systems optimization and noise suppression can be achieved using relatively simple computational and chemical approaches [42] (Figure 1.6).

Several comprehensive review articles have already covered to various degrees the molecular computing systems (mostly addressing chemical aspects of switchable signal-responsive systems operating as logic gates and small circuits) [19]. A good collection of review articles covering chemical and biochemical computing systems has been recently published in the special issue of *Israel Journal of Chemistry* (Wiley-VCH) – "Molecular and Biomolecular Information Processing Systems" (February 2011, Vol. 51, Issue 1, Guest Editor – E. Katz). However, taking into account rapid developments in this area, the editor and the publisher believe that

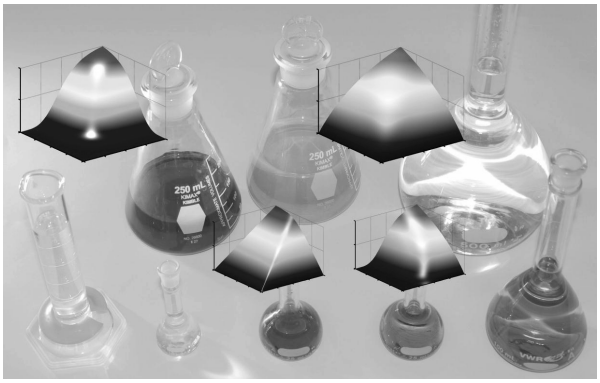

Figure 1.6 Theoretical and experimental response functions of a chemical AND logic gate representing noise-suppressing (top-left schematic) and noise-amplifying (top-right schematic) operation. Two experimental response surfaces recently realized in the parameter regime of no noise amplification are also shown (lower schematics).

another comprehensive summary of the results would be beneficial for the multidisciplinary research community, which includes fields of chemistry, materials science, and computer science, thus bringing to your attention the present book.

This book represents a unique collection of review accounts written by major contributors to this newly emerged research area overviewing the state of the art in unconventional chemical computing and its potential applications. In this book, following introductory Chapter 1, Chapters 2–6 authored by A. Credi *et al.*, J. Andréasson and D. Gust, A.P. de Silva, D.C. Magri, C.P. Carvalho and U. Pischel represent an overview of a broad research area utilizing molecular and supramolecular species for chemical computing. Chapter 7 written by K. Szaciłowski *et al.* extends the chemical computing research area to semiconductive species (thin films and nanoparticles). Theoretical and experimental approach to reaction-diffusion computing systems is described in Chapter 8, written by A. Adamatzky *et al.* Various aspects of theoretical approaches to novel computing algorithms based on chemical computing can be found in Chapters 9 and 10, written by V. Kreinovich *et al.* A very unusual approach to unconventional chemical computing is offered by A. Schumann in Chapter 11. In this chapter, he connected Kabbalah, the esoteric teaching of Judaism, with massively parallel chemical computing, coming to the conclusion that any physical, chemical, or biological phenomena could be simulated with the help of chemical computing. Chapter 12, authored by V. Privman, offers theoretical consideration and practical realization of noise management in chemical computing systems. Electrochemical systems employed for information processing are outlined in Chapter 13 of S. Sadeghi and M. Thompson, while Chapter 14 prepared by E. Katz describes electrode interfaces switchable by external signals considering them as a platform for information processing systems. Chapter 15 offers the Editorial (E. Katz) conclusions and speculates about future perspectives of chemical computing systems.

The Editor (E. Katz) and Publisher (Wiley-VCH) express their gratitude to all authors of the chapters, whose dedication and hard work made this book possible, hoping that the book will be interesting and beneficial for researchers and students working in various areas related to unconventional chemical computing, including chemistry, materials science, computer science, and so on. It should be noted that the field of chemical unconventional computing extends to the fascinating area of biomolecular systems, consideration of which is outside the scope of the present book. This complementary area of biomolecular computing is covered in another new book of Wiley-VCH: *Biomolecular Information Processing: From Logic Systems to Smart Sensors and Actuators* – E. Katz, Editor. Both books are a must for the shelves of specialists interested in various aspects of molecular and biomolecular information processing.

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