

Technomimetics versus Biomimetics

Technomimetics versus Biomimetics:

*An Application towards
Artificial Intelligence*

By

Ruby Srivastava

**Cambridge
Scholars
Publishing**



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This book first published 2020

Cambridge Scholars Publishing

Lady Stephenson Library, Newcastle upon Tyne, NE6 2PA, UK

British Library Cataloguing in Publication Data
A catalogue record for this book is available from the British Library

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ISBN (10): 1-5275-4971-2

ISBN (13): 978-1-5275-4971-5

To my parents

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PREFACE

Welcome to the first edition of the book: *Technomimetics versus Biomimetics: An application towards Artificial Intelligence*. The goal of this book is to help readers and researchers of almost any field to get an idea of the role of manmade devices; nature's mimicking devices; how silicon chip technology has shifted to molecular computers; natural and/or artificial molecular devices where macromolecules, including proteins and nucleic acids, mediate necessary functions; autonomous systems and their biomedical applications; machine learning; Big Data; deep learning; and the role of artificial intelligence in industrial applications.

Innovations in biomedical device design have advanced to thin adhesive bandages; soft conductive gels; collecting accurate recordings of cardiac, brain, and muscle activity; epidermal sensors; biochemical signatures; autonomous systems; protosensors; and many more devices. New bioelectronic designs have been made to implant programmable devices with unique modes of operation due to their ability to bypass the blood-brain barrier. These systems are designed to interface directly with internal organs, thereby allowing targeted and programmed drug delivery and reducing the possibilities of drug toxicity and/or side effects. These bioelectronic implants are able to deliver electrical stimulation to the heart and brain to treat cognitive disorders and other related conditions. Also, bioelectronics devices help in the treatment of disease and healing processes. Additionally, these devices are able to replace many inefficient body parts due to their efficient functions. This device's autonomy, which has made significant advances in deep learning algorithms and artificial intelligence-based diagnostics, is already being used by highly trained physicians for certain tasks. It is not possible to cover all of this in one book, but we have tried to cover the essential topics and the use of artificial intelligence more generally.

I am very thankful to Helen, book publishing manager at Cambridge Scholars Publishing, for her prompt response to all queries and her immense support at every level. *Thank you so much Helen*. I would like to acknowledge the DST WOS A project (SR/WOS A/CS-69/2018) and Dr. Shrish Tiwari, my mentor scientist, from the Bioinformatics Division, CSIR-

CCMB, for the support. Foremost, I would like to thank my husband, Amit; daughter, Arghyaa; son, Aryan; and my entire family for their continuous encouragement and understanding at every stage to complete this book. Finally, I would like to acknowledge a few eminent scientists in this field who have guided me at every stage when writing this book.

ACKNOWLEDGEMENTS

1. Prof. Dmytro M. Hovorun
Department of Molecular and Quantum Biophysics, Institute of Molecular
Biology and Genetics, National Academy of Sciences of Ukraine, Kyiv,
Ukraine.

2. Prof. Yoseph Bar-Cohen
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Drive, Pasadena, CA 91109-8099, USA. JPL/Caltech/NASA.

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I would also like to thank Ms. Joanne Ella Parsons for proof-reading the
manuscript. She has finished the task in a highly efficient manner. *Thank
you so much Jo.*

CHAPTER 1

INTRODUCTION

Technomimetics represent a limited subclass of molecular devices, which constitute a more general family of individual molecules and molecular systems capable of providing valuable device-like functions. Similarly, research on nanoscale semiconductor devices elicits a novel understanding of biological systems. There are so many areas where nature is superior in its ability to recognize patterns and objects. However, some human inventions that appear to be biomimetic may not have been due to adapting nature's ideas. So, for more effective use, we need a database to establish a logical catalog of nature's capabilities, specifications, mechanisms, processes, tools, and functions in terms of its principles, materials, dimensions, and limitations. Nature offers numerous examples of materials that serve multiple functions. The multifunctionality of biological materials (sensing, healing, actuation, and other functions) occurs at the macro and nanoscale, as well as on various temporal and compositional levels. Effective packing and deployment techniques make the best use of nature's resources because they use the minimum amount to produce maximum results. This also allows the organisms to fit the environment in which they need to operate. This technology is used to produce scalable mechanisms ranging from miniature (nanometer scale) to large (several meters).

Molecular electronics has significant potential as this technology is very useful as well as very challenging. Its challenges include the difficulty of integrating molecules with bulk materials so that the limitations of the latter do not dominate the device's operation. The second challenge is to achieve sufficient performance so that molecules can outscale silicon in metrics other than size. As there is an increased understanding of molecular design and performance, together with the improved ability to fabricate nano-ordered materials, molecular electronics is still considered to be a promising future technology. Molecular motors are also well-established nanoscale molecular machines present in living systems. They are responsible for various dynamic processes that transport single

molecules over small distances to cell movement and growth. Molecular motors are self-guiding and ideal systems because of their small size, perfect structure, and efficiency. Active biomimetic systems based on molecular motors and filaments have many potential applications in the fields of bioengineering, pharmacology, and medicine. Molecular motors are formed by using bottom-up approaches to construct active structures and provide maintenance at the nanometer scale. Though mimicking nature is challenging, it also has endless possibilities. Biomimetics is a very useful source of inspiration for inventors and scientists. Researchers are in continuous search of robots that are highly flexible and dexterous, can operate intelligently and autonomously, can crawl, can camouflage themselves, are able to amend their shape according to their surroundings, can be used to see clearly without blind spots, and which have many multifunctional components that can perform multiple tasks simultaneously.

Multifunctional macromolecular biological assemblies are essentially all exquisitely designed molecular machines. For example, hemoglobin, polymerases, ATP synthase, membrane channels, and ribosomes. Natural processes are capable of designing an enormously diverse range of fabrication materials and molecular machines, which have high precision, flexibility, and error correction. These machines can self-organize into refined structures, and also are self-sustaining and evolving. Nature builds molecular assemblies effortlessly, within a well-defined scaffold and using a bottom-up approach. But recreating them in the laboratory is highly challenging for scientists. In biomimetics, we use natural bottom-up fabrication processes to mimic these phenomena to create new and varied structures with novel utilities. Basically, two distinctive and complementary fabrication technologies are used to produce the materials and tools. In a top-down approach, these materials are manufactured by stripping an entity into its parts, while the bottom-up approach requires a deep understanding of individual molecular structures, their assembling properties, and their dynamic behaviors. At the nanoscale, two levels of mimetics are considered. "Machine nanomimetics" applies mechanical principles to create nanomachine components, which are inspired by the equivalent machine components at the macro-scale and "bionanomimetics", where biotechnical principles are applied to the biological entities, such as proteins and DNA to create nanomachine components. Furthermore, all of these features are applied in nanorobotics to design machines with various characteristics, design logics, advantages, and limitations. Interestingly, biology has joined forces with technological advancement and is now ready to challenge human identity.

Living organisms are the perfect example of nature's advanced nanotechnological manufacturing. Therefore, there is much interest in building artificial organs that mimic nature. Nanotechnology can provide molecularly manipulated nanostructured materials, which mimic the natural surfaces. Sensing and control are also used to design novel interface technologies. Drug delivery systems [1]; molecular self-assembly at the surface; geometry via polymeric patterning, adhesion, and migration [2, 3]; the extracellular matrix containing glycosaminoglycans; and glycoproteins supporting cell growth and proliferation [4] are a few examples. The National Institute of Health (NIH) has undertaken a big initiative for the development of nanotechnology in drug delivery, cell repair, anticancer methodologies, and biomachines. The energy issues can also be solved by developing micro-machines, which can derive energy from substances, such as oxygen and glucose, which are easily available from the body.

Molecular machines that resemble other objects from our everyday world have a seductive appeal. However, numerous mechanisms that work at the macroscopic scale are physically impossible at the molecular level. The logical progression of the mono-molecular electronics approach is that it integrates many electronic elements, such as wires, switches, and amplifiers, in a single molecule or individual supramolecular assembly. There are many unresolved issues and opportunities for molecular electronic devices in the architectural field where a conventional analysis of a molecular device appears to be invalid due to the linear superposition of its components. This will make molecular electronics a prime contributor to the building of nanoscale quantum machines using the power of quantum-state superposition. Indeed, as synergistic and cooperative effects in complex molecular systems are understood and controlled, new electronic devices based on unconventional operating principles need to be developed. In short, it seems that applying conventional electronic concepts and approaches is not necessarily the best way to achieve functional molecular devices operating on a dimensional scale where quantum mechanics dominates.

Nanotechnology acts as a toolkit for the electronics applications as it allows us to make nanomaterials with special properties modified by ultra-fine particle size, crystallinity, structure, or surfaces. A semiconductor is a material that can be produced or fabricated by nanotechnology with a top down or a bottom up approach. These nanotechnology-based semiconductor materials are now being used to produce materials with extremely large surface areas. One of the most important areas used in semiconductor is

solar energy harvesting. Solar cell or photovoltaic materials are produced by nanotechnology with increasing efficiency with regard to photon trapping and converting to electric energy by making materials such as quantum dots, quantum wires, and quantum wells.

In recent years, there has been a lot of interest in intelligent systems as they have been used in applications from customer support to curing cancer. However, the term “AI” can be sometimes used as a trigger to increase the likelihood of accessing funding. Reports about its positive and negative roles declare that AI is going to steal our jobs and that the US government is concerned about the prospect of super-intelligent killer robots. The government is also worried about how to address wealth disparity. So, there are several questions regarding the ethical employment of technology. Furthermore, will robots be afforded rights? What happens if they become conscious or smarter than us?

Comparatively, the positive impact of artificial intelligence is rarely discussed with regard to how it is going to actually affect business. Terms including AI, machine learning, automation, Big Data, cognitive computing, and deep learning are basically about a machine’s ability to fulfill objectives based on data and reasoning. Big Data and deep learning are the most important aspects, and they are already significantly changing business in practically every industry. In spite of all the progressive claims, there are still several core problems where little progress has been made, such as learning by analogy and natural language understanding. At some point we still have to accept that machine learning is not the solution to all problems, as we have neither the data nor the necessary understanding to build machines that make routine decisions as well as human beings [5]. So, it is better to focus on all the positive characteristics of artificial intelligence in order to design smarter devices, which could be useful to mankind in the future.

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CHAPTER 2

TECHNOMIMETICS: FROM MACROS TO NANODEVICES

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 - 2.2 Examples of Technomimetic Devices
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 - 2.2.2 Molecular gears
 - 2.2.3 Belts and Tubes
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2.1 Introduction

Technomimetic materials are created by individual molecules and molecular systems that can mimic manmade devices in their design, functions, and modes of operation. Despite the fact that these materials started to be used in the 1970s, major advancements have only occurred in the past thirty years. Yet, technomimetic materials have established themselves as a distinct class for applications in biological and material field over the past ten years [1]. However, the major impact of this technology is the construction and fine-tuning of complex functional technomimetic molecules, which is expected to occur in the near future. Technomimetics have a limited group of molecular devices and molecular machines. Molecular devices represent a family of individual molecules and molecular systems, which are capable of providing device-like functions that are mostly used in industrial applications. Technomimetics can be identified as distinct conventional prototypes materials. These sets include simple molecular devices as container compounds [2, 3], gearing systems [4], belts and tubes [5], tweezers [6, 7], molecular brakes [8] and chemically driven motors [9], molecular wheelbarrows [10], cars [11], and scissors [12]. Further examples are molecular pumps [13], spoked wheels [14-17], pinwheels [18], molecular hinges [19], caterpillar tracks [20], and elevators [21]. We have tried to cover these vast topics in two chapters (2 and 3), as well as to give brief introductions about the material devices.

2.2 Examples of Technomimetic Devices:

The simplest conventional devices are molecular containers that mimic the functions of containers, and which can be filled with guest molecules or ions. These molecular carrier vehicles are used in biomedical applications.

2.2.1 Molecular Containers

The inner space of these container act as “a novel reaction environment” [23] or “molecular reaction flask” [24], which can easily fit various guest molecules, such as small organic molecules, reactive intermediates [25], nanotubes, benzaldehyde, and entrapped fullerene C₆₀. The research has now shifted towards using endohedral fullerenes [26–29] as guest molecules, which are characterized by their tightly meshed all-carbon network sidewalls. The empty internal cavities of fullerenes are filled via the implementation of modern ion implantation and “surgical” open-and-close synthetic methodology. N@C₆₀ is commercially costly compound,

which is used in miniature atomic clock applications [30].

2.2.2. Molecular gears

Molecular gearing systems [31, 32] are an important class of technomimetic molecules. Molecular gearing systems are constructed with gear slippage and various braking elements, so that the rotation can be controlled externally [33]. A pictorial representation of molecular gears is given in Figure 2.1.

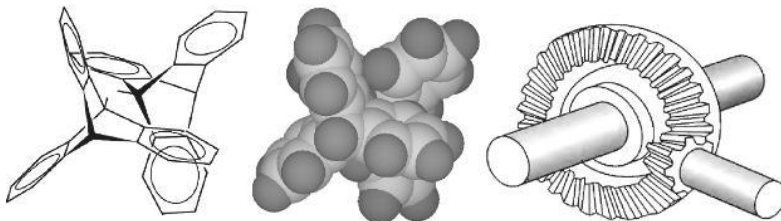


Figure 2.1: Schematic representation of molecular gears. Courtesy of Prof. Yoseph Bar-Cohen, JPL/Caltech/NASA.

2.2.3. Belts and tubes

Belt and tubes are used for the transportation of gases and liquids, and also as the parts of various mechanical devices. An example is cyclo [34] fluorene, which has a distinct green fluorescence.

2.2.4. Molecular tweezers

These are developed classes of technomimetics with potential applications ranging from advanced chemical sensors to novel biomedical agents [10, 11]. Conventional mechanical tweezers are guided by human or artificial intelligence, so that the desired “intelligent” selectivity can be attained by including multiple functional groups. Dynamic molecular tweezers, such as molecular tweezers with porphyrin pincers, are controlled allosterically with the presence of certain chemical species in a particular environment or by responding to light, electrochemical, and mechano-chemical stimuli [11].

2.2.5 Scissors and pliers

Molecular scissors and pliers are externally controlled molecular devices, which undergo scissor-like transformations in certain stimuli, such as narrow-band electromagnetic radiation [16]. Though scissors can only mimic their conventional mechanical prototypes' mode of action and not their cutting function. Molecular scissors are used to cut chemical bonds. However, the advanced version of molecular pliers can mimic conventional mechanical counterparts both in terms of their action and functional mode (see Figure 2.2).



Figure 2.2: Pictorial representation of molecular scissors. Figure adapted from en.wikipedia.org.

2.2.6 Molecular wheelbarrows, cars and trucks

Molecular wheelbarrows are sophisticated technomimetic molecules with wheels, axels, a supporting frame, and handles.

Molecular cars and trucks [35, 36] are the logical extension of molecular wheelbarrow designs. Molecular cars usually have four wheels, which

allows unrestricted movement along the applied external force [37]. Several variants of car design include the use of fullerene C_{60} [38], adamantane [39], p-carborane [40-42], and organometallic complexes, which mimic car wheels. Light-driven [43] and electrically driven [44] motorized molecular cars are also available. As molecular cars do not permit the attachment of a useful payload, “nanocars” are considered to be replicas of conventional cars but only with regard to their mode of action. Their payload functionality is achieved by the addition of a functionalized “cargo bay” (for picking up and dropping off the payload); therefore, these machines are categorized as molecular trucks.

2.2.7 Rotary devices

The extended family members of rotary devices [45] are molecular gyroscopes [46–52], turnstiles [53–57], and compasses [58, 59] where the rotors are embedded in a stationary molecular frame (see Figure 2.3). Molecular gyroscopes and ball bearings are molecular systems that allow some form of partially restricted rotation of a smaller, internal part of the molecular assembly.

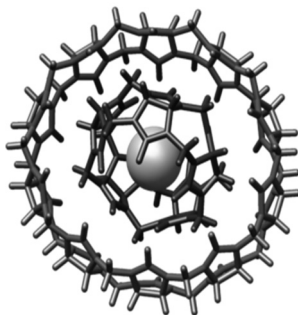


Figure 2.3: Molecular gyroscopes with the chloride ion in green, the rotor in red, and the stator in purple. Figure adapted from en.wikipedia.org.

The only difference between the molecular gyroscopes and the ball bearings is the degree of rotational restriction, which is lower for molecular ball bearings. An example is when fullerene C_{60} and cyclo [4] chrysenylene form a strong complex ($\log K_a = 12.3$ in benzene) where the internal C_{60} can rotate freely in all directions within the cyclo [4] chrysenylene framework (see Figure 2.4). The dual mode rolling mechanism was observed in a substituted fullerene C_{60} ball, which produced two types of distinctive rolling dynamics (spin and precession)

with relatively low activation energies 4–5 kcal/mol [60].

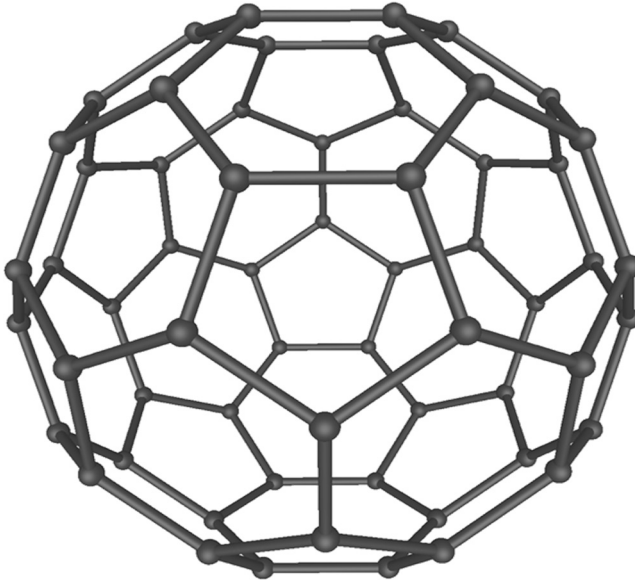


Figure 2.4: Molecular representation of Fullerene. Figure adapted from en.wikipedia.org.

2.3 Manufacturing Technomimetics

The manufacturing of molecular devices can be successfully accomplished by using modifications of traditional synthetic methods that are successfully employed in organic chemistry and biochemistry. The earlier development occurs with the “repair replication” method [61], which was in the form of the “polymerase chain reaction”, or PCR [62]. PCR is a combination of two synthetic approaches: (a) template-directed synthesis and (b) repetitive synthesis. The existing PCR protocol can only be applied for the production of DNA copies. Template-directed and repetitive synthesis methods are used to manufacture a variety of technomimetic molecules. The simplest repetitive polymerization reaction is used in the production of polyethylene, while the controllable oligomerization is used for the synthesis of belt molecules. Repetitive synthesis occurs for “folding stairs” molecular ribbons. Benzene rings align in a parallel staircase-like manner, which has been observed as the longest molecular ribbon prepared with a metacyclophane oligomer with

nine benzene rings. The synthesis is independent of the ribbon length and processed due to its good solubility. Template manufacturing is also a technological approach that fabricates the complex artificial object, which includes the construction of buildings, bridges, concrete and ceramic items, and others objects at the macro level. It is used in enzyme catalysis and manufacturing molecularly imprinted polymers in chemistry. An example is the preparation of container compounds from properly functionalized resorcin [4] arenes [63]. Larger semipermeable container compounds (e.g., with four $(\text{CH}_2)_4$ links instead of four CH_2 links) are used where the template molecules are difficult to remove from the closed molecular containers. This allows the removal of the template molecule at elevated temperatures [64]. Template-directed repetitive synthesis is found in giant porphyrin-based molecular tube fragments and all-carbon molecular tubes with metal clusters and coded hetero polymerization [65, 66]. It is also able to add chemically homomorphic units in a controllable manner.

Though there are some self-replicating systems, which involves the spontaneous assembly of molecules into structured, stable, noncovalently joined aggregates [67], these systems are of little values to technomimetics. Some technomimetics require covalent bonding of functional fragments, which means they cannot be produced via self-assembly. These molecular capsules can be prepared by self-assembling two complementary half-spheres. This is the key development in technomimetics.

Now, we will discuss the latest technomimetic molecules related to modern electronic and computer devices, including molecular wires, transistors, diodes, and other components. These molecular electronic components' modes of action and structures are quite different compared to the devices discussed above.

2.4 Modern Technomimetics

The development of high-performance semiconductor devices, such as Si, GaAs, and InP, have improved our lives significantly during the last century. The wide-bandgap semiconductors, such as ZnO, SiC, GaN, Ga_2O_3 , and diamond, are considered to be the next-generation semiconductors due to their excellent physical and chemical properties. These devices have wide applications in the fabrication of optoelectronic devices and semiconductor electronics, such as light emitters, solar cells, solar blind detectors, high-temperature and high-power electronics, gas sensors, high power microwave transistors, and microelectromechanical systems (MEMS). Several research fields are being developed with

changes in their basic design, such as high-quality bulk or epitaxial layer growth, n-type and p-type doping, surface crystal quality improvement, interface quality of metal/semiconductor or insulator/semiconductor junctions, and the optimization of device fabrication processes. There has been significant progress in semiconductor growth and device technology, which would be valuable and meaningful for the industrial purposes.

The semiconductor industry continues to produce ever smaller devices that are more complex in shape and contain more types of materials. The ultimate size and functionality of these new devices will be affected by fundamental and engineering limits, such as heat dissipation, carrier mobility, and fault tolerance thresholds. At this stage, it is difficult to analyze the particular parameter or the best measurement methods needed to evaluate the nanometer-scale features of such devices; it is also unclear how the fundamental limits will affect the required metrology.

The power electronic devices act as solid-state switches in circuits or as a switch without any mechanical movement in the semiconductor industry. The following are examples of these types of devices: Power Diodes, Metal-Oxide-Semiconductor Field-Effect Transistor (MOSFET), Bipolar-Junction Transistor (BJT), Insulated-Gate Bipolar Transistor (IGBT), and Thyristors (SCR, GTO, MCT). The pictorial representation of these devices is given in Figure 2.5.

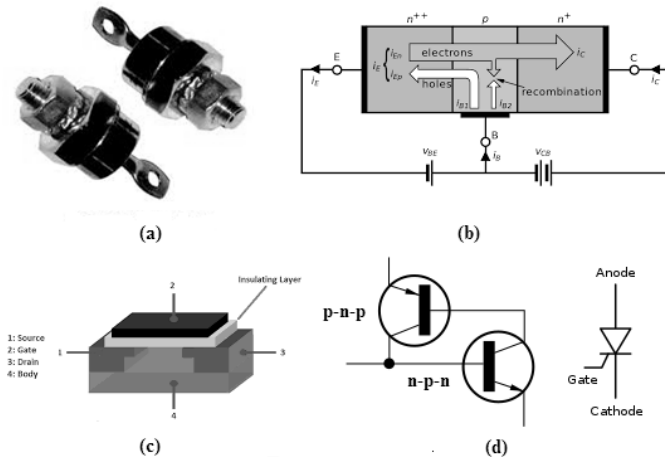


Figure 2.5: The device structure of (a) a power diode, (b) a bipolar junction transistor (BJT), (c) a MOSFET, and (d) a SCR-thyristor.

Solid-state devices are made from a solid material and their charge flow is confined within this solid material. The term “solid state” is used to differentiate it from earlier vacuum and gas-discharge tube devices, and also to exclude them from electro-mechanical devices (relays, switches, hard drives and others).

The first solid state device “transistor” was designed by Bell Labs in 1947, and it was later used commercially in the 1960s. The first working prototype transistor was invented by John Bardeen, Walter Brattain, and William Shockley at Bell Labs in 1947. This device was known as a point contact transistor. It was further improved by the addition of the bipolar junction transistor. Other similar types of solid-state devices are as follows: power diodes; power transistors; MOSFETs; the thyristor and its two-transistor model; triacs; gate turn-off thyristors (GTO); and insulated-gate bipolar transistors (IGBT). In power electronics circuitry, these switches act in the saturation region; however, they work in the linear region in the analog circuitry for power amplifiers and linear regulators. These switches are highly efficient as they lose less power.

Semiconductors are smaller, lighter, more reliable, and less expensive to build compared to the vacuum tubes. Furthermore, numerous transistors are combined in an integrated circuit to form a single device. These devices’ extensions are used for many practical applications, such as cell phones, GPS devices, laptop computers, tablets, and global communications infrastructure.

Semiconductors are made up of two types: Intrinsic and Extrinsic. Intrinsic semiconductors are neither good conductors nor insulators, and their conduction is largely dependent on the temperature. The material’s properties can be altered by injecting foreign substances or impurities (dopants) into the crystal. A crystal with an added dopant is known as an extrinsic semiconductor or doped material. A small amount of impurity could be added (one part per million). A dopant could be added through a gaseous diffusion process or it could be allowed to “seep into” the target crystal. The other alternative is ion implantation where the impurities are accelerated and smash into the target, thereby dislodging and replacing some of the original atoms in the crystal.

There are two different types of semiconductors: N-type material and P-type material. N-type material is created by adding pentavalent impurities, such as a dopant with five electrons in its outer shell. For

example, As, P, and Sb. P-type materials contain a trivalent impurity and have three electrons in their outer shell. Examples of trivalent impurities include B, Ga, and In.

The PN junction is the fundamental building block of solid-state semiconductor devices. The PN junction is created by a single zone of N material adjacent to a zone of P material. The basic device built from the PN junction is known as the diode. Diodes are designed for a wide variety of uses, including rectification, lighting (LEDs), and photodetection (photodiodes). Examples of these diodes are as follows: Zener diodes, light emitting diodes (LED), photodiode, Schottky and varactor diodes, clippers, and clampers. PN junctions can be found in a variety of devices, which include bipolar junction transistors (BJTs) and junction field effect transistors (JFETs). Signal amplification, such as boosting the signal level from a sensor or increasing driving loads via loudspeakers or antennas, is used for these models. The salient feature of an ideal amplifier is to multiply the amplitude of the input signal by a constant. It should not change the frequency of the signal, alter its shape, add noise, or distort the signal in any way. Complex amplifier circuits include input and output impedances along with a controlled source that exhibits a signal gain or amplification factor.

Detailed state-of-the-art dimensional metrology methods for integrated circuits, as well as their advantages, limitations, and potential improvements, can be found in any semiconductor devices book. In this book, we have elaborated on the technical and biological aspects of technomimetics in detail.

2.5 Molecular Electronics: Devices and Circuits

The term “molecular-scale electronics” refers to creating functional electrical circuits using individual or ensemble molecules, which not only meets the increasing technical demands of the miniaturization of traditional Si-based electronic devices, but also provides an ideal window through which to explore the intrinsic properties of materials at the molecular level. It has provided new insights into the development of efficient platform methodologies for building reliable molecular electronic devices with the desired functionalities through the combination of programmed bottom-up self-assembly and sophisticated top-down device fabrication. Molecular-scale electronics create functional electrical circuits based on the properties of individual or ensemble molecules with several unparalleled advantages. The advantages are as follows: an extremely

reduced molecule size; heightened capacities; faster performances; the ability to surpass the conventional limit of silicon semiconductors; abundant diversity in their molecular structures; universal availability of molecules; and low-cost manufacturing. Molecular-scale electronics refer to the use of single molecules or nanoscale collections of single molecules as electronic components.

Molecular electronics devices [68] has several potential advantages: their small size (a few nm); they can self-assemble onto surfaces; it is a very low-cost process; and they can be designed at the atomic level. This device allows the precise control of electronic properties at the atomic level. Research has been carried out to measure and predict the transport of electricity through these organic devices. Organic materials are metallic and have semiconducting carbon nanotubes, silicon nanowires, oligo(phenylene ethynylene) (OPE) based bistable molecular switches, insulating alkanethiol chains, slightly more conductive OPEs and oligo(phenylene vinylene)s (OPVs), and charge storage molecular systems, such as ferrocenes. Electron transport and charge storage are used to engineer molecules for specific applications. The chemical structure for a molecular switch is given in Figure 2.6.

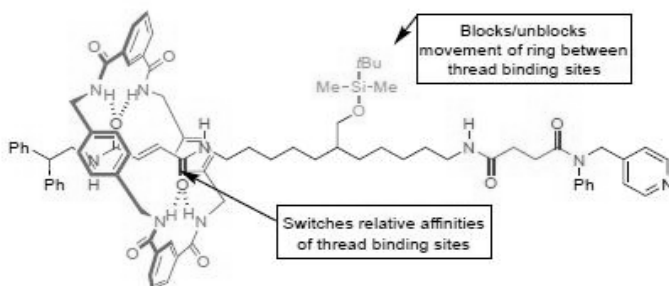


Figure 2.6: The chemical structure of a molecular switch. Adapted with permission from reference [68]

2.6 Silicon Devices

Silicon device characteristics are engineered by varying the carrier density using doping techniques and designing molecular devices which involve modifying electronic wavefunctions at the metal-molecule-metal junction.

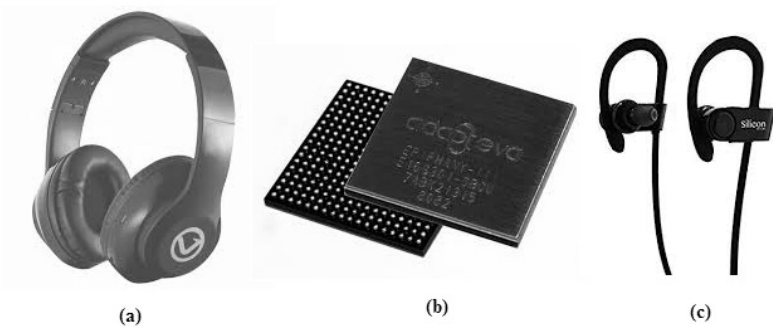


Figure 2.7: A pictorial representation of silicon devices: (a) head phones; (b) silicon chips; and (c) ear phones.

A significant development occurred with the development of scanning probe microscopy (SPM) [69] which addressed both surface topography and transport information issues [70]. A few examples of silicon devices are given in Figure 2.7. Various other techniques, including mechanically controllable break junctions, electromigration breakdowns, electrochemical depositions, and surface diffusion-mediated depositions have also been developed [71-74]. Additional new effects, including electronmechanics, thermoelectrics, optoelectronics, quantum interferences, and spin transports, were discovered at the single molecule level [75-78]. Nonmetal materials, such as conducting polymers and carbon-based materials, possess natural compatibility and excellent mechanical flexibility [79, 80] with nanotubes and graphene; they are used as point contacts when creating robust single-molecular junctions with desired functions. The “transmission coefficient” and formulations that use the nonequilibrium Green’s function (NEGF) approach, Breit-Wigner formula, and Simmons model have been used to interpret electron transport behaviors through a molecule [81-84]. The NEGF approach is used to demonstrate elastic and inelastic effects with the metal-electrode coupling and gating effects [85]. A small variation in each process may result in large changes in molecular devices. The current variation is sensitive to environmental changes, such as contamination, radiation, humidity, temperature variations, and other external influences. The resulting challenges are its reproducibility due to molecular aging and the mass production of single-molecule devices at low cost. STM and AFM have revealed many interesting phenomena in single molecule junctions, such as large magnetoresistance [86, 87], spin split molecular orbitals [88], Kondo resonance [89], the Coulomb blockade effect [90],

negative differential resistance behavior [91, 92], strain-induced binding configuration [93], and the redox switch [94, 95], which accelerates the development of molecular electronics. Molecular junctions fabricated via a hole, such as a nanopore or a nanowell, were first introduced by Reed et al. [96-98]. A promising device architecture that could achieve next-generation memory and logic devices based on metal-molecule-metal junctions may be the crossbar/crosswire latch [96, 99, 100].

2.7 Hybrid-molecular and mono-molecular devices

The semiconductor industry has seen a remarkable miniaturization trend with many scientific and technological developments. The size of microelectronic circuit components has reached the scale of atoms or molecules. The concept is that a few molecules or even a single molecule could be embedded between electrodes to perform the basic digital electronics functions such as rectification, amplification, and storage. This idea was developed in 1970s, but it is still challenging because of the difficulty in connecting molecules to one another. Therefore, the problem is rectified by “mono-molecular” electronics, where a single molecule will integrate the elementary functions and interconnections required for computation. A single molecule with a donor-spacer-acceptor (d-s-a) structure was suggested in studies conducted by Aviram and Ratner [101]. This structure behaves like a diode placed between two electrodes; the electrons can easily flow from the cathode to the acceptor, and donor electrons are then transferred to the anode. This device’s working principle involves manipulating the electronic wavefunction of the metallic electrodes to extend through the d-s-a molecule, rather than the carrier density in a semiconductor material.

Hybrid molecular electronic (HME) devices, which are comprised of molecules embedded between several electrodes, have applications in dye lasers, light-emitting diodes (LEDs), liquid-crystal displays, and soft plastic transistors. The design of these structures poses the challenge of integrating the functions required for advanced processing (computing), within the same molecule in a mono-molecular electronics (MME) approach. Due to the inability to establish electrical contact between individual molecules, experimental investigations in processes involved in electron transfers has focused on gas-phase and liquid-phase systems. The fabrication of a circuit using HME devices requires the following steps: (1) fabrication of millions of multi-electrode nanojunctions with interelectrode distances (of a few nanometers); (2) wiring these junctions

to form interconnections; (3) the deposition/assembly of one molecule or a supermolecule at the nanojunction; (4) the fabrication of the input/output and driving power interconnections; and (5) packaging the circuit.

Various techniques can be used on many types of molecule to form organized molecular monolayers on suitable substrates [102]. The scanning tunneling microscope (STM) approach, along with controlled two-terminal measurements, has allowed new experimental approaches for demonstrating and probing electron transport through individual molecules [103], such as the electrical single-atom switch, which was realized using a Xe atom [104]. A variety of experimental techniques, such as the Coulomb blockade [105], nanopore [106], break junction [107, 108], electrodeposition [109], and nanolithography [110, 111], have been used to determine the electronic transparency of single molecules. Electrodeposition techniques are used for suspended electrodes in a pseudo-planar configuration to trap molecules electrostatically in and on the junction. Nanolithography is used for mesoscopic electrodes [112, 113] and nanojunctions for HME. This technique is also used to measure the conductance of single-wall carbon nanotubes (SWCNTs).

Furthermore, the conductance of the metal-SWCNT-metal junction is determined by metal-SWCNT contacts. Quasi-ideal rectification characteristics have been experimentally observed in SWCNT [114] and electrically contacted MWCNTs [115]. In recent studies, a single, planar SWCNT comprising of tube sections with different tube helicities has shown rectification behavior at the molecular level [116]. Magnetic phenomena associated with single atoms or molecules [117] has also been investigated in device scaling and quantum micro-reversibility [118]. These materials' hysteresis behavior can be used for information storage applications. The studies on HME transistors are numerous [119], yet the realization [120] of these devices is difficult and challenging because logic circuit applications require a three-electrode configuration with high gains. The circuit's design is a crucial aspect in the development of future molecular electronic systems. Input/output interconnections, clock frequency, and the increasing logic complexity are challenging issues. The other proposed architectures are quantum cellular automata [121] and quantum dots [122].

2.8 Molecular Robotics

Molecular robotics uses molecules to manipulate other molecules in a robotic fashion. For example, in metazoan fatty acid synthase, a growing

fatty acid chain is tethered to an embedded carrier protein; it is then passed between enzyme domains in the protein superstructure in the same way that a robotic arm manipulates objects on a factory assembly line [123]. These robots are made by integrating the actions of several simple molecular machine functions. Two distinct gripping/release actions and a “robotic arm” are used to perform particular functions. The transportation of the substrate is controlled by inducing sequential conformational and configurational changes within an embedded hydrazone rotary switch [124] that steers the robotic arm. In this way, it is possible to program the molecular machine for selective transport, by taking control of each simple machine’s function. These machines can also adapt to produce different outputs from a series of molecular robot-mediated chemical reactions. The molecular robot can be programmed to stereoselectively produce an excess of any of the four possible diastereoisomers by the addition of a thiol and an alkene to a α,β -unsaturated aldehyde in a tandem reaction process.

2.9 Nano-Structured Materials:

Nanotechnology is now a key area of technology and it is concerned with creating and manipulating materials at the nanometre (nm or 10^{-9} m) scale either from the bottom up (using single groups of atoms to increase matter) or from the top down (by reducing bulk materials to a group of atoms).

Two common techniques can be used to create nano-structured materials: the top-down technique and the bottom-up technique. This is where the difference is based on the size of the primary entities used to build the nano components with or without atomic level control [125-127]. The main applications of nanotechnology are related to nanoscience in the electronics industry. Over the past few decades, the transistor has been continually miniaturized in modern integrated circuits [128].

The ability to fabricate structures with nanometric precision is of fundamental importance. Nanotechnology’s great promise is the ability to do more in the same space; this means that it will advance our current technologies through miniaturization, so that each device will be smaller, faster, and more powerful than the previous one. Nanomaterials have small dimensions and an extremely large surface area to volume ratio, which results in more "surface" dependent material properties. According to the dimension parameter, nanomaterials are classified as (a) 0D spheres and clusters, (b) 1D nanofibers, nanowires, and nanorods, (c) 2D films, plates, and networks, and (d) 3D nanomaterials.