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An Unconventional Pathway to Develop Artificial Intelligence: The Chemical AI

Pier Luigi Gentili [1,*]

[1] Università degli Studi di Perugia, Department of Chemistry, Biology, and Biotechnology, Via Elce di Sotto 8, 06123 Perugia, Italy.

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Abstract

Artificial Intelligence is a valuable technology for addressing this century's global challenges. Chemists can concretely contribute to AI by promoting the development of Chemical AI. Unlike traditional AI, CAI integrates hardware and software within reactive chemical 'wetware' that is maintained far from thermodynamic equilibrium. Inspired by living systems viewed as Information-Gathering and Utilizing Systems, CAI seeks to reproduce aspects of biological intelligence, such as sensing, processing, and action. A conceptual knowledge map is presented, spanning molecular and supramolecular chemistry, systems chemistry, and multiscale chemistry, and encompassing the sensory, cognitive, and motor domains. Three main strategies for developing CAI are discussed, which are: chemical logic-based computation, neuromorphic wetware systems, and emerging Quantum AI inspired by quantum phenomena in living matter. By exploiting self-organization and information processing in chemical systems, CAI offers a pathway toward autonomous "chemical robots" and provides new insights into both artificial intelligence and the origin of life.

Keywords: Reaction networks, Neuromorphic engineering, Molecular logic gates, Quantum biology, Fuzzy molecules, Systems chemistry.

1. Introduction

The rapid advancement of information and communication technologies, together with modern transportation systems, has profoundly transformed human society. People are now more interconnected than ever, forming an extensive, tightly linked global network. This unprecedented connectivity requires humanity to confront challenges that affect the entire planet. Commonly referred to as global challenges, these issues have been formally identified by United Nations member states within the framework of the 2030 Agenda [1-3]. Such challenges involve highly interconnected systems that encompass individuals, societies, urban environments, the global economy, natural ecosystems, and the climate [4-6]. Understanding and managing these systems poses major challenges for scientific research because they fall under the broad class of Complex Systems. Studying them involves epistemological complexity arising from multiple factors [7]. One important source is computational complexity: many problems involving Complex Systems are effectively intractable, since exact solutions cannot be obtained within a reasonable time even using the most advanced supercomputers [8]. A second challenge concerns pattern recognition. Processes such as facial and voice identification, medical diagnosis, and analysis of large-scale biological or social phenomena depend on emergent properties arising from numerous interacting components. Despite decades of research, no universal and computationally efficient algorithm capable of recognizing all classes of patterns has yet been developed [9]. Since the beginning of the twenty-first century, Artificial Intelligence (AI) has emerged as one of the most promising approaches for addressing these challenges [10-12]. AI technologies aim to extract meaningful information from complex datasets, recognize patterns, generate predictions, and support decision-making processes. Current AI research can be broadly divided into three major strategies, schematically illustrated in **Figure 1**. The first strategy is based on the implementation of AI algorithms in software running on general-purpose computers or dedicated electronic hardware. Some approaches emulate human reasoning through formal logical operations applied to numerical or linguistic information, whereas others are inspired by biological neural networks and learn from data through adaptive training procedures. Additional methodologies reproduce natural phenomena such as biological evolution, resulting in alternative computational paradigms [13-15]. The second strategy seeks to embody intelligence directly in physical hardware. In this approach, neural architectures are implemented using silicon-based circuits, inor-

***Corresponding author:** Pier Luigi Gentili, email: pierluigi.gentili@unipg.it

ganic memristive devices, or organic semiconductors [16-19]. These technologies are increasingly used in neuroprosthetics and in developing neuromorphic computing platforms, which challenge the conventional von Neumann architecture by integrating data storage and information processing on the same physical substrate, often in three dimensions. More recently, a third strategy has emerged that exploits wetware, namely liquid-based systems that constitute the fundamental medium of life. This approach, often referred to as Chemical Artificial Intelligence (Chemical AI), employs molecules and macromolecules as hardware components, while the dynamic physicochemical processes occurring within the medium, including chemical reactions, diffusion, migration, convection, advection, and wave propagation, perform computational functions [20-23]. Unlike conventional computing architectures, where hardware and software are clearly separated, wetware systems blur this distinction by integrating both within a single reactive chemical environment. Chemical AI is attracting growing interest because it offers a fundamentally different route to information processing, inspired not by electronic devices but by the mechanisms operating in living systems. By exploiting the intrinsic ability of chemical systems to self-organize, adapt, and process information in parallel, Chemical AI may provide innovative solutions for addressing complex real-world problems and open new opportunities at the interface between chemistry, biology, and artificial intelligence.

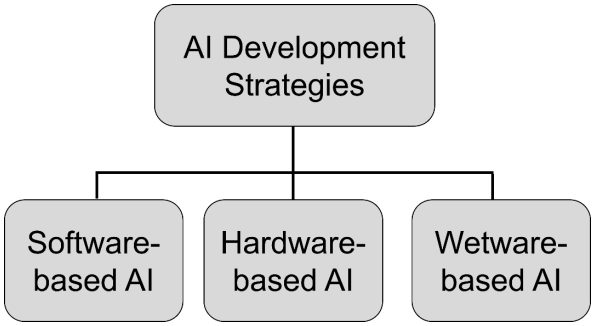


Figure 1 | The three principal strategies for developing AI.

2. Life-Inspiring Chemical AI

Living systems exhibit remarkable properties that continue to inspire scientists across disciplines. Although no universally accepted definition of life exists, many influential theories converge on a set of common characteristics. Living systems are generally understood to be (1) self-bounded, (2) self-sustaining, (3) maintained far from thermodynamic equilibrium, and (4) purposive [24-26]. Among these attributes, purposefulness is the feature most directly relevant to the emerging field of Chemical AI (CAI) [27]. The primary goals pursued by living systems are survival and reproduction. To achieve these goals, organisms continuously exploit matter and energy to acquire, store, process, communicate, and utilize information. In this perspective, living beings can be regarded as *Information Gathering and Utilizing Systems* (IGUSs) that display diverse forms of intelligent behavior, collectively referred to here as biological intelligence. Such intelligence emerges through learning processes, including adaptation, acclimation, and evolution, and through the capacity to generate actions that are not completely determined by local environmental conditions [28-31]. From this viewpoint, CAI can be defined by a simple but profound question:

Which aspects of biological intelligence can be reproduced using non-living chemical systems operating in wetware, that is, in the liquid environments characteristic of living matter [27,32]*?*

This objective clearly distinguishes CAI from the already established field of AI in chemistry. During the last decade, artificial intelligence has transformed chemical research by accelerating molecular design, molecular characterization, and data analysis, developments recognized by the 2024 Nobel Prize in Chemistry [33]. AI has also enabled the emergence of autonomous laboratories and robotic synthesis platforms capable of performing chemical experiments with minimal human intervention [34]. Chemical AI, however, seeks something fundamentally different. Rather than using AI to improve chemistry, it aims to realize intelligence directly within chemical matter itself.

3. A Knowledge Map for Chemical AI

A useful framework for understanding CAI is provided by the three-dimensional knowledge map proposed in **Figure 2** [27]. This conceptual space organizes the field along three axes. The *x*-axis represents the domains of CAI, the *y*-axis its fundamental paradigms, and the *z*-axis (encoded through saturation of the green color) the complexity of the biological intelligence competencies that have been, or may eventually be, reproduced in chemical systems. The *x*-axis encompasses three increasingly complex domains:

1. Molecular and Supramolecular Chemistry [21]
2. Systems Chemistry [35]
3. Multiscale Chemistry [27]

The first two domains are already established research areas, whereas multiscale chemistry represents a largely unexplored frontier. Multiscale chemistry investigates systems capable of self-organizing across multiple spatial and temporal scales while exhibiting both bottom-up and top-down causation. Under suitable thermodynamic conditions, such systems can generate dissipative structures [36-38] and active matter [39,40], phenomena that are likely essen-

tial for reproducing the structural and functional organization characteristic of living systems. The progression along this axis is accompanied by increasing complexity, which can be quantified through three interrelated properties: the multiplicity of components, the density of interactions, and the degree of integration manifested through emergent behavior. As complexity increases, so does the potential to reproduce increasingly sophisticated forms of biological intelligence [41,42]. This progression mirrors the hierarchical organization of life itself. Living systems process information at multiple levels, ranging from molecules and organelles to cells, tissues, organs, entire organisms, and even collective systems such as societies and swarms [43]. Reproducing biological intelligence therefore appears to require chemical systems capable of operating across multiple organizational scales. The *y*-axis of the knowledge map (**Figure 2**) reports the fundamental functional components of every IGUS. These can be described as:

1. Sensors, which acquire information from the environment
2. Brains, which process information and support decision-making
3. Effectors, which translate decisions into actions

The specific realization of these paradigms depends on the biological system used as a reference. In single cells, they correspond to membrane receptors, intracellular signaling networks, and genetic machinery, respectively. In higher organisms, they are represented by sensory organs, nervous systems, and effector systems such as muscles and glands [44,45]. Current achievements in CAI are concentrated primarily within the sensing domain. Molecular and supramolecular systems already perform sophisticated sensing functions by responding selectively to external physicochemical stimuli. Systems chemistry extends these capabilities through cooperative network effects that enhance sensitivity, selectivity, and information-processing capacity. The realization of higher-level cognitive functions remains considerably more challenging. Perception, for example, requires memory together with the ability to extract meaningful patterns from sensory inputs. Such capabilities are likely to depend on multiscale architectures capable of integrating information across different organizational levels. Likewise, although various forms of chemical computation and decision-making have been demonstrated, major challenges remain in the implementation of functions such as knowledge representation, reasoning, and planning. The effector dimension represents perhaps the most ambitious frontier of CAI. Chemical systems have already demonstrated primitive forms of action and communication; however, the ultimate goal is the creation of systems capable of autonomous goal-directed behavior. In other words, future chemical systems should be able to pursue objectives and adapt their actions in order to maximize expected outcomes.

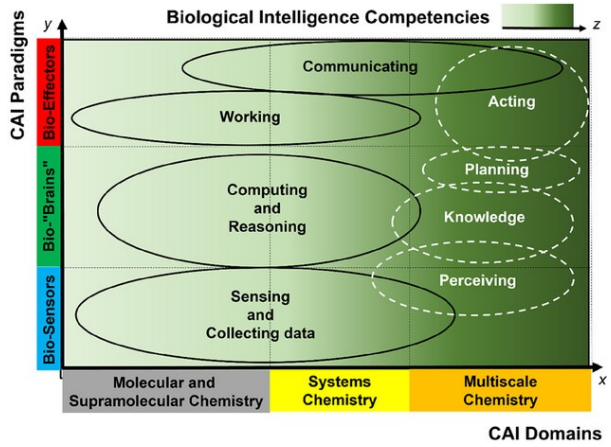


Figure 2 | The Chemical AI knowledge map, published in [27] under the Creative Commons Attribution License (CC BY).

Achieving this capability would open the possibility of developing genuine chemical robots: autonomous systems implemented entirely in wetware and operating through chemical rather than mechanical processes [46]. Such systems would constitute the chemical analogues of conventional robots, but potentially at scales comparable to living cells. Their prospective applications could be transformative, encompassing targeted medicine, environmental remediation, synthetic biology, regenerative technologies, and longevity research. Beyond its technological implications, CAI may contribute to addressing one of the deepest questions in science: the origin of life. Life is often viewed as a major phase transition that occurred approximately four billion years ago, when non-living matter acquired the capacity to process information, pursue goals, and sustain autonomous organization [47]. The mechanisms underlying this transition remain largely unknown and have yet to be reproduced experimentally. From this perspective, Chemical AI is more than a new paradigm for artificial intelligence. By attempting to construct intelligent chemical systems from the bottom up, it offers a unique experimental framework for investigating how purposive behavior and information processing can emerge from matter itself. Consequently, advances in CAI may simultaneously expand the boundaries of artificial intelligence and deepen our understanding of the processes that transformed chemistry into biology.

4. Approaches Toward Chemical Artificial Intelligence

To date, three major approaches to CAI have emerged, so far (**see Figure 3**). The earliest approach is based on the chemical implementation of the different forms of causality animating living matter. Inspired by classical computer science, this strategy seeks to reproduce deductive reasoning through chemical logic gates, including both Boolean and fuzzy architectures, with the long-term

goal of constructing chemical analogues of Turing machines [48,49]. In this framework, chemical reactions perform information-processing operations, enabling decision-making directly within molecular systems. Some molecules have also been proposed to reproduce circular causality that is at the core of molecular cybernetics [46,27]. A second major direction is neuromorphic engineering in wetware, which draws inspiration from the structure and dynamics of biological nervous systems. Rather than implementing symbolic logic, this approach aims to reproduce the behavior of neurons and neural networks in wetware, exploiting the rich nonlinear dynamics of chemical reactions and reaction networks to generate adaptive and learning-like behaviors [50]. By emulating information processing in biological brains, chemical neuromorphic systems may provide a route toward more flexible and robust forms of intelligence than those achievable through purely logic-based architectures. For instance, they are expected to be particularly well-suited for pattern recognition, as demonstrated [51-55]. More recently, a third and highly speculative research direction has begun to emerge: Quantum AI. This approach is motivated by growing evidence that both coherent and incoherent quantum phenomena may contribute to the functioning of living systems, although the precise role of such processes remains incompletely understood [56,57]. Rather than reproducing neural or logical architectures alone, Quantum Chemical AI seeks to exploit quantum effects as computational resources for intelligent behavior. The emergence of this third paradigm coincides with increasing interest in the broader convergence between artificial intelligence and quantum information science [58,59]. Quantum computing, sensing, and communication technologies exploit uniquely quantum phenomena such as superposition, entanglement, interference, and tunneling, offering the potential to solve specific classes of problems more efficiently than classical approaches. At the same time, AI techniques are expected to facilitate the design and control of quantum systems, creating a mutually reinforcing relationship between the two fields. Despite their promise, however, qubit-based quantum technologies remain technologically demanding and often require substantial energetic and experimental resources. In this context, CAI may provide an alternative pathway toward Quantum AI. Rather than relying exclusively on highly controlled qubit architectures, chemical systems could exploit quantum phenomena that naturally occur in molecular systems, particularly those associated with incoherent quantum mixed states. Such an approach may offer new opportunities for implementing quantum-inspired forms of intelligence within chemically active environments. Taken together, these three complementary strategies illustrate the breadth of the CAI research landscape. Although they differ substantially in their theoretical foundations and implementation methods, all share the common objective of realizing intelligence directly in chemical matter. Their continued development may ultimately provide unprecedented capabilities for sensing, computation, decision-making, and autonomous action in the molecular world, opening new avenues for both fundamental research and technological innovation.

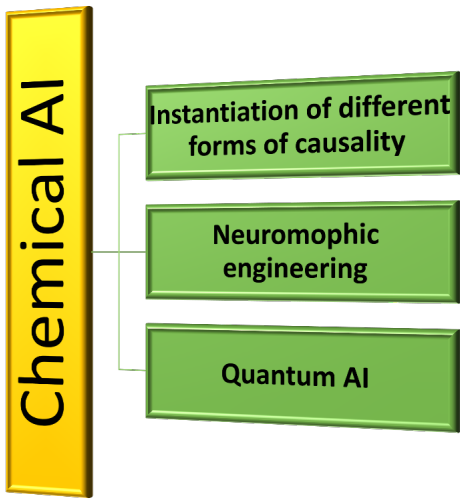


Figure 3 | The three pathways proposed to develop Chemical AI.

5. Concluding Remarks

Chemical Artificial Intelligence (CAI) represents an unconventional route toward the realization of intelligent systems. Unlike conventional digital AI, where hardware and software constitute distinct entities, CAI integrates both within the wetware of reactive chemical systems operating far from thermodynamic equilibrium. In these systems, molecules simultaneously provide the physical substrate and participate in the information-processing dynamics, blurring the traditional distinction between computation and material implementation. This distinctive feature places CAI at the intersection of chemistry, artificial intelligence, complex systems science, and the study of life itself. Rather than merely using computational tools to accelerate chemical research, CAI seeks to endow chemical matter with progressively more sophisticated information-processing capabilities, ranging from sensing and memory to learning, decision-making, and autonomous action. In doing so, it extends the traditional scope of chemistry from the study and manipulation of matter toward the engineering of intelligent chemical systems. The development of CAI is still at an early stage, and many conceptual and technological challenges remain unresolved. Among the most important are the design of chemical

architectures capable of storing and processing information across multiple spatial and temporal scales, the implementation of robust learning mechanisms, the emergence of goal-directed behavior, and the realization of effective coupling between sensing, computation, and action. Addressing these challenges is indeed translational because it will require close interaction among chemists, physicists, materials scientists, biologists, computer scientists, and engineers, as no single discipline possesses all the conceptual and experimental tools needed to advance the field. At the same time, the opportunities offered by CAI are substantial. Future intelligent chemical systems could operate in environments inaccessible to conventional electronic devices, perform autonomous tasks at microscopic scales, and interact seamlessly with biological systems. Such capabilities may open new avenues in areas including precision medicine, smart therapeutics, environmental monitoring and remediation, adaptive materials, synthetic biology, and autonomous chemical manufacturing. Beyond its technological potential, CAI may also provide a unique experimental framework for exploring fundamental scientific questions. Living organisms are the only known examples of matter capable of acquiring information, pursuing goals, adapting to changing conditions, and reproducing themselves. Understanding how these properties emerge from collections of interacting molecules remains one of the greatest challenges in science. By attempting to reproduce selected aspects of biological intelligence in non-living chemical systems, CAI offers a bottom-up strategy for investigating the transition from chemistry to biology and, ultimately, the origin of life. In this perspective, CAI should not be viewed simply as another branch of artificial intelligence. Rather, it represents a new scientific frontier that seeks to understand and engineer intelligence as an emergent property of matter. Whether it ultimately leads to chemical computers, chemical robots, or entirely unforeseen forms of intelligent matter, CAI promises to deepen our understanding of both intelligence and life while expanding the horizons of chemistry in the twenty-first century.

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