

The Molecule as an Epistemic Object: An Ontosemiotic Perspective on Its Historical Emergence¹

Juan D. Godino

Universidad de Granada, España

Corresponding author. E-mail: jgodino@ugr.es

Abstract. This article presents an epistemological and historical analysis of the emergence and evolution of the concept of molecule, adopting the Ontosemiotic Approach to knowledge and instruction as its theoretical framework. From this perspective, the meaning of “molecule” is not conceived as a static entity, but rather in a pragmatic sense: as a system of operative and discursive practices oriented toward the resolution of specific problems within historically situated contexts. Through a diachronic study, the paper identifies and characterizes a series of partial meanings of the concept—ranging from early intuitions of Daltonian “compound atoms” and Avogadro’s distinction, to the structural representations of organic chemistry and the contemporary quantum-mechanical elaboration of molecular theory. The analysis examines how these partial meanings are articulated into a holistic meaning of the molecular object, revealing the discontinuities, semiotic mediations, and ontological shifts that have enabled its consolidation. By situating this evolution within the History and Philosophy of Chemistry, the study provides a robust methodological tool for understanding the complexity of chemical thought and offers new perspectives for the teaching and communication of this fundamental concept.

Keywords: Ontosemiotic approach; concept of molecule; holistic meaning; history of chemistry; epistemology.

INTRODUCTION

The concept of molecule constitutes a cornerstone of the intellectual architecture of modern chemistry. While the atom is commonly presented as the fundamental unit of the elements, it is the molecule that functions as the unit of identity of chemical substance in all its complexity.^{1, 2} Its historical emergence did not amount to a mere empirical discovery, but rather entailed a genuine ontological revolution that enabled chemistry to move beyond a purely classificatory discipline toward a predictive science capable of creating its own object of study.³ Nevertheless, the determination of the ontological status of the molecule remains one of the most persistent problems in contemporary philosophy of chemistry. This difficulty does not stem from a lack of empirical evidence, but from the multifaceted nature of the concept itself, whose essence appears to shift depending on the experimental context, the level of theoretical approximation, and the representational system employed.^{4, 5} Fundamental chemical concepts do not possess a univocal ontology; rather, they emerge from the interaction between theory, practice, and representation, as shown by Scerri and Ghibaudi⁶ in the case of the chemical element.

¹ Godino, J. D. (2025). The Molecule as an Epistemic Object: An Ontosemiotic Perspective on Its Historical Emergence. Manuscript under review.

Traditionally, this tension has been articulated as a contrast between a naïve realist stance, which conceives the molecule as a discrete physical entity independent of the observer, and a pragmatic instrumentalism that interprets it as an operational construct⁷. The latter view arises from the collision between realist assumptions and everyday chemical practice; for instance, in systems where the notion of a discrete molecule dissolves, the chemist is compelled to resort to alternative models such as the unit cell.^{4, 8} In this scenario, the molecule emerges not as a static “thing-object,” but as a mental and semiotic model designed for the resolution of specific problems.

In order to address this complexity, the present study adopts the theoretical architecture of the Ontosemiotic Approach (OSA) to mathematical and scientific knowledge^{9, 10} in order to carry out a historical and epistemological reconstruction of the genesis and evolution of the concept of molecule. From this perspective, the meaning of a construct is not understood as an abstract definition, but pragmatically: as a system of operative and discursive practices oriented toward the resolution of problem situations within historically situated contexts. The central aim is to identify and characterize the various partial meanings that have emerged—from early intuitions of Daltonian “compound atoms” to contemporary quantum-mechanical sophistication—and to analyze how they are articulated into a holistic and systemic meaning. By situating this evolution within the History and Philosophy of Chemistry, the study provides a robust methodological tool for understanding the complexity of chemical thought and offers new perspectives for teaching and learning processes in the discipline.

Section 2 presents the Ontosemiotic Approach (OSA) as a tool for historical and epistemological analysis, which conceives scientific constructs as emergent from systems of practices and their holistic meaning as a complex and systemic network integrating and coordinating partial meanings. Section 3 describes the diachronic analysis of epistemic configurations as the methodological core of ontosemiotic analysis, identifying the historical periods that mark points of inflection or rupture in the systems of practices characterizing the four partial meanings identified. Section 4 constitutes the core of the paper and contains the analysis of the partial meanings of the molecule: protomolecular, physicochemical, structural, and electronic-quantum. In Section 5, we discuss how these partial meanings are articulated into a holistic meaning and compare this holistic conception of the molecule with contemporary perspectives in the history and philosophy of chemistry. Finally, Section 6 presents the conclusions and discusses the implications of the study for the philosophy of chemistry and for teaching and learning processes in the discipline.

THE ONTOSEMIOTIC APPROACH AS A TOOL FOR HISTORICAL AND EPISTEMOLOGICAL ANALYSIS

Within the Ontosemiotic Approach (OSA), the concept of *practice* constitutes the elementary component of analysis¹¹. Practice is not understood as a mere “activity,” but rather as any action or manifestation—linguistic or otherwise—carried out by an agent in order to solve a problem, communicate a solution, or validate a result. From this standpoint, the molecule is not defined by what it “is” ontologically in a metaphysical vacuum, but by what chemists do with it in their professional practice.

The OSA and the Nature of Knowledge

The Ontosemiotic Approach to knowledge and instruction originated in the field of mathematics education; however, its robust ontological, semiotic, and epistemological

architecture allows for its effective transfer to the analysis of complex scientific concepts, particularly in chemistry. This theoretical framework distances itself from Platonic or purely idealist conceptions of knowledge, proposing instead a pragmatic and anthropological paradigm.^{12,13} Under this premise, scientific knowledge is not understood as access to pre-existing entities in a noumenal world, but as the outcome of human problem-solving activity. Accordingly, the meaning of an object such as the molecule is defined by the system of operative and discursive practices enacted by a scientific community when confronting a specific problem situation. This perspective enables the historian of science to trace not only the “discovery” of an object, but also the evolution of the languages and modes of reasoning that endowed it with functional existence.¹⁴

The Ontosemiotic Configuration of the Concept

In order to understand the evolution of a construct such as the molecule, the OSA proposes the identification of a configuration of primary objects⁹ involved in scientific practices. These objects do not operate in isolation, but are interwoven within a complex semiotic network. First, one considers the languages—terms, expressions, notations, and graphical representations—that allow the chemical entity to be represented on paper or in the laboratory. These are accompanied by the problems that drive chemical activity, and by the definitions (conceptualizations) that seek to delimit the identity of the object. The analysis gains rigor through the integration of propositions, procedures, and arguments that serve to validate scientific conclusions. In the transition from classical to quantum chemistry, for example, one can observe how changes in computational procedures and validation arguments drastically reconfigure the ontology of the molecule, transforming it from an aggregate of atoms with fixed positions into a system of electronic densities and probabilities.

Dualities and Meanings: From Partial to Holistic Meaning

A fundamental aspect of this analytical framework is the consideration of epistemic and cognitive dualities, particularly the dialectic between the unitary and the systemic. The OSA makes it possible to understand that a concept is not an indivisible unit, but rather a system composed of multiple partial meanings that have emerged at different historical moments. Each of these partial meanings corresponds to a specific ontosemiotic configuration: the molecule as a unit of volume in gases is distinct from, though related to, the molecule as a three-dimensional stereochemical structure. The richness of historical–epistemological analysis lies in identifying how these partial meanings are articulated—and at times come into tension—to give rise to what we term the holistic meaning of the object.⁹ This approach is particularly fruitful in chemistry, where theoretical models from different periods coexist and are used pragmatically by scientists depending on the problem at hand, demonstrating that scientific progress does not always entail the replacement of one meaning by another, but rather the expansion and refinement of a system of practices.

METHODOLOGY: DIACHRONIC ANALYSIS OF EPISTEMIC CONFIGURATIONS

The methodology employed in this study is based on diachronic ontosemiotic analysis, a tool that allows for the reconstruction of the evolution of a scientific object through the identification of its epistemic configurations across different historical periods. Rather than offering a linear narrative of discoveries, this approach focuses on the study of the systems of practices that a scientific community mobilizes in order to

solve specific problems.¹¹ The analysis is structured around the notion of ontosemiotic configuration, which systemically groups the problems, languages, concepts, procedures, propositions, and arguments that confer meaning on the molecule at a given stage. This methodology captures not only what is “known” about the molecule, but also how such knowledge is mediated by instruments and semiotic representations.¹⁰

To carry out this reconstruction, four fundamental milestones in the history of chemistry have been selected, each representing a significant ontological shift. The process begins with an analysis of the emergence of the concept within early chemical atomism, examining practices related to the determination of equivalent weights and combining volumes.¹⁵ The analysis then turns to the consolidation of structural meaning in nineteenth-century organic chemistry, a period in which the mediation of graphical representations and physical models¹⁶ reconfigured the ontology of the molecule as an entity endowed with internal architecture.¹ This historical tracing does not aim at the replacement of one model by another, but rather at identifying the partial meanings that have persisted and transformed up to the advent of quantum mechanics.

The rigor of the methodological analysis resides in the application of the cognitive dualities of the OSA, particularly the unitary–systemic duality. In examining each period, attention is paid to how the molecule functions as a unitary entity for certain experimental purposes, while revealing itself as a complex system of relations for others. The triangulation between primary historical sources and the theoretical framework of the OSA ultimately enables the construction of a holistic meaning of the concept. This methodological approach not only facilitates an epistemological understanding of conceptual evolution, but also offers a model for analyzing the inherent complexity of other fundamental concepts in chemistry.

ANALYSIS OF THE PARTIAL MEANINGS OF THE MOLECULE

The Protomolecular Meaning: “Compound Atoms” (1803–1811)

The first partial meaning of the concept of molecule emerged in the context of the atomistic revolution of the early nineteenth century, shaped by the need to account for the laws of definite and multiple proportions.¹⁷ In this period, the meaning we term *protomolecular* manifests itself through the practices of Dalton, who, although not employing the term *molecule* in its modern sense, introduced the notion of “compound atoms” as the minimal units of chemical substances.^{15, 18} From the perspective of the Ontosemiotic Approach, this epistemic configuration is strongly anchored in a duality between the macroscopic and the microscopic: the problem situations of the time were essentially gravimetric—namely, the determination of combining weights—yet their resolution required the invention of an ontological model of discrete particles endowed with specific relative weights.

Semiotic mediation at this stage was rudimentary but revolutionary. Dalton introduced an iconic language composed of circular symbols to represent the atoms of the elements, whose physical combination gave rise to simple geometrical configurations.¹⁹ This practice, however, was constrained by the “rule of maximum simplicity,” an argumentative presupposition according to which, if only one compound between two elements was known, it had to be binary.¹⁵ This procedural limitation prevented Dalton from distinguishing between atoms of an element and diatomic molecules, generating semiotic conflicts when attempting to account for the combining volumes of gases.¹⁷

In terms of OSA ontology, the Daltonian “compound atom” is not yet a molecule in the structural sense, but rather a mass point endowed with the capacity for chemical

combination. The system of practices of this period focused on elemental composition and weight, omitting any consideration of the internal arrangement of components. Despite these limitations, this protomolecular meaning was fundamental to the establishment of chemistry as a quantitative science, providing the first rules of correspondence between the world of substances and that of microscopic entities—rules that would later enable the transition toward more complex and differentiated meanings.

The Physicochemical Meaning: The Avogadro–Cannizzaro Distinction (1811–1860)

The transition toward what we term the *physicochemical* meaning of the molecule was marked by the resolution of a profound crisis of coherence within the system of practices of early atomism. At the core of the problem lay the contradiction between Gay-Lussac's law of combining volumes and Dalton's model, which rejected the possibility that equal volumes of different gases could contain the same number of particles.¹⁷ In this context, Avogadro proposed in 1811 a fundamental ontological distinction by differentiating between the “elementary molecule” (atom) and the “integral molecule” (the independent gaseous entity), thereby allowing for the existence of diatomic molecules in gaseous elements.¹⁸ From an ontosemiotic standpoint, this proposal was not merely a physical hypothesis, but a semiotic reconfiguration that introduced a new rule of correspondence between the macroscopic behavior of gases and the microscopic constitution of matter.

Despite its clarifying potential, Avogadro's proposal was not immediately accepted by the chemical community, giving rise to a period of terminological and methodological confusion that lasted nearly half a century. During these decades, the lack of consensus regarding atomic weights and molecular formulae generated a well-known “chaos of formulas” that hindered scientific communication.²⁰ The system of practices of this period became fragmented between those who prioritized chemical equivalents and those who sought a physical foundation for the molecule. It was not until the Karlsruhe Congress of 1860 that Cannizzaro, by recovering Avogadro's hypothesis and grounding it in the law of Dulong and Petit, succeeded in presenting a coherent and logically consistent system of arguments that allowed for the unambiguous determination of atomic weights and molecular formulae.³

From an ontosemiotic perspective, the meaning consolidated after Karlsruhe represents a qualitative leap: the molecule ceases to be a mere Daltonian “compound atom” and becomes an entity with an independent physical status, defined by its behavior in the gaseous phase and by its molecular mass. This epistemic configuration integrated languages (rationalized chemical formulae), procedures (vapor density determinations), and arguments (the clear distinction between atomic and molecular weight), conferring upon chemistry an unprecedented degree of conceptual stability. This physicochemical meaning allowed the molecule to be recognized not only as a unit of combination, but as a real and measurable entity, laying the foundations for subsequent investigations into its internal architecture.

The Structural Meaning: Three-Dimensional Architecture (1860–1920)

The consolidation of the structural meaning represented one of the most significant ontological shifts in the history of the discipline, transforming the molecule from a unit of mass into an entity endowed with internal architecture and defined geometry.² This paradigm shift was driven by the need to resolve the problem of isomerism: the existence of substances with identical elemental composition but divergent chemical properties.¹

From the perspective of the Ontosemiotic Approach, this period is characterized by the emergence of a new representational language—the structural graph—and by the development of the concept of valence as an operative property of atoms.²¹ The practices of chemists such as Kekulé enabled the molecule to be understood as a system of bonds, in which atomic connectivity determines the chemical identity of a substance.

The structural epistemic configuration reached its full expression with the introduction of three-dimensionality by van 't Hoff and Le Bel in 1874. The proposal of the tetrahedral carbon atom constituted an unprecedented semiotic mediation: the use of physical models and spatial diagrams to account for the optical activity of organic compounds.¹ In this sense, the meaning of the molecule expanded to include stereochemistry, integrating the relative spatial position of atoms in Euclidean space as a constitutive property of the object. As Meinel¹⁶ has shown, the use of molecular models in this period was not merely a didactic resource, but a necessary tool of thought that enabled chemists to mentally “manipulate” entities that could not yet be directly observed. Indeed, this transition toward spatial reasoning proved so effective that contemporary textbooks adopted three-dimensional representations almost immediately after their original formulation.²²

From an ontosemiotic perspective, this structural meaning operates as a system of practices linking chemical reactivity to form. The molecule ceased to be an invisible point and became an object endowed with “shape” and “bonds,” allowing classical organic chemistry to predict and synthesize millions of new compounds on the basis of geometrical combination rules. This stage consolidated a fundamental duality: the molecule as a discrete unit for physics and, simultaneously, as a complex system of spatial relations for chemistry. This distinction underscores the need, in both the classroom and the laboratory, to clearly differentiate the symbolic level of representation from the physical reality of the object—an epistemological precaution already presents in the earliest structural treatises.²² Far from being supplanted by the advent of quantum physics, the structural meaning continues to constitute the core of the operative language of synthetic chemistry today.²⁰

The Quantum Meaning: The Dematerialization of Structure (1920–Present)

The emergence of quantum mechanics in the early decades of the twentieth century entailed the most profound revision of the ontological status of the molecule. With the discovery of the electron and the development of the Schrödinger equation, the system of practices of theoretical chemistry shifted from the manipulation of mechanical models toward the mathematical treatment of energetic interactions.⁴ In this new scenario, the molecule ceased to be an assembly of spheres and rods and became a stationary system of nuclei and electrons in dynamic equilibrium.^{23, 5} From the standpoint of the Ontosemiotic Approach, this quantum meaning introduced a highly abstract form of semiotic mediation, in which the language of molecular orbitals and potential energy surfaces replaced classical graphical representations.

This paradigm shift posed a fundamental epistemological challenge: the tension between molecular structure— heir to the nineteenth-century structural meaning—and quantum formalism.⁵ Whereas classical chemistry assigned fixed positions to nuclei, quantum mechanics, in its strictest formulation, dissolves the notion of shape into probability distributions. The operational resolution of this conflict was achieved through the Born–Oppenheimer approximation, a cornerstone of the contemporary system of practices that allows nuclear motion to be “frozen” in order to recover the notion of molecular geometry.⁴ Thus, the quantum meaning does not annul previous meanings, but

rather subsumes them within a broader explanatory framework in which the chemical bond is redefined as a region of high electronic density.²⁰

From an ontosemiotic perspective, the quantum epistemic configuration represents the highest degree of complexity of the object. The holistic meaning of the molecule is completed by integrating the predictive power of quantum mechanics with the heuristic strength of classical structure. As a result, the contemporary molecule emerges as a multifaceted object: it functions as a graph for the synthetic chemist, as an energy surface for the physicist, and as a system of densities for the crystallographer. This plurality of partial meanings, far from being contradictory, reflects the richness of contemporary chemical thought and the effectiveness of the Ontosemiotic Approach in mapping the evolution of a concept that has progressed from an atomistic intuition to a complex mathematical and functional entity.

DISCUSSION: ARTICULATION OF THE HOLISTIC MEANING

In contemporary chemistry, the transition between the partial meanings described above does not occur through hierarchical replacement, but rather through what the Ontosemiotic Approach terms the *articulation of meanings*. The professional chemist does not rely on a single definition of the molecule, but instead mobilizes an ontological “toolbox” that is activated according to the problem situation at hand. Table 1 synthesizes the constitutive elements of the holistic meaning of the concept of molecule as reconstructed from the Ontosemiotic Approach. Its purpose is to show, in a comparative manner, how the different partial meanings—protomolecular, physicochemical, structural, and quantum—are configured as differentiated praxeological systems, each with its own problems, practices, languages, definitions, propositions, procedures, and arguments. This articulation makes it possible to highlight the ontosemiotic plurality of the concept while simultaneously revealing the relations of dependence, complementarity, and reorganization that are established among different levels of theorization.

Model Alternation as Semiotic Competence

The diachronic analysis developed in the preceding sections reveals that the evolution of the concept of molecule does not follow a linear replacement of obsolete theories by more accurate ones, but rather a process of accumulation and coexistence of partial meanings. In contemporary chemical practice, the ability to move between Kekulé’s structural meaning and the quantum meaning of molecular orbitals is not perceived as a contradiction, but as a fundamental form of semiotic competence. From the perspective of the Ontosemiotic Approach, this alternation of models constitutes a pragmatic use of different epistemic configurations, in which the subject selects the system of practices—and, consequently, the meaning of the object—that proves most efficient for solving a given problem situation. This capacity to integrate divergent levels of information has been described as a form of “*schizovision*”, enabling practitioners to process theoretical and experimental dimensions simultaneously.²⁴

Table 1. Elements of the holistic meaning of the concept of molecule

Meaning elements	Protomolecular meaning	Physicochemical meaning	Structural meaning	Quantum meaning
Problems	Explaining the laws of proportions and the behavior of gases.	Determining atomic/molecular weights and empirical formulae.	Explaining isomerism and the spatial arrangement of atoms.	Explaining chemical bonding and stability from first principles.
Practices	Weighing reactants and measuring gaseous volumes.	Elemental analysis and determination of vapor densities.	Organic synthesis, crystallography, and three-dimensional modeling.	Spectroscopy, quantum computation, and theoretical modeling.
Languages	Dalton's symbols, incipient empirical formulae.	Molecular formulae, Berzelian notation.	Lewis diagrams, Fischer projections, ball-and-stick models.	Wave functions (ψ), electronic densities, orbitals.
Definitions	Ultimate particle of a compound that preserves its properties.	Minimal unit of a substance capable of independent existence.	Aggregate of atoms linked by chemical bonds with fixed geometry.	System of nuclei and electrons in energetic equilibrium.
Propositions	Avogadro's hypothesis; law of combining volumes.	Dulong–Petit law; existence of diatomic molecules.	Tetrahedral carbon theory; chirality; covalent bonding.	Schrödinger equation; Pauli exclusion principle.
Procedures	Comparison of relative masses in chemical reactions.	Application of the ideal gas law and stoichiometry.	Structural deduction through reactivity and diffraction.	Energy level calculations and geometry optimization.
Arguments	Inductive justification based on the discontinuity of matter.	Logical deduction from experimental pressure–temperature data.	Structural inference from optical activity and isomerism.	Deductive justification grounded in wave mechanics.

Ontological flexibility allows an organic chemist to employ two-dimensional Lewis representations to predict the reactivity of a functional group, while simultaneously using electronic density calculations to understand a transition state. As Meinel (2004) emphasizes, molecular models function as operative tools mediating between theory and experimentation; their value lies not exclusively in their fidelity to an underlying physical reality, but in their heuristic power. From this perspective, molecular images act as conjectures that mediate abductive reasoning, revealing functional aspects that purely numerical data would otherwise conceal.²⁴ Within the OSA framework, the chemist is understood to handle a unitary–systemic duality: the molecule is treated as a simplified functional unit in certain contexts and as a complex quantum system in others, demonstrating that disciplinary expertise entails mastery of these semiotic translations.¹⁰

Consequently, the formation of chemical thinking should not aim at imposing the quantum model as the only “true” one, but at developing the capacity to manage this plurality of meanings. The articulation of the holistic meaning of the molecule resides precisely in the awareness that each partial meaning captures a distinct facet of chemical reality. This competence in alternating between semiotic registers and ontosemiotic configurations defines the rigor of scientific practice and enables chemistry to maintain its autonomy from physical reductionism, preserving models that, although simplified, retain an indispensable operative validity in the laboratory. The essays collected by Scerri and Ghibaudi⁶ underscore the role of instruments, models, and representations in the stabilization of chemical entities.

Ontological Leaps and Semiotic Discontinuities

Throughout the diachronic analysis, it becomes evident that the evolution of the concept of molecule is marked by semiotic discontinuities that have compelled profound reconfigurations of chemical ontology. From the perspective of the Ontosemiotic Approach, these ruptures are not mere changes in nomenclature, but rather *ontological leaps* generated by the emergence of new problem situations that previous languages and procedures were unable to resolve. A paradigmatic example is the transition from Dalton’s compound atom to Avogadro’s molecule: the conflict was not resolved through the accumulation of experimental data, but through the introduction of a new grammatical and conceptual category—the distinction between elementary and constituent molecules—which made it possible to restore coherence to the system of physicochemical practices.¹⁸

These discontinuities are particularly evident in the transition from structural to quantum chemistry. Whereas the structural meaning was grounded in a semiotic mediation of a mechanical and visual character (graphs and three-dimensional models), the quantum meaning introduced a radical rupture by shifting the focus from the position of nuclei to energy density and probability.²⁰ In OSA terms, this leap entailed a transformation in the meaning of the object: the molecule ceased to be a “body” with a fixed form and became an *emergence* of a dynamic field of forces. As suggested by Bensaude-Vincent³, this process of dematerialization compels the chemist to undertake an effort of abstraction in which the object is no longer “seen”, but rather “calculated” through mathematical operators.

Nevertheless, these ruptures do not imply a total disconnection. Ontosemiotic analysis reveals the persistence of underlying meanings that ensure the stability of the discipline. Despite ontological leaps, the molecule retains its identity as a unit of substance, guaranteeing continuity across different theoretical frameworks. Understanding these discontinuities is crucial for the philosophy of science, as it demonstrates that chemical progress is not a process of passive accumulation, but a series of active transformations in the systems of representation and argumentation that define, in each historical period, what counts as a real chemical entity.¹⁶

From the Molecule as a Thing to the Molecule as a Process

The culmination of the diachronic trajectory of the concept of molecule reveals a fundamental shift in its ontological character: the transition from a conception of the molecule as a “thing” or static entity to its understanding as a “process” or a complex mathematical model. In the early stages of structural chemistry, the molecule was interpreted within a mechanical realist framework, in which atoms were conceived as

spheres connected by rigid bonds. However, the system of practices of contemporary quantum chemistry and computational chemistry has compelled a redefinition of the object. Within the architecture of the Ontosemiotic Approach, this shift implies that the molecule is no longer defined by its substantiality, but by the semiotic functions that link experimental data with mathematical operators.

This dematerialization of the chemical object has led several philosophers to argue that the molecule is, strictly speaking, an operative construct. As Meinel¹⁶ notes, the use of models in chemistry has evolved from pictorial representation to simulation tools, in which the molecule appears as a response to specific boundary conditions within a Hamiltonian. In this sense, the molecule does not “exist” as a fixed structure, but as a dynamic system of electronic densities and probabilities that acquires a “form” only when the system of practices—for instance, through the Born–Oppenheimer approximation—decides to freeze its dynamism in order to render it intelligible.³

From the ontosemiotic perspective, this transformation can be described as a shift from an ostensibly accessible object to one mediated by extreme abstraction: whereas in the nineteenth century the molecule was meant to be “seen” through physical models, today it is primarily “understood” through highly abstract semiotic mediations.²⁰ The molecule as a “process” implies that its identity depends on the temporal and energetic scale of observation, reinforcing the idea that the holistic meaning of the concept is systemic and context-dependent.

Comparing the Holistic Meaning of the Molecule with Contemporary Perspectives in the History and Philosophy of Chemistry

The holistic meaning of the molecule proposed in this study, grounded in the ontosemiotic articulation of partial meanings, can be situated in dialogue with several contemporary positions concerning the nature of the molecular concept. In particular, it is fruitful to compare it with the perspectives of Hoffmann²⁵, Bensaude-Vincent³, Nye²⁰, Chang¹⁵, and Scerri¹⁷, whose contributions have shaped current debates on the ontological and epistemological status of molecular objects.

First, the plural and pragmatic conception of the molecule advocated by Hoffmann²⁵ converges with the central OSA idea that the object lacks a fixed essence and instead emerges from the coexistence of heterogeneous models and practices. However, whereas Hoffmann articulates this plurality primarily in narrative and phenomenological terms, the Ontosemiotic Approach provides an explicit analytical architecture for explaining how such models are integrated into a holistic meaning through the coordination of languages, procedures, and arguments. In this respect, the present approach systematizes what in Hoffmann appears as a philosophical intuition regarding the multifaceted nature of the molecule.

Bensaude-Vincent’s sociotechnical perspective³, which conceives the molecule as a cultural artefact mediated by instruments and representations, aligns closely with the ontosemiotic notion of meaning as a system of practices. Both approaches emphasize that molecular identity depends on the semiotic and material mediations that allow its manipulation and stabilization. Nevertheless, while Bensaude-Vincent foregrounds the historical and material dimensions of these mediations, the OSA extends the analysis by systematically integrating epistemic components—problems, languages, definitions, propositions, procedures, and arguments—that configure the meaning of the object at each historical stage.

Nye’s contribution²⁰ operates at a complementary level. Her analysis of chemistry as a cultural practice helps explain how certain molecules acquire symbolic and social

meanings that transcend their scientific definition. Although the OSA does not explicitly address this cultural dimension, its conception of meaning as a network of practices allows such aspects to be incorporated as part of the languages and social uses of the object. In this sense, the ontosemiotic proposal offers a broader framework capable of integrating the cultural dimension highlighted by Nye into a general theory of scientific meaning.

Chang's methodological pluralism¹⁵ arguably represents the position closest to the holistic meaning defended in this work. His notion of *epistemic iteration* describes how scientific concepts stabilize through historical cycles of refinement, which resonates with the idea of partial meanings that are articulated rather than replaced. The OSA, however, provides a more fine-grained structure for analyzing this articulation by explicitly identifying the semiotic and epistemic components involved in each historical configuration. In this way, the ontosemiotic proposal may be understood as a formalization of Chang's iterative pluralism applied to the specific case of the molecule.

Finally, Scerri's position¹⁷, grounded in a moderate structural realism that seeks to anchor molecular identity in electronic structure, stands in contrast to the pluralist orientation of the OSA. Whereas Scerri defends a relatively stable and physically grounded molecular ontology, the holistic meaning proposed here maintains that molecular identity is contextual and depends on the function the molecule performs within a given system of practices. This divergence reflects two distinct conceptions of chemical ontology: one oriented toward physical unification, and the other toward the pragmatic autonomy of chemical models.

Taken together, this comparison shows that the holistic meaning of the molecule formulated from the ontosemiotic perspective stands in continuity with the pluralist and pragmatic views of Hoffmann, Bensaude-Vincent, and Chang, complements the cultural dimension emphasized by Nye, and offers an explicit alternative to Scerri's structural realism. Its distinctive contribution lies in providing a systematic theory of the articulation of meanings that allows the molecule to be understood as a complex, historical, and operative object, whose identity emerges from the dynamic coordination of heterogeneous scientific practices.

CONCLUSIONS AND PERSPECTIVES

The diachronic reconstruction presented in this study shows that the concept of molecule has not followed a linear trajectory of refinement toward an absolute "truth", but has instead evolved through a series of epistemic configurations responding to specific operative needs. From the perspective of the Ontosemiotic Approach, the emergence of the molecule can be understood as the result of a progressive sophistication of scientific practices and of the interactions among their primary objects. Ontosemiotically, the molecule is consolidated as a complex object arising from the dialectic between thought and action. The OSA allows us to observe that each historical stage does not erase the previous ones, but rather adds a layer of partial meaning that remains functional in specific contexts. Moreover, the evolution of the concept is marked by the resolution of semiotic conflicts—such as the atom–molecule confusion or the nature of chemical bonding—in which the creation of new languages and arguments proved decisive for scientific progress.

In conclusion, the ontosemiotic lens supports the claim that the molecule is a holistic construct: a network of meanings that enables the professional chemist to operate with equal competence when weighing a substance (stoichiometric meaning), predicting a reaction (structural meaning), or simulating an electronic property (quantum meaning).

The history of the molecule is, in essence, the history of the expansion of human capacities for representation and action.

Implications for the Philosophy of Chemistry: Pragmatic Realism versus Structural Realism

The ontosemiotic analysis of the molecule offers an original contribution to the debate on realism in contemporary philosophy of chemistry. The diachronic trajectory of the concept shows that chemists do not adhere to a naïve realism seeking a one-to-one correspondence between the term “molecule” and an immutable physical entity, but rather to what may be described as a pragmatic and plural realism. From this standpoint, the reality of the molecule does not reside in its ultimate “substantiality”, but in the effectiveness of the systems of practices that allow it to be manipulated and transformed. As the OSA framework maintains, the ontology of a scientific object is inseparable from the network of semiotic functions that constitute it in a given context⁹; accordingly, the molecule is “real” insofar as epistemic configurations—whether structural or quantum—enable the prediction of phenomena and the synthesis of new substances.

This approach offers a way to mediate the tension between structural realism and instrumentalism. While structural realism holds that what persists across theoretical change are the mathematical and structural relations among entities, the ontosemiotic analysis suggests that what truly persists is a holistic meaning composed of the articulation of partial meanings. In this view, molecular “form” is not an intrinsic property invalidated by quantum physics, but an emergent property of a specific system of practices that retains its operative validity. Philosophy of chemistry thus benefits from an understanding of ontology as dynamic and relational, avoiding extreme physical reductionism that often overlooks the autonomy of chemical models.³

Finally, the OSA distinction between the molecule as a “thing” and as a “model” reinforces the idea that chemistry is a science of mediations. Chemical reality is mediated by instruments, languages, and representations that do not merely describe the world, but actively configure it.²⁰ By understanding the molecule as a system of practices, philosophy of chemistry can better account for how the discipline maintains internal coherence despite theoretical discontinuities. This perspective not only grants chemical concepts a robust epistemological status, but also recognizes that the richness of chemistry lies precisely in its capacity to operate simultaneously at multiple levels of reality, from the laboratory scale to the abstraction of mathematical formalism.

Toward a Chemistry Education Based on the Plurality of Meanings

The conclusions derived from this ontosemiotic analysis have direct implications for science education, calling for a rethinking of how the architecture of matter is communicated in the classroom. Traditionally, chemistry education has presented atomic and molecular models as a sequence of superseded errors, often generating ontological confusion in students attempting to reconcile apparently contradictory representations. In contrast to this linear approach, the results of this study point to the need for an education grounded in the management of a plurality of meanings. In line with OSA principles, learning chemistry should be understood as the progressive acquisition of systems of practices that enable students to identify which meaning of “molecule” is most appropriate for a given problem situation.

High-quality science education should not conceal semiotic discontinuities, but rather make them explicit, allowing students to understand that the “ball-and-stick”

molecule and the “electron density” molecule are intellectual tools with distinct domains of validity. As Izquierdo-Aymerich and Adúriz-Bravo²⁶ have argued, science education requires an epistemological foundation that gives meaning to school models and prevents them from becoming empty dogmas devoid of operative content. The diachronic trajectory presented here makes it possible to design instructional sequences in which students traverse ontological shifts—from gravimetric proportion to structural architecture—thus fostering a deeper and more systemic understanding of the object.¹⁰

Ultimately, recognizing the molecule as a holistic and evolving meaning allows educators to present chemistry as a living, creative, and continuously reconfiguring discipline. By fostering a semiotic competence that enables the alternation among models, future professionals are prepared not merely to apply formulas, but to participate in the construction of new knowledge. This approach, which places practice and semiotic mediation at the center of learning, not only narrows the gap between professional and school chemistry, but also equips students with a critical understanding of the nature of science—one in which the complexity of the molecular world is addressed through the richness and diversity of our representational systems.²⁷

The didactic orientation proposed here finds strong support in the work of Mocellin and Labarca²⁸, who advocate a deep dialogue between chemistry education and philosophy of science as a means of overcoming the “scientific monism” that often dominates classrooms. By integrating a pluralist perspective, chemistry is no longer presented as a “mummified” discipline—a catalogue of finished truths free of problems—but as a field in which students are invited to explore historical tensions, contradictions, and unresolved questions. For these authors, the plurality of definitions—such as Lavoisier’s macroscopic ontologies versus modern particle-based ones—should not be seen as a conflict to be resolved, but as a pedagogical opportunity to demonstrate that scientific reality encompasses multiple domains and constructions. In this way, an education grounded in plurality not only clarifies conceptual content, but also fosters a critical and argumentative stance in students, preparing them to manage the complexity inherent in the molecular world.

Use of AI statement: During the preparation of this work the author used Gemini and NotebookLM artificial intelligence tools in order to search for documentary sources, suggest translations and refine wording for clarity and precision. AI was not involved in conceptualizing research goals and methodology. After using these tools, the author reviewed and edited the content as needed and takes full responsibility for the content of the publication.

REFERENCES

1. A. J. Rocke, *Image and Reality: Kekulé, Kopp, and the Scientific Imagination*, University of Chicago Press, **2010**.
2. S. J. Weininger, Contemplating the Finger: Visuality and the Semiotics of Chemistry., *HYLE* **1998**, *4(1)*, 3-27. <https://www.hyle.org/journal/issues/4/weinin.htm#f0>
3. B. Bensaude-Vincent, *Matière à Penser. Essais d'Histoire et de Philosophie de la Chimie*, Éditions du Seuil, **2008**.
4. J. Hunger, How Classical Models of Explanation Fail to Cope with Chemistry—The Case of Molecular Modeling, in *Philosophy of Chemistry: Synthesis of a New Discipline* (Eds.: D. Baird, E. Scerri, L. McIntyre), Springer, **2006**, pp. 129–155.

5. R. G. Woolley, Is There a Quantum Definition of a Molecule?, *J. Math. Chem.* **1998**, 23(1), 3-12.
6. E. Scerri, E. Ghibaudi (Eds.), *What is a Chemical Element? A Collection of Essays by Chemists, Philosophers, Historians, and Educators*, Oxford University Press, **2020**.
7. E. R. Scerri, Normative and Descriptive Philosophy of Science and the Role of Chemistry., in *Philosophy of Chemistry: Synthesis of a New Discipline* (Eds.: D. Baird, E. Scerri, L. McIntyre), Springer, **2006**, pp. 119–128.
8. J. Schummer, The Philosophy of Chemistry: From Infancy Toward Maturity., in *Philosophy of Chemistry: Synthesis of a New Discipline* (Eds.: D. Baird, E. Scerri, L. McIntyre), Springer, **2006**, pp. 19–39.
9. J. D. Godino, *Ontosemiotic Approach in Mathematics Education. Foundations, Tools, and Applications*, DIGIBUG Author edition, **2024**. <https://hdl.handle.net/10481/93738>
10. J. D. Godino, C. Batanero, V. Font, The Onto-semiotic Approach to Research in Mathematics Education., *ZDM Int. J. Math. Educ.* **2007**, 39(1-2), 127–135. <https://doi.org/10.1007/s11858-006-0004-1>
11. J. D. Godino, C. Batanero, Clarifying the Meaning of Mathematical Objects as a Priority Area of Research in Mathematics Education, In *Mathematics Education as a Research Domain: A Search for Identity* (Eds.: A. Sierpiska, J. Kilpatrick), Kluwer, **1998**, pp. 177-195.
12. C. S. Peirce, *Collected Papers of Charles Sanders Peirce*, Harvard University Press, **1931–1958**.
13. L. Wittgenstein, *Philosophical Investigations*, Basil Blackwell, **1953**.
14. V. Font, J. D. Godino, J. Gallardo, The Emergence of Objects from Mathematical Practices., *Educ. Stud. Math.* **2013**, 82, 97–124. <http://dx.doi.org/10.1007/s10649-012-9411-0>
15. H. Chang, *Is Water H2O? Evidence, Realism and Pluralism*, Springer, **2012**.
16. C. Meinel, Molecules and Croquet Balls, in *Models: The Third Dimension of Science* (Eds.: S. de Chadarevian, N. Hopwood), Stanford University Press, **2004**, pp. 242–275.
17. E. R. Scerri, *The Periodic Table: Its Story and Its Significance*, 2nd ed., Oxford University Press, **2020**.
18. A. J. Rocke, *Chemical Atomism in the Nineteenth Century: From Dalton to Cannizzaro*, Ohio State University Press, **1984**.
19. S. H. Vollmer, Space in Molecular Representation; or How Pictures Represent Objects, in *Philosophy of Chemistry: Synthesis of a New Discipline* (Eds.: D. Baird, E. Scerri, L. McIntyre), Springer, **2006**, pp. 293–308.
20. M. J. Nye, *From Chemical Philosophy to Theoretical Chemistry: Dynamics of Matter and Dynamics of Disciplines, 1800-1950*, University of California Press, **1993**.
21. C. A. Russell, *The History of Valency*, Leicester University Press, **1971**.
22. M. Chioccioli, An Investigation into the Role and Importance of Three-dimensional Representations through an Analysis of Late 19th and Early 20th Century Chemistry Textbooks, *Substantia* **2025**, 9(2), 99-109. <http://dx.doi.org/10.36253/Substantia-3430>

23. J. R. Woodyard, A New Paradigm for Schrödinger and Kohn., in *Philosophy of Chemistry: Synthesis of a New Discipline* (Eds.: D. Baird, E. Scerri, L. McIntyre), Springer, **2006**, pp. 245–271.
24. E. M. Ghibaudi, An Exercise of Applied Epistemology: Peirce’s Semiosis Implemented in the Representation of Protein Molecules, *Substantia* **2024**, 8(2), 45-56. <https://doi.org/10.36253/substantia-2558>
25. R. Hoffmann, *The Shame and Not the Same*, Columbia University Press, **1995**.
26. M. Izquierdo-Aymerich, A. Adúriz-Bravo, Epistemological Foundations of School Science., *Sci. Educ.* **2003**, 12(1), 27–43. <http://dx.doi.org/10.1023/A:1022698205904>
27. J. K. Gilbert, D. F. Treagust (Eds.), *Multiple Representations in Chemical Education*, Springer, **2009**.
28. R. C. Mocellin, M. Labarca, For a Dialogue between the Teaching of Chemistry and the History and Philosophy of Chemistry: The Case of the Concept of ‘Chemical Element’, *Substantia* **2024**, 8(1), 81-89. <https://doi.org/10.36253/substantia-2324>