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Structures and Equations: The History of Theoretical Chemistry and Its Epistemological Challenges

Estruturas e Equações: A História da Química Teórica e Seus Desafios Epistemológicos

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Theoretical chemistry was developed in the twentieth century not as a mere application of quantum mechanics, but as a hybrid field sustained by divergent models of molecular structure. From the 1928 Solvay Conference of Chemistry and the seminal publication by Heitler and London, the first application of quantum mechanics to a molecule, this article examines the formation of a discipline marked by tensions between classical structural chemistry and quantum formalism. Key historical debates, the role of Valence Bond and Molecular Orbital models, their reception within the chemical community, and the epistemological obstacles that persist in chemical education are reviewed. Drawing on Alex Johnstone's epistemology and empirical studies with university students, the article argues that widespread misinterpretations of quantum concepts reflect both historical inheritances and pedagogical practices.

Keywords: history of science; quantum chemistry; structural chemistry; epistemological obstacles; chemical education.

1. Introduction

The consolidation of theoretical and quantum chemistry in the first decades of the twentieth century occurred in a context marked by profound conceptual tension. Although the development of quantum mechanics in physics was marked by controversies, it became established as the fundamental framework for microscopic phenomena. In chemistry, however, quantum mechanics was incorporated through hybrid models that preserved pre-existing structural concepts rather than replacing them. Structural models proposed by Lewis, became not only explanatory tools but also a shared language for chemical reasoning, prediction, and pedagogy.

The emergence of quantum mechanics did not immediately replace this tradition. Instead, quantum chemistry developed as a hybrid field, situated between classical structural chemistry and quantum formalism. From its inception, it relied on approximations, visual models, and semi-empirical interpretations that allowed chemists to preserve familiar conceptual frameworks while selectively incorporating mathematical results derived from physics. This hybridization proved both productive and problematic: while it enabled the rapid dissemination of quantum ideas within chemistry, it also generated persistent epistemological ambiguities.

A pivotal moment in this process was the publication of the Heitler-London paper in 1928, which applied quantum mechanics to the hydrogen molecule and is often regarded as the foundational work of theoretical chemistry. Rather than overthrowing Lewis's concept of electron sharing, the Heitler-London approach, as revisited by Linus Pauling, provided a mathematical justification for it, while simultaneously revealing a fundamental gap between mathematical formalism and chemical meaning. The interpretation of wavefunctions in terms of bonds, resonance, and electron exchange was not dictated by the equations themselves, but constructed through conceptual negotiation grounded in pre-existing chemical models.

Historical debates surrounding the reception of quantum mechanics in chemistry, particularly those documented at the 1928 Solvay Conference of Chemistry, demonstrate that the formation of quantum chemistry was not merely a technical or ontological matter, but also a problem of communication, representation, and pedagogy. Divergent traditions emphasized different balances between mathematical rigor and empirical visualization, shaping the subsequent development of Valence Bond and Molecular Orbital theories.

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These historical dynamics continue to influence contemporary chemical education. The widespread use of semi-empirical models, visual representations, and algorithmic rules has facilitated learning at introductory levels, but has also contributed to enduring difficulties in distinguishing classical from quantum concepts. Drawing on historical analysis, epistemological frameworks, and empirical studies on student learning, this review examines how the hybrid origins of quantum chemistry have generated persistent epistemological obstacles. By situating these difficulties within their historical context, the article aims to clarify the conceptual foundations of theoretical chemistry and to contribute to more reflective approaches in teaching and learning quantum chemical concepts.

2. Structural Chemistry and the Limits of Classical Explanation

Quantum and theoretical chemistry as a subfield of chemistry had a conflicted birth. In the 1920s-30s, it emerged not as physics, or quantum mechanics applied to chemistry, but as an in-between field that was never able to abandon its roots in structural chemistry. When we look at structural chemistry from the end of the 19th and beginning of the 20th century, it is undeniable the amount of success it achieved describing molecules and explaining empirical evidence. Therefore, we have to acknowledge and understand why the ideas of Lewis, Langmuir and Kossel are still so entrenched in modern chemistry, having become a key set of algorithms and even a necessary language. In this section, we will explore two of the most influential papers in structural chemistry, published by G. N. Lewis in 1913 and 1916, all along the dawn of Quantum Theory.[1,2]

2026 marks the 110th anniversary of the publication of G. N. Lewis's 1916 paper entitled "The Atom and the Molecule", in which Lewis describes chemical bonding as the sharing or pairing of two electrons in a valence shell and the octet rule. Those ideas shed a light in explaining certain molecular structures and improved the concept of valence, already discussed in his 1913 paper, "Valence and Tautomerism".[1,2]

The idea of bond between atoms was largely understood as a consequence of forces acting between those atoms to keep them together. Since the 18th century, electrostatic interactions have been regarded as the main driving force between bodies. Lewis's 1913 paper alludes to the idea of chemical bonding, classifying chemical compounds in three types, depending on the nature of their chemical combination: polar, non-polar, and metallic. To arrive at this conclusion, Lewis expands the common idea of valence at the time as valence and polar number. Valence, in structural chemistry, was regarded as the number of bonds one atom could have in a chemical combination, and was strongly based on periodic properties. In order to accommodate different types of compounds, organic and inorganic, Lewis splits the concept of valence in two: i) the number of positions on the atom in which attachment to other atoms occurs (valence number); and ii) the number of negative electrons an atom has lost (polar number). From those two concepts, Lewis classifies two types of chemical combinations, which he regards as different both in kind and in degree, polar and non-polar, in a striking resemblance to what we currently know as ionic and covalent bond. It is important to note that Lewis's classification is based entirely on empirical evidence. His rationale can be summarized as follows. Polar compounds are characterized as mobile, with atoms moving freely, predominant in inorganic compounds; and non-polar compounds, as immobile, with a frame structure and fixed arrangement of atoms, predominant in organic compounds. Therefore, tautomerism occurs when a compound assumes at least in part some polar form. Moreover, since polar compounds have free charges at certain points, it explains the high dielectric constants of ions.

In his famous 1916 paper, The Atom and the Molecule, Lewis starts with a recollection of the previous paper, showing chemical and physical properties that distinguish polar and non-polar compounds, suggesting this nomenclature is a better option than inorganic and organic, and assuring those distinctions are fundamentally due to one single cause, the strength to which electrons are held by individual atoms in the presence of another atom in a chemical combination. Therefore, correcting his previous paper, he argues the two types of chemical combination, polar and non-polar, are distinct only in degree: and that a single molecule, or even a part of a molecule, may pass from one extreme type to another, not by a sudden and discontinuous change, but by imperceptible gradations.[2] Then, his Theory of Atomic Structure is presented to explain such an assumption. The theory of the Cubicle Atom explains laws of chemical behavior through six postulates, which we will briefly illustrate to confirm Lewis's theory still is the cornerstone of explaining chemical bonding in many areas of chemistry.

1. The first postulate is that each atom possesses a kernel with an excess of positive charges corresponding to the group in the periodic table to which the element belongs. This kernel remains unaltered in any chemical change. This postulate, based on the Thomson's atom, gives rise to the representation of the atom as the symbol of the element to represent the kernel, followed by the symbol + in superscript to represent the ionic charges.

2. The neutral atom is composed of an outer shell with negative electrons equal in number to the excess of positive charges of the kernel, and the number of outer shell electrons can vary between 0 and 8 in a chemical combination. This postulate is justified by the understanding of reduction and

oxidation processes, explained as increase and decrease in the number of electrons in the outer atom of the element, respectively.

3. The atom tends to hold an even number of electrons in the outer shell, symmetrically arranged in the corners of a cube. To rationalize this assumption, Lewis generalizes the outer shell of the atom as an element of electricity, represented by the symbol E which in combination with the positive number of the kernel (postulate 1), should account for the total charge of the compound. Analyzing formulae of inorganic and organic compounds, Lewis sustains this postulate with several examples, such as lithium fluoride, LiF. Lithium has one positive charge in the kernel, and fluorine has seven, so that the neutral molecule is represented as LiFE8. In lithium sulfate, S and O each has six positive charges, thus Li2SO4 = Li2SO4E32. This generalization engenders the very successful and popular Rule of Eight or Octet Rule.

4. Two atomic shells are mutually interpenetrable. This assumption explains Lewis's new idea, correcting his 1913 paper, that polar and non-polar compounds differ only in degree, not in kind. Here, Lewis dismisses the idea of electrons of one atom passing completely into another atom, and that the different charged parts of the molecule thus produced are held together by electrical forces. It is interesting to note the reader will find this definition of ionic bond in any general chemistry textbook, in all levels of education – secondary, post-secondary, and even graduate.

5. Electrons can move from one outer shell to another, and this movement is dependent on the magnitude of the constraints which hold them in position. This postulate is justified by the fact that there is no empirical evidence of the existence of electronic isomers, ie, compounds that differ by the localization of electrons in one atom or another. Therefore, there is a considerable freedom of movement of electrons in a chemical compound. Moreover, this assumption is in agreement with postulate 4, that chemical combination of the polar and non-polar types differ in the degree to which the electrons are held by one atom or another, and leads to postulate 6.

6. Electric forces between particles which are very close together do not obey the simple law of inverse squares which holds at greater distances. This postulate is perhaps the most interesting, as it is not frequently found in modern chemistry textbooks alongside the others to explain chemical bonding according to Lewis's theory. Lewis declares there are only two ways in which one body can be held by another, one being governed by attraction and repulsion at long and short distances, respectively, with a rest point where the net attraction or repulsion is zero. The other is the one "in which the planets are held by the sun". Lewis asserts this idea is employed by Bohr based on Planck's theory, when Bohr's electron moving in a fixed orbit (according to Planck's elementary oscillator which maintains its motion at the absolute zero) does not produce any effect upon external charges, in disagreement with the laws of electromagnetism. Furthermore, Lewis claims to have an upper hand over Bohr and Planck:[3]

He (Bohr) explains the spectral series of hydrogen by assuming that an electron can move freely in any one of a series of orbits in which the velocities differ by steps, these steps being simply expressed in terms of ultimate units (in his theory Planck's h is such a unit), and that radiation occurs when the electron passes from one orbital velocity to the next. It seems to me far simpler to assume that an electron may be held in the atom in stable equilibrium in a series of different positions, each of which having definite constraints, corresponds to a definite frequency of the electron, the intervals between the constraints in successive positions being simply expressible in terms of ultimate rational units.

Following, Lewis admits the unknown status of the forces driving chemical combination:[2]

Indeed it seems hardly likely that much progress can be made in the solution of the difficult problems relating to chemical combination by assigning in advance definite laws of force between the positive and negative constituents of an atom, and then on the basis of these laws building up mechanical models of the atom.

Lewis suggests we must first understand the structure and arrangement of atoms from the perspective of chemical combination, to then, accordingly, modify generalizations on the nature of the forces governing chemical combination. Nevertheless, he believes when it comes to the electron in a molecule, Coulomb's law of inverse squares must fail at small distances.

Preceding his exposition on molecular structure, Lewis connects his rationale citing Parson's magneton theory.[4] According to Lewis, the fundamental assumption that the electron is a charge and a small magnet, and therefore the existence of electric and magnetic forces, leads to the conclusion that the most stable condition for the atomic shell is the one in which eight electrons are held at the corners of a cube.

The form how Lewis wrote and presented his ideas in the "Atom and the Molecule" leads the reader to presume the six postulates of Lewis's Theory of Atomic Structure inevitably create rules for explaining (in some cases, determining) molecular structure. Using the postulate of the cubic atom, Lewis shows as an example the chemical combination of liquid iodine to form the iodine molecule I_2 with a graphical representation, reproduced as follows.

The cubic representation shown in Figure 1 depicts the Octet Rule, as explained:[2]

A represents the molecule as completely ionized, as it undoubtedly is to a measurable extent in liquid iodine.

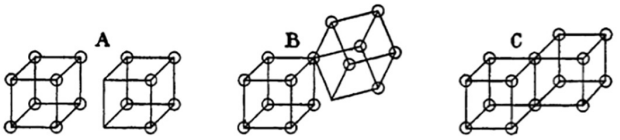


Figure 1. Representation of chemical combination to form I_2 molecule according to Lewis[2]

Without ionization we may still have one of the electrons of one atom fitting into the outer shell of the second atom, thus completing its group of eight as in B. But at the same time an electron of the second atom may fit into the shell of the first, thus satisfying both groups of eight and giving the form C which is the predominant and characteristic structure of the halogens.

Subsequently, Lewis presents the theory in symbols: a colon (or two dots) representing a pair of electrons shared freely between two connected atoms, being each formula a representation of the many tautomeric states of the structure, meaning each tautomeric form could be associated with a different polarization of the electron pair. Thus, Lewis's formulae explain not only polar compounds, but non-polar (and a range of semi-polar in between), in which each 2 dots represent 2 electrons held in common by two atoms, as in structural organic chemistry is represented by a line understood as a single bond. Extending the cubic atom to a tetrahedron, Lewis is able to explain triple bonds, in which two tetrahedra, attached by one, two or three corners of each, represent respectively the single, the double and the triple bond.

The success of Lewis's ideas is indisputable, as it presently constitutes the main core of chemical bonding, especially in introductory and general chemistry. Their simplicity, in terms of fundamental concepts and representational tools; ability to describe many chemical structures and explain some empirical observations transformed a set of rules and algorithms of structural chemistry into a widely accepted theory of chemical bonding, in spite of the advent of Quantum Chemistry.

The transfiguration of Lewis's structural theory into quantum chemical bonding theories was not a simple transposition or translation of concepts. Quantum Mechanics, and subsequently, Quantum Chemistry, appeared to shed a new light on how chemists interpreted the chemical bond. In the next section, we will attempt to understand how the historical context shaped this quasi-revolutionary movement.

In a very interesting documental analysis, Gillespie and Robinson[5] describe the development of Lewis's ideas concerning the chemical bond and in particular the concept of the electron pair bond and the octet rule, showing that the conceptual language which arose from Lewis's theories, such as resonance structures, endure in modern chemistry to describe molecules. It is interesting to note the authors, aiming to evince the success of Lewis's theories, chose statements like the following:

"*Today it is realized that bonding electron pairs in many molecules are not as well localized as Lewis believed, nevertheless resonance structures, i.e., plausible alternative Lewis structures, are still often used to describe such molecules*."

And: "*Moreover electrons are not always found in pairs*, (...)"

The wording of these statements, as presented in the abstract of the cited article, suggests that the authors endorse a descriptive view of the chemical bond, one that is validated and interpreted through quantum mechanics, in a way highly reminiscent of Linus Pauling's approach, which we will address in a later section.

3. Quantum Mechanics and the Solvay Conference of 1928

The quantum approach to chemical problems was not received in open arms by a greater community of chemists, especially experimentalists who were very well satisfied with structural chemistry. At the 1928 Solvay Conference of Chemistry (the third in the Chemistry cycle of conferences), discussions on valence revealed the tension between classical images and new electronic descriptions. Lewis and Langmuir's octet theory resonated with organic chemists, while Kossel's electrostatic theory appealed to physicists. The central dilemma was: are electrons particles, waves, or simply representational tools? Chemists welcomed quantum mechanics but worried about losing touch with chemical practice, and an intense debate was reported in the annals of the meeting.[6]

Georges Urbain, a renowned French chemist, gave a lecture titled Chemical Valences, fundamentally rooted on the structural chemistry theories of Lewis, Langmuir, and Kossel. Following the lecture, the English chemist Frederick George Donnan seemed to be very open to the new ideas, bringing to the discussion of Urbain's lecture the question of how chemists would now interpret the electron, given Schrödinger's theory:

I listened with great interest to Mr. Urbain's excellent presentation. It is a very clear outline of the comings and goings of chemical theories. I would like to make a few remarks about modern theories of valence. Of Bohr's primitive theory, all that remains today is the idea of stationary states of the atom. I believe that the concept of electron orbits has completely vanished. In fact, electrons themselves no longer exist, at least in the form previously imagined. According to Schrödinger's theory, that is, according to wave mechanics or the micromechanics of

atoms, we have in the atom a stationary and vibratory distribution of electric charges that Schrödinger analyzed by a new combination of the ideas and theories of Hamilton, Fermat, and Planck. In my opinion, it is by developing this theory that we can find an explanation of valence. I think we will find it in the distribution of the nodes of the Schrödinger wave system.

It is very interesting to note that Donnan was essentially an experimental chemist, having devoted most of his career to the field of chemistry engineering, and is known for the Gibbs-Donnan effect, which describes the equilibrium of charged particles on a semipermable membrane. It was the first and last time Donnan attended a Solvay Conference. Donnan continues, stating:

It should be noted that this way of conceiving things is not likely to restrict the role of chemists. On the contrary, I believe that the disappearance of Bohr's highly complex electron orbitals will give them new possibilities for existence.

One can notice how enthusiastically Donnan introduced the subject of quantum theory in chemistry. It should be noted that the 1928 Solvay Conference of Chemistry was the third since 1922. The Solvay Conferences are important meetings in physics and chemistry that have been held since 1911, when the famous "Radiation and the Quanta" conference was chaired by Nobel Laureate Hendrik Lorentz, who also chaired the subsequent conferences in 1913, 1921, 1924, and 1927. In 1922, the first Solvay Conference in Chemistry was chaired by Sir William Pope, who also chaired the following four meetings. A parallel between the conferences in physics and in chemistry should be made at this point: whereas the very first conference in physics had already discussed quantum theory (the famous picture of quantum physicists, popularly known as "Probably the Most Intelligent Picture Ever Taken" was taken at the 5th Solvay Conference in Physics in 1927), the third conference in chemistry (in 1928, the one we are discussing in this paper) had barely alluded to the subject of quantum mechanics.

Jean Perrin, the French physicist who had been awarded the 1926 Nobel Prize in Physics for his experimental studies of Brownian motion, which provided decisive evidence for the atomic nature of matter, replied to Donnan by drawing a distinction between chemists and physicists. He states that chemists are concerned about bonds, counting them, representing them. In his own words:

It seems to me that the study of chemistry is a study of the discontinuity of matter (simple bodies, molecules, atoms, material quanta, energy quanta). All this seems very characteristic of the minds of chemists. The notion of valence fits well within this framework. Chemists have imagined, in rigid molecules, assembly bars. These bonds, whose number and angles are fixed, … can be counted; confusion can arise from the fact that they may not all be used. We are generally concerned with the maximum number of bonds used.

He then notes there was still no unified theory to account for the chemical bond between atoms: *"The stationary states of hydrogen were explained by Bohr by variations in quanta, but while we have a theory that accounts for emission spectra, we don't have one that explains the phenomena of attraction between atoms, that is, the valence mechanism*."

Following Perrin's contribution to discussion, Georges Urbain expresses some frustration towards the concerns voiced by Donnan. He mentions that chemistry has always taken advantage of the new developments in physics, although physics (or physicists) often impose their discipline on the chemistry of electrons and valence. On this matter, Urbain states:

Initially hesitant, chemists welcomed the new doctrines. But now physicists are telling them that they don't really know what electrons are. There are five or six authoritative theorists in the world who tell us that electrons are "clusters of waves," that is, perhaps something completely immaterial, and about which, at the present time, little can be said.

It appears that Georges Urbain refers to Schrödinger's interpretation, as it was mentioned by Donnan, and is clearly against it. Erwin Schrödinger is known for defending a realistic interpretation of the electron since his first publication on the new wave mechanics.[7] Urbain expresses his concerns about the implications of such interpretation in chemistry: "*It is therefore prudent not to seek, at least temporarily, to overly specify electronic images*." He explains that electrons should not be regarded as concrete realities, but as "*a system of signs, a language, which would conventionally translate immediate experimental facts*". Here, Urbain is in agreement with a positivist interpretation of the electron, very much aligned with the Copenhagen interpretation of quantum mechanics. On the other hand, Urbain also mentions that "*structures in chemistry can either represent real architectures or schematize possible reactions*", suggesting a realistic view on molecular structures.

Nevil Sidgwick, English theoretical chemist who published a very important textbook on chemical bonding, The Electronic Theory of Valency (1927),[8] is at most "a little" skeptical about the use of quantum mechanics to treat chemical problems. Sidgwick's report followed Urbain's and was titled "Variable Valences". He concludes his report responding to two objections raised during the discussion of Urbain's report, one to Donnan:

Mr. Donnan seems to me to be going a bit far when he criticizes chemists for using electronic theory, while physicists have now gone so far as to deny the existence of these electrons, which, according to them, are merely the nodes of a wave system. Indeed, the new theory is

not yet sufficiently advanced for us to be able to assert its incompatibility with the classical conception of the electron.

From this speech, Sidgwick implies to agree with a realistic and corpuscular view of the electron, which retains the realistic (but wave) approach of Schrödinger. Indeed, in his 1927 book, The Electronic Theory of Valence, Sidgwick tries to unify the language of chemists and physicists, and acknowledges that wave mechanics had given solutions to atomic spectra, but he stresses *"there is no proof that it should be taken so literally as to be incompatible with the conception of the nature of electrons and nuclei to which the work of the last thirty years has led."*

Donnan very politely asserts, disagreeing with Sidgwick, that quantum mechanics is not incompatible with the reality of electrons, as chemists would find in the nodes of the wave systems of Schrödinger's theory specific evidence to validate valence theory. Donnan says: *"I simply believe that Schrödinger's theory constitutes an important advance, and will, in the very near future, be of great value to the chemist."*

Sidgwick then replies, excusing himself for having misinterpreted Donnan's words. However, from the remainder of his speech, it can be understood he maintained his position of somewhat denying quantum mechanics in chemistry. In his words: *"I agree with him that the development of wave mechanics will allow us to better understand the behavior of covalent compounds. But it has not yet been demonstrated that this theory is physically incompatible with the concept of real electrons. F. London has already begun to apply wave mechanics to the case of shared electrons."*

This last commentary evinces Sidgwick's outlook on quantum mechanics. If it was a matter of taking sides, he would be on the side of structural chemistry, defending the theories of Lewis even more than Lewis himself.

4. Heitler, London, and the Model-Based Nature of Quantum Chemistry

Gavroglu and Simões[9] interpret the emergence of quantum chemistry not simply as the application of quantum mechanics to chemistry, but as the consolidation of a hybrid discipline shaped by epistemological, institutional, philosophical, and historical factors. In particular, they argue that its development involved multiple styles of reasoning, reflected in the coexistence of different approaches to chemical bonding proposed by Lewis, Heitler and London, Mulliken, Slater, and Pauling. This perspective provides an appropriate framework for understanding the model-based nature of quantum chemistry discussed in this section.

Within this context, the publication of Heitler and London's 1928 paper is widely regarded as marking the birth of theoretical chemistry. Unlike physics, quantum chemistry evolved through the coexistence of multiple models rather than the refinement of a single theoretical framework. Valence Bond and Molecular Orbital theories offered complementary, yet sometimes conflicting, representations of molecular structure, both relying on quantum approximations whose chemical interpretation frequently translates mathematical results into classical descriptive concepts, as exemplified by the Born-Oppenheimer separation of electronic and nuclear motion. Thus, quantum chemistry is hybrid: it combines quantum formalism with classical structural concepts.

Heitler and London[10] address the chemical bond through the interaction between two hydrogen atoms, interpreted from the perspective of the then newly established quantum mechanics. From the outset, the authors highlight the limitations of earlier ideas, particularly those proposed by Lewis, in explaining covalent bonding. While Lewis postulated that a bond was formed through the sharing of electrons, his theory lacked a mathematical foundation capable of explaining how this sharing occurred. Nevertheless, this limitation did not undermine the practical success of the theory, which functioned effectively within its intended scope.

The advent of quantum mechanics triggered a series of revisions and so-called "new" discoveries concerning chemical and physical phenomena. Chemistry gradually ceased to be an exclusively descriptive and experimental discipline and began to acquire a deep theoretical foundation through quantum mechanics and, subsequently, quantum chemistry, which emerged in this period. This transition was neither immediate nor complete; rather, it was a slow, revolutionary, and still ongoing process.

Heitler and London applied quantum mechanics to the simplest molecular system, the hydrogen molecule,[10] and provided a theoretical demonstration of electron sharing. From a practical standpoint, this did not substantially alter chemical practice: with explanations that were far simpler, Lewis (although theoretically incorrect) had already arrived at qualitatively accurate conclusions. The contribution of Heitler and London thus did not revolutionize chemical bonding in an operational sense, but rather established a new level of theoretical justification. Their work raises an important counterfactual question: what would have changed in the teaching of chemical bonding had the Heitler and London's paper never been published?

At the core of the paper lies a question that encloses its broader implications: are we witnessing the beginning of a fully mathematical chemistry, in which chemical reactions can be calculated directly from quantum mechanics?

Heitler and London began with Lewis's qualitative ideas and, for the first time, applied quantum mechanics to the

problem of the chemical bond, producing a mathematically consistent equation that accounted for both Lewis's conceptual framework and experimental observations. However, the equation itself does not carry inherent verbal meaning. It does not explicitly refer to electron sharing, resonance, or electron exchange. Such terms do not emerge directly from the mathematical formalism.

Interpretations involving resonance, electron exchange, and sharing were introduced by Heitler and London themselves as attempts to assign linguistic meaning to the equation, thereby connecting it to both Lewis's bonding model and known experimental results. In this sense, a pre-existing conceptual framework guided the interpretation of the equation. While the wavefunction yields results, the meaning attributed to those results is constructed by physicists and chemists and is mediated by the scientific culture of the time. Thus, verbal content, cognitive imagery, and the linguistic signs associated with the chemical bond are not contained within the equation itself, but rather arise from human interpretation.

Subsequent physicists and chemists sought to address the limitations of the original equation, as well as earlier limitations in Lewis's framework, often focusing on highly specific issues.[11] A central difficulty in imposing a mathematical description within a verbal and human interpretative framework lies in the attempt to render it universally meaningful. Scientific disciplines repeatedly strive to encapsulate their results within conceptual "boxes" and elevate them to the status of general laws. When results deviate from expectations, new exceptions, extensions, or approximations are introduced. It is possible, however, that these are not true exceptions, but rather mathematical outcomes that resist explanation within our modes of communication and conceptual categorization. From this perspective, the difficulty may lie not in the mathematics itself, but in human attempts to translate mathematical language into natural language.

As discussed by Gavroglu and Simões,[12] quantum chemistry did not arise simply from the direct application of quantum physics to chemical problems. Although quantum equations were capable of reproducing previously observed phenomena, the attribution of meaning to these equations depended on chemists and physicists. Quantum chemistry thus emerged not as a straightforward application of physics, but as a process of intellectual and methodological negotiation.

This process involved reinterpreting phenomena previously understood only through experimentation and transforming quantum formalism applied to chemical systems into visual and verbal representations. The debate concerning the relationship between physics and chemistry was not primarily ontological. There was little explicit discussion about what constituted quantum chemistry as a conceptual domain, what defined physics, or even what chemical bonds fundamentally were. Instead, what initially appeared to be an internal theoretical debate was, in fact, largely external: a debate about communication, pedagogy, and representation.

The period of early development of theoretical chemistry was marked by confrontation between two schools of thought, often regarded in modern textbooks as the Valence Bond *versus* Molecular Orbital clash. Nevertheless, Gavroglu and Simões[12] argue that instead of contrasting the Heitler-London-Pauling-Slater method of valence bonds and the Hund-Mulliken method of molecular orbitals, we should approach the matter from an epistemological point of view: Heitler-London *versus* Mulliken-Pauling, or the Germans *versus* the Americans. While Heitler and London were more inclined to support Dirac's reductionist pronouncement of 1929, in which he stated:

The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble,[13]

Pauling and Mulliken had a strong inclination toward semi-empirical methods. The American theoretical chemists did not reject quantum physics or its mathematical apparatus, which they regarded as essential. Rather, they emphasized the importance of grounding interpretation in observable phenomena. For instance, spectroscopy existed and functioned prior to quantum mechanics, and quantum theory did not replace it; instead, it provided a theoretical foundation. The question, however, is whether every spectroscopic analysis must be grounded primarily in mathematical formalism, or whether it is legitimate to employ visual and verbal translations compatible with human cognition and the researcher's cultural framework to explain observable phenomena.

German scientists, by contrast, favored a more explicitly mathematical language, minimizing jargon and abstract chemical terminology, and maintaining a stronger commitment to quantum formalism and mathematical rigor. Chemists, with a long-standing resistance to excessive mathematization, tended to privilege visual interpretation and flexibility in mathematical treatment. Consequently, this debate was less about theoretical ontology and more about scientific communication and education, about how quantum chemistry should be presented, taught, and made intelligible.

A critical counterpoint emerges, however: when experimental results are interpreted using symbols and vocabulary that may not correspond rigorously to the underlying mathematics, what is the scientific validity of such interpretations? What is gained by publishing results

that are knowingly imprecise? Is the desire to know *what* happens more important than understanding *how* and *why* it happens?

In G. N. Lewis and the Chemical Bond,[14] Linus Pauling presents not only a historical account of Lewis's contributions but also a retrospective justification of his own theoretical program in chemical bonding. Throughout the article, Pauling consistently frames Lewis's theory as the foundational conceptual structure upon which modern quantum theories of the chemical bond could and should be built, rather than as a pre-quantum heuristic to be overruled. Pauling explicitly identifies Lewis's 1916 paper, "The Atom and the Molecule", as revolutionary for introducing the idea that a chemical bond consists of a pair of electrons jointly held between two atoms. This notion, according to Pauling, established a chemically meaningful representation of bonding that was structurally intuitive, capable of guiding chemical reasoning well before the advent of quantum mechanics. Rather than abandoning this framework, Pauling's later work sought to demonstrate that quantum mechanics could validate and refine it.

A central strategy in Pauling's approach was the construction of a hybrid theory of the chemical bond, combining Lewis's classical and structural concepts with quantum-mechanical formalism. Pauling emphasizes that features such as directed bonds, electron pairing, and partial ionic character, already implicit in Lewis's theory, could be rigorously justified using wave mechanics. His discussion of partial ionic character, electronegativity, and bond stabilization illustrates this point as he argues that the stabilizing effect of partial ionicity was conceptually anticipated by Lewis's shifting electron-pair model.

Mostly, Pauling resists framing quantum mechanics as a conceptual rupture. He explicitly notes that some ideas later attributed to quantum mechanics are not intrinsically quantum-mechanical, but rather became quantitatively treated through quantum theory. This rhetorical move reveals Pauling's broader epistemological commitment: quantum mechanics is presented as a confirmatory and legitimizing framework, not as a replacement for chemical intuition.

Pauling's treatment of resonance further illustrates his effort to preserve Lewis's relevance. While acknowledging that Lewis himself did not formulate resonance theory, Pauling portrays resonance as a natural extension of Lewis structures. In doing so, he retroactively integrates Lewis's representations into a quantum-mechanical ontology, transforming classical structural formulas into physically meaningful components of the wavefunction in his textbook The Nature of the Chemical Bond (1939).[15]

Overall, Pauling's narrative demonstrates a sustained and deliberate effort to ensure that Lewis's theory of the chemical bond remained central to chemical theory in the quantum era. By embedding Lewis's concepts within quantum mechanics, Pauling constructed a continuity narrative in which modern quantum chemistry appears as the natural culmination of classical chemical thought. This synthesis not only preserved the pedagogical and conceptual utility of Lewis structures but also reinforced Pauling's own descriptive approach to chemical bonding, in which quantum mechanics serves to justify chemically intuitive models rather than to eliminate them.

According to Ana Simões,[16] Pauling's textbook The nature of the chemical bond (1939)[14] was only challenged by Coulson's Valence (1952),[17] a textbook that was published more than a decade later. Simões establishes a strong connection with the preceding discussion by addressing the impact that a textbook can have on education, whether at the secondary or elementary level or in higher education. Textbooks do not necessarily exhibit strict mathematical scientific rigor in their content, as their primary purpose is to help students consolidate concepts. When such materials are used without a proper presentation of the mathematics underlying the phenomena, it becomes possible, over successive generations of chemists, for these representations to be taken as faithful depictions of reality.

This oversight is not merely linguistic. Coulson, in attempting to address a theory of bonding with less visual appeal, repeatedly encountered the conceptual limitations imposed by his own framework.[16] He frequently ended up interpreting molecular orbitals in terms of valence bonds. When Pauling sought to cultivate a "chemical intuition", capturing the reader's attention through images that appear conceptually plausible but contain contradictions (acknowledged by Pauling himself), he transformed his pedagogical approach into a hegemonic one. This hegemony arose not from coherence, but from ease of assimilation.

There were, therefore, two distinct approaches, both of which achieved considerable success within the academic community. Pauling, by constructing a body of work grounded in classical chemical concepts,[15] with simple and easily comprehensible mathematics, managed to eternalize certain images and to set the terms of the debate on chemical bonding, even though these were presented as idealizations intended for chemists. Coulson also achieved success in his work by relinquishing excessive mathematization and by using images as interpretative tools rather than as visually faithful representations of what physically occurs, without assigning them an ontological status. Although Pauling also attempted to frame the use of images as merely supportive elements, he was unable to prevent his interpretation from being elevated to an ontological level. In this sense, Coulson was more successful in his approach.

Accordingly, Simões proposes a debate on the impact of this homogeneity. Whom does it serve? For a professional

or an academic, is a more didactic and less theoretically grounded approach appropriate, or is it preferable for a researcher to have deeper knowledge of the foundations? For a secondary-level student, which approach is more suitable? The concept of resonance plays a fundamental role in explaining the structures of chemical compounds, but knowing that it does not correspond to physical reality, what is the validity of this knowledge?

It is also necessary to recognize that moving directly from a visual approach to abstract mathematization may deter readers. A gradual construction, such as that adopted in valence-based approaches, demonstrates the success of mathematical treatments when combined with visual elements and other didactic devices, understood strictly as pedagogical tools rather than as faithful representations of reality.

Over time, the abandonment of quantum formalism and its models has led to significant consequences for the understanding of chemical bonding and quantum chemistry. One outcome has been the need to study increasingly extensive theories to explain each new phenomenon. What began as a debate over form has gradually become ontological in nature. Chemical bonds have been transposed to hybridization, overlap, or interference, and as mathematical formalism was progressively abandoned, the distinction between physical reality and symbolic representation became blurred.

This discussion points toward a broader epistemological debate, aligned with perspectives developed by Bachelard, Kuhn, and others,[18,19] which view scientific models as instruments rather than literal descriptions of reality. From this standpoint, critical questions arise regarding chemical education: what is the impact of these conceptual frameworks on the teaching of chemistry? Does the practical success of approximations render mathematics obsolete? Is mathematics merely a visible instrument of validation that can be replaced by observable models? Is it worthwhile to relinquish mathematical formalism altogether?

While the use of symbols and images to represent chemical bonds is both normal and pedagogically useful, treating these representations as physically real entities raises significant epistemological concerns. Understanding where representation ends and reality begins remains a central challenge in both quantum chemistry and its teaching.

5. Quantum Chemistry Teaching and Epistemological Obstacles

The hybrid nature of quantum chemistry that arose from divergent views, which also includes a strong attachment to structural chemistry, leads to an uncountable amount of epistemological obstacles when we teach chemistry. The hybrid quantum/classical nature of theoretical chemistry and the epistemological obstacles created by such nature raise questions: How does this reach our classrooms? In organic chemistry, we teach resonance and hybridization, which are semi-empirical tools. In inorganic and physical chemistry, molecular orbitals and approximate methods. In spectroscopy, the Born-Oppenheimer approximation is used without dispute. We pass on a mosaic of pragmatic models, but rarely address their autonomy or epistemological tensions.

One of the major problems in teaching quantum chemistry lies in the difficulty that some students have in establishing a clear distinction between what is classical and what is quantum. Among the examples is the representation of the atom. According to Allred and Bretz,[20] students are able to conceive two contradictory models simultaneously, such as the Bohr model, which retains classical features, and the quantum model, which describes electrons not as classical particles but through the concept of wave–particle duality. The problem described above does not originate from students' ideas and conceptions. According to Gómez and Martín,[21] quantum chemistry is an academic discipline and, as such, is not clearly related to the broad chemical knowledge developed in inorganic chemistry, organic chemistry, or analytical chemistry laboratories. Real chemical problems require in-depth mathematical knowledge to be addressed from the perspective of quantum chemistry, making their solution difficult for students with only basic mathematical knowledge.

On the other hand, for the resolution of such problems, it is sufficient to understand a simple visual model, independent of quantum mechanics. The consolidation of chemical bonding concepts using such models in textbooks, particularly through the influence of Linus Pauling, established a hybrid quantum-classical language in chemical education. While pedagogically effective, it obscured underlying epistemological tensions. This hybrid quantum-classical language created a myriad of visual models, strongly based on the structural chemistry developed before modern Quantum Mechanics.

Gómez and Martín[21] refer to Folk Molecular Theory (FMT) as "an informal set of structural ideas and semi-empirical rules." According to FMT, the bonds that occur between atoms are concrete; there is something linking the atoms, like a spring, and these bonds are represented by rules such as Lewis dot structures, atomic orbital hybridization, or the Valence Shell Electron Pair Repulsion (VSEPR) theory. FMT is the theoretical basis of many teachers, as it is able to describe a variety of chemical systems at the microscopic level. However, it lacks the mathematical formalism present in quantum theory, and its many exceptions mislead students.[22]

For instance, Lewis dot structures are used to determine molecular geometry through a procedure with a few simple steps, such as: defining the central atom (the least electronegative atom), inserting bonds between the central atom and the other atoms, completing the octet of these other atoms, and distributing the remaining electrons on the central atom.[23] Many pedagogical issues may arise from the use of the Lewis model,[21] such as:

- It is not a model derived from the physical-mathematical formalism of quantum mechanics. Instead, it is a semi-empirical structural model that successfully accounts for chemical behavior through heuristic rules and representations.
- Results are dimensionless: number and type of atoms; molecular charge; polarity; ionic character; geometry. For instance, it is possible to state which atom in a compound is more polar by observing the molecular structure. Furthermore, regarding resonance, it is possible to say that a compound is more stable simply by observing the length of the chain of alternating double and single bonds. However, this same behavior can be explained by solving the Schrödinger equation for the particle-in-a-box model and concluding that the larger the box, the lower the energy of the system.[24]

With respect to Valence Bond theory (VB) from the FMT perspective, Lamoureux and Ogilvie[25,26] discuss the problems caused by the use of hybridization in organic chemistry teaching. Among the criticisms, the authors stress that hybridization is presented to students as being based on quantum mechanics, which is false. Taber argues that what is called hybridization in chemistry textbooks is a flawed model limited by a simple trigonometric approach.[27] Another problem lies in terminology that loses its original meaning. For example, in VB, terms such as "atomic orbital," "overlap," "orbital hybridization," or "resonance" are interpretations of mathematical results of Schrödinger's equation. However, in FMT these same terms possess a physical reality.[21] One example is the atomic orbital, which some students describe as a physical region or understand orbital and shell as synonyms.[28]

The main epistemological obstacle in teaching quantum chemistry arises from the fact that quantum terms have been endowed with classical meanings. As new chemical data and observations emerge, FMT is updated so that it continues to function. In this sense, new rules or even exceptions to the rules are added and FMT is maintained and perpetuated.[21]

It is well accepted that Chemistry is a discipline that involves forms of knowledge that are difficult to understand for they are particularly abstract. Thus, it is essential that chemistry teaching be conceived under three aspects of knowledge: phenomenological, theoretical, and representational.[29] The phenomenological aspect encompasses what can be seen, felt, or measured, such as changes in physical state, changes in temperature, or the measurement of energy released in a reaction. The theoretical aspect comprises discussions of abstract concepts and topics that cannot be visualized, as is the case of quantum chemistry. Finally, the representational aspect is related to chemical language through symbols, equations, and model representations. Similarly, Alex Johnstone[30-32] describes three levels of knowledge in chemistry: macro, sub-micro, and symbolic. The macro level is tangible and visible. The sub-micro level corresponds to the atomic level or that which is invisible to the human eye. The symbolic level is represented by formulas, equations, symbols, and graphs. During the teaching process, teachers move through these three levels with ease; however, students have difficulty doing the same. According to Johnstone, concepts should start at the macro level and progressively be updated with the sub-micro and symbolic levels, so that students can gradually follow these concepts. In this sense, quantum chemistry should be introduced in a more concrete way, for example, through everyday applications, and from there be gradually related to the symbolic and sub-micro levels.

The evergoing quest for visualization and giving physical meaning to abstract concepts in chemistry can be understood in terms of the ontological inversion of the levels of knowledge in the epistemology of Johnstone. As an example, we consider the use of images as the sole bearer of conceptual knowledge. Figures 2 and 3, below, show the images we will further discuss.

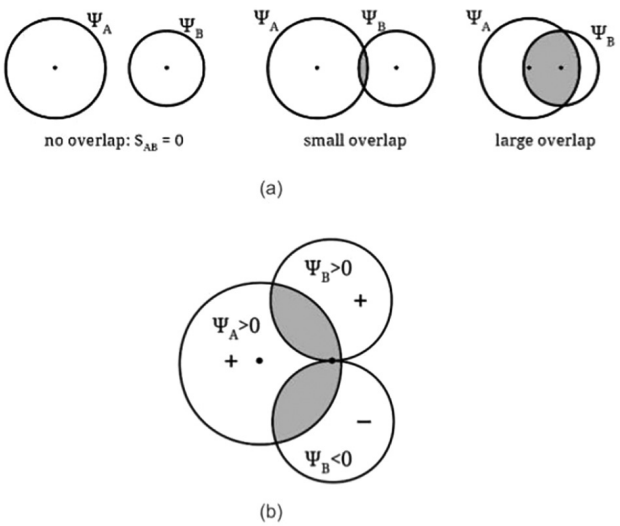


Figure 2. (a) Representations of overlap integrals for two orbitals, and (b) A diagram used to illustrate the vanishing of the overlap integral for symmetry reasons when Ψ_A is an s orbital and Ψ_B is a p orbital. Adapted from Barradas-Solas and Gómez (2014)[33]

In Figure 2, we can see two images used to support the equations and mathematical development of chemical bonding in the VB theory. In other words, they were

used so the student could visualize the equations and give meaning to them in a chemical context. On the other hand, we see images in Figure 3 which represent atomic orbitals approaching each other to "form" a bond when they physically overlap. The ontological inversion is clear: the chemical bond then becomes the physical, real, touchable overlap of other physical entities. When showing images that represent orbitals, it is important to clearly distinguish orbitals from electron density. Electron density is a measurable physical quantity, whereas orbitals are graphical representations of wavefunctions, typically depicted as isodensity surfaces defined by an arbitrary cut-off value, since the wavefunction extends asymptotically to infinity. The epistemological issue is not the physical reality of electron density, but the interpretation of these representations as physical objects that literally overlap to form chemical bonds.[34]

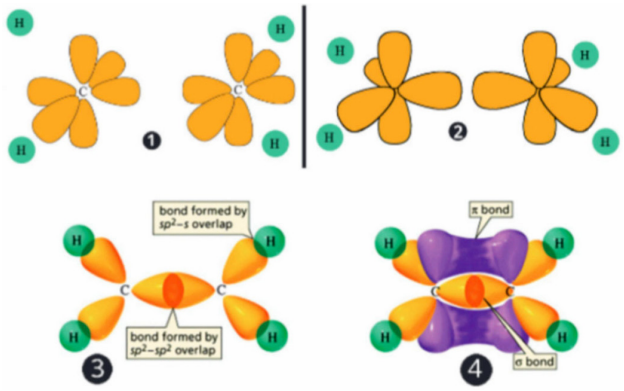


Figure 3. Images representing different molecular orbitals to form bonds by overlapping the orbitals. Adapted from Barradas-Solas and Gómez (2014)[33]

In 2023, as a result of a master's dissertation, we published in the Journal of Chemical Education the paper The Electronic Structure of the Atom: (Mis)Interpretations of Quantum Concepts by Brazilian University Chemistry Students,[35] in which we measured the level of knowledge of university students on quantum chemistry concepts throughout the chemistry programme, and identified the collapse of the epistemology of Johnstone. We applied 2 questionnaires, one in the beginning of the term, and one in the end, to 75 undergraduate students in 3 courses of the 2nd and 3rd year, namely Advanced Inorganic Chemistry and Quantum Chemistry. The questions were divided as representational and conceptual (quantum) questions. The main conclusion was that it was not possible to notice an improvement in the comprehension of students regarding the electronic structure of the atom. Even though students performed better with representational questions when compared to conceptual questions, the majority of students could not correctly interpret information from images, diagrams, and graphs. A reproduction of a multiple-choice question in questionnaire 1 is shown below in Figure 4:

Students showed a lack in understanding and interpreting the energy diagram, as 54.5% of them chose incorrect answers for question 6. Notably, the alternative "the electron is attracted to the nucleus" was selected as correct by 36.4% of the students. It is possible to identify that the students resort to classical ideas to explain quantum knowledge, suggesting that the students think according to FMT, that is, they evaluate the question through rules such as "charges of opposite signs attract each other" rather than the concept of energy quantization, a more abstract concept.

Those epistemological obstacles also appear in chemistry textbooks. For example, certain textbooks used at a Brazilian university in first-year chemistry programs contain terms or statements that compromise learning of quantum chemistry. In "Inorganic Chemistry: atoms, molecules, liquids, and solids", for example, one can read: *"from this point onward, the electron can no longer be conceived as a particle, but rather as a region with a given volume in space that has a high probability of containing the electric charge"*.[23] Through this and similar statements, the textbook appears to suggest that the electron is a region in space, which may lead to the interpretation that the orbital is the electron itself, as

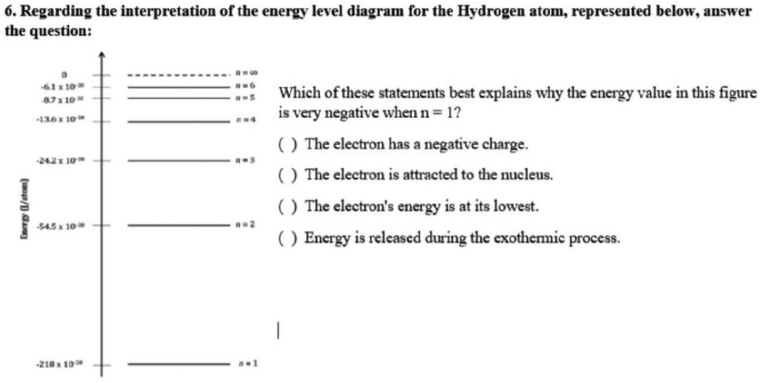


Figure 4. Question in questionnaire 1, in which students should interpret an energy level diagram. Reproduced from Goulart da Cunha and collaborators[20]

observed among students in a previous study.[35] In addition, several texts[23,36-38] employ terms such as shell, subshell, core, or the representation of orbitals as boxes, not mentioning they are representations or interpretations of mathematical results. Moreover, essential concepts in wave mechanics, such as momentum, diffraction, wavefunction, probability, interference, electron density, complementarity, are not defined, distancing even more the chemical reasoning from the mathematical rationale.[23,36,37]

The ontological inversion between the levels of knowledge – symbolical, macro, and sub-microscopic causes a loss in understanding the theoretical dimension of the chemical problem. The electron becomes a cloud of dots around the nucleus, the orbital becomes an arrangement of party balloons, and the chemical bond becomes the overlap between those balloons. It is not surprising that chemists frequently choose this ontological inversion, as it is the means of creating a hybrid quantum-classical language, or the set of semi-empirical rules Gómez and Martín call FMT. The relationship between FMT and quantum mechanics constitutes an obstacle to the teaching of disciplines involving quantum chemistry. FMT does not (or should not) function as a conceptual basis, and one way to counter the relationship between quantum chemistry and FMT is through teaching the history of science. In this way, students can gain an understanding of how the processes of theory and model development occurred over the years, recognizing the importance of more current theories when compared to earlier ones. A simple way to introduce the history of science is through a course outside the curriculum, avoiding the work of reformulating an entire curriculum to include this aspect, and incorporating research as a teaching strategy in the classroom. For instance, the research papers cited in this work could be used as means to discuss the validity of the models. Nascimento explains the nature of the chemical bond using a historiographical account of three main dogmas - the sharing of an electron pair; the electron spin; and the reduction of potential energy. Those three dogmas, which are originally built one on to another from structural chemistry through FMT, are finally deconstructed using the relatively simple example of the hydrogen ion molecule, giving rise to a new understanding of chemical bonding based on evidence from quantum mechanics.[39]

This historical development gave quantum chemistry a hybrid character, combining classical models, semi-empirical approaches, and quantum mechanics. Although this plurality contributed to the consolidation of the discipline, it also created epistemological challenges for chemistry education, as students often struggle to distinguish heuristic chemical models from concepts derived directly from quantum theory.

6. Final Remarks

The historical development of theoretical and quantum chemistry reveals that the field did not arise from a single, unified theoretical framework, but from the coexistence and pragmatic integration of divergent models. Structural chemistry, with its visual and semi-empirical tools, was not displaced by quantum mechanics; instead, it was reinterpreted and partially legitimized by mathematical formalism. This hybrid character, established in the early twentieth century, continues to shape chemical reasoning, representation, and pedagogy.

The analysis presented in this review highlights that many of the conceptual difficulties observed in the teaching and learning of quantum chemistry are not merely cognitive or didactic in nature, but deeply rooted in the epistemological structure of the discipline itself. The attribution of classical meanings to quantum concepts, the reification of representational models, and the ontological inversion of symbolic, sub-microscopic, and macroscopic levels of knowledge are historical inheritances rather than isolated pedagogical failures.

Recognizing scientific models are representational instruments that mediate between mathematical formalism and chemical interpretation, as emphasized in epistemological perspectives associated with Bachelard and Kuhn, is essential for addressing these challenges. The success of semi-empirical approximations does not render mathematical formalism obsolete, nor does visualization alone suffice to convey quantum concepts. Instead, a reflective balance between formalism, interpretation, and representation is required.

From an educational standpoint, we attempt to reinforce the importance of explicitly addressing the historical and epistemological dimensions of quantum chemistry. Incorporating the history of science into chemical education offers a viable strategy for contextualizing models, clarifying their limits, and preventing the naturalization of symbolic constructs as physical entities. Such an approach may help students and educators alike to better distinguish between mathematical structure, representational convenience, and physical interpretation. Ultimately, understanding the hybrid origins of quantum chemistry is not merely a matter of historical interest, but a necessary step toward improving conceptual clarity and epistemological coherence in both theoretical chemistry and its teaching.

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