Foundations of Chemistry
https://doi.org/10.1007/s10698-024-09508-y

Clashing perspectives: Kantian epistemology and quantum chemistry theory

Ricardo Vivas-Reyes[1]

Accepted: 9 April 2024

Abstract
In this contribution, the role of epistemology in understanding quantum chemistry is discussed. Quantum chemistry is the study of the behavior of atoms and molecules using the principles of quantum mechanics. Epistemology helps us evaluate claims to knowledge, distinguish between justified and unjustified beliefs, and assess the reliability of scientific methods. In quantum chemistry, the epistemology of knowledge is heavily influenced by the mathematical nature of quantum mechanics, and models can be tested, proven, and validated through experimentation. This paper also discusses key concepts used in quantum chemistry, such as the wave-particle duality of matter and the uncertainty principle. This work utilizes Kant's philosophy of science to frame debates and discussions in quantum chemistry, particularly with regard to the interplay between empirical observation and theory. Additionally, the text explores how Kant's ideas about the role of the mind in constructing our understanding of the world can help us comprehend the counterintuitive phenomena of quantum mechanics and its applications in quantum chemistry theory.

Keywords Epistemology · Quantum chemistry · Scientific knowledge wave-particle duality · Uncertainty principle

Introduction

Recently, there has been significant interest in studying quantum chemistry, leading to new insights and approaches in understanding chemical substances and their properties. One of these approaches is the philosophy of molecular chemistry, which focuses on the molecular structure and composition of substances and the interactions between molecules (Scerri 2011; Hendry and Needham 2014). This approach aims to comprehend the nature of chemical substances, their reactions, and properties, and their relationship with other fields of study such as physics and biology (Torretti 2013; Hacking 1983)

✉ Ricardo Vivas-Reyes
rvivasr@unicartagena.edu.co

[1] Grupo de Química Cuántica y Teórica, Programa de Química, Facultad de Ciencias Exactas y Naturales, Universidad de Cartagena, Campus San Pablo, Cartagena, Colombia

Published online: 14 May 2024

In addition to these approaches, there has also been a growing interest in the role of visualization and simulation in quantum chemistry (Computational Quantum Chemistry and Theory). The development of computational chemistry has been closely linked to advancements in computing hardware and software, as well as the growing use of artificial intelligence (AI) and machine learning (ML) techniques. These developments have enabled researchers to perform increasingly complex calculations and simulations, providing insights into the behavior of atoms and molecules that were previously unattainable. These tools can help researchers understand and explore the behavior of atoms and molecules, as well as develop and test new theoretical models. However, there are also important questions to consider regarding the accuracy and reliability of these tools, as well as their relationship to empirical observation, need to be considered (Scerri and McIntyre 2014).

The use of visualization and simulation tools in quantum chemistry has revolutionized the field, but it also raises important epistemological questions that need to be addressed. Understanding the sources and criteria for knowledge and the accuracy and reliability of these tools is crucial for ensuring that the results obtained from these tools are trustworthy and can be used to advance our understanding of the behavior of molecules and chemical reactions. Epistemology provides a means for addressing these questions and can guide the development of scientific knowledge, allowing us to gain a better understanding of the world around us (Boghossian 2006; Ladyman and Ross 2007). By providing a framework for distinguishing between justified and unjustified beliefs, assessing evidence, and evaluating scientific methods, epistemology plays a crucial role in the advancement of scientific inquiry (Kuhn 2012).

Moreover, understanding the answers to these questions is vital for comprehending how we gain knowledge about the world, evaluate the truth of our beliefs, and make decisions based on our knowledge (Sosa 1991). It is essential to develop epistemological frameworks that allow us to evaluate the reliability and accuracy of these tools and to understand the sources and criteria for knowledge in quantum chemistry (Baird and Shew 2004; Cleland 2001).

Let's now consider how epistemology relates to quantum chemistry mechanics. In quantum chemistry, epistemology is concerned with the ways in which we can understand the behavior of atoms and molecules, as well as the methods by which we can test and validate our knowledge. Quantum chemistry is a branch of chemistry that uses the principles of quantum mechanics to study the behavior of atoms and molecules (Levine, 2022). Computational chemistry involves the use of mathematical algorithms and computer simulations to model and predict the behavior of chemical systems. This approach can be used to investigate a wide range of chemical phenomena, from the properties of individual molecules to the behavior of complex materials and biological systems.

A key area for the development of computational quantum chemistry has been the use of high-performance computers computing (HPC) systems, which provide researchers with the computational power needed to perform complex simulations and calculations. Advances in HPC hardware, such as the development of parallel processing and graphics processing units (GPUs), have allowed researchers to perform simulations on an unprecedented scale, enabling the study of complex systems that were previously out of reach.

In this case, the epistemology of knowledge in quantum chemistry is heavily influenced by the mathematical nature of quantum mechanics. Mathematical equations and models are used to describe the behavior of atoms and molecules, and these models can be tested and validated through experimentation.

Within the realm of computational chemistry, discussions regarding different computational approaches have sparked debates leading to both the creation and destruction of categories. Kant's philosophical principles of unity find resonance in these discussions, particularly in the pursuit of a unified understanding of computational methods. The process of unifying diverse computational approaches initiates the creation of new categories that encompass previously disparate perspectives. However, as researchers delve deeper into these discussions, they may encounter contradictions or limitations within existing frameworks, leading to the destruction or revision of outdated categories. (Boge 2021) Through rigorous analysis and debate, the field of computational chemistry evolves, with categories being refined, merged, or discarded to better capture the complexities of computational methods. This dynamic process reflects Kant's philosophical approach, wherein the creation and destruction of categories are integral to the advancement of knowledge and understanding (Gueto et al. 2009; Mercado-Camargo 2020; Morales-Bayuelo and Vivas-Reyes 2013; Morales-Bayuelo et al. 2012; Vivas et al., 2008, 2009, 2013, 2020; Vivas-Reyes et al. 2003, 2008).

In quantum chemistry, the fundamental concept of wave-particle duality suggests that particles can exhibit wave-like behavior and vice versa. This duality can make it challenging to predict the behavior of atoms and molecules with certainty, creating obstacles for scientists seeking to understand the properties and behavior of chemical systems. Additionally, the uncertainty principle states that the more precisely the position of a particle is known, the less precisely its momentum can be known, and vice versa. This principle places limits on the precision of measurements and can have a significant impact on the accuracy of predictions made using quantum mechanical models (Cassidy 1992).

To address these challenges, Kant's philosophy of science highlights the critical importance of empirical observation and theoretical constructs in scientific modeling. Kant's perspective asserts that scientific theories are grounded in both empirical evidence and conceptual frameworks. In the realm of computational chemistry, for instance, theoretical models based on abstract concepts and mathematical formulations play a pivotal role in elucidating the behaviors of subatomic particles. Kant's philosophical approach acknowledges the inherent limitations of human cognition, shedding light on our ability to faithfully represent reality. (Kant 2003)

Kant's philosophical framework provides a systematic guide for addressing the complexities of scientific inquiry, including computational chemistry. By recognizing the symbiotic relationship between empirical observation and theoretical constructs, we gain a deeper understanding of the essence of reality within the bounds of human comprehension (phenomenon and noumenon). Furthermore, Kant's principles find tangible applications in computational chemistry, as they reveal the epistemological constraints inherent in computational methodologies. Despite these limitations, computational chemistry retains its capacity to simulate complex chemical processes and provide predictive capabilities (Kant 2003; Westphal 2003).

Kant's ideas and quantum chemistry

Since Kant's time, there has been significant progress in the field of science, shedding light on the complexities of the world around us and reaffirming some of Kant's foundational intuitions and concepts. For instance, the groundbreaking works of figures such as W. Heisenberg and K. Gödel have highlighted some of Kant's ideas, especially in the fields of quantum mechanics and mathematics. Heisenberg's uncertainty principle, a cornerstone of quantum physics, challenges the very foundations of scientific predictability, revealing the inherent limitations of the deterministic worldview of classical physics. (Heisenberg 1927) This epistemological dilemma forces us to confront the notion that perhaps our understanding of reality is fundamentally circumscribed, as framed in Kantian philosophy regarding the limits of human cognition. On the other hand, Gödel's incompleteness theorem strikes at the heart of mathematical formalism, demonstrating the inherent incompleteness of mathematics. (Gödel 1931) This profound insight underscores the intrinsic limitations of our intellectual endeavors, reminding us that even the most rigorous mathematical frameworks are subject to the limitations of human finitude.

As is widely recognized, quantum mechanics challenges our most fundamental intuitions regarding the behavior of matter, as asserted by Albert (1994). For instance, wave-particle duality contradicts our expectation that particles exist as discrete objects with well-defined properties. Although this concept may initially perplex our intuitive understanding of reality, Kant's perspective on the active role of the mind in constructing our comprehension provides a framework for interpretation. Certain interpretations of quantum mechanics propose that particles lack definite properties until observed or measured, echoing Kant's notions that the mind imposes categories and structures on our experience. The act of measurement imposes a specific category on the particle and "collapses" the wave function into a particular outcome.

Additionally, in line with the preceding discussion, N. Bohr's principle of complementarity challenges the law of excluded middle by asserting that a particle can manifest both as a particle and a wave simultaneously. This principle underscores the inherent limitation of our understanding of the world, stemming from the irreducibility of subjectivity during the act of observation, thus preventing us from attaining a wholly faithful and objective representation of reality. This acknowledgment of our finitude is reflected even in the loftiest pursuits of scientific inquiry. In this context, Kant's ideas of phenomenon and noumenon become pertinent, elucidating that our limitations cannot be rationalized as we might desire, but rather stand as fundamental aspects of our existence. Furthermore, these reflections on our subjective condition are not divorced from the practical applications of quantum physics, such as computational chemistry, and their implications (Bohr 1913, 1922; Friedman 1992)

Kant's ideas about the role of the mind in constructing our understanding of the world are relevant for making sense of the counterintuitive phenomena of quantum mechanics (Ishikawa 2011). The concept of wave-particle duality in quantum mechanics challenges our intuition that particles should exist as discrete objects with definite properties. In this framework, particles are also described as waves and may exhibit wave-like behavior under certain conditions. This can be difficult to reconcile with our everyday experience of the world, but Kant's ideas can help us understand how our minds construct our understanding of the world and how our intuition may not always align with the underlying reality.

The study of computational quantum chemistry is concerned with accurately predicting the behavior of molecules and their interactions with other molecules or electromagnetic fields. This is a significant challenge, and the field has developed methods to address this problem, including solving the Schrödinger equation, which describes the quantum mechanical behavior of the electrons and nuclei that make up the molecule (Cramer and Truhlar 1999; Parr 1989).

The pursuit of accurately predicting molecular behavior and interactions has led to significant advancements in computational chemistry. The increasing computing power and development of efficient algorithms have allowed for the application of quantum chemistry methods to larger and more complex molecules. Moreover, the field has embraced the use of artificial intelligence and machine learning techniques to enhance the accuracy of molecular predictions.

However, it is important to recognize the philosophical implications of these advancements. As we gain a deeper understanding of the quantum world, we must remain mindful of the limitations of our methods and the questions they raise about the nature of reality. Additionally, we must not lose sight of the importance of empirical observation and experimentation in the pursuit of knowledge.

Taking a holistic approach to knowledge, including empirical observation, experimentation, and theoretical modeling, we can continue to deepen our understanding of the quantum world and its complexities. The study of computational quantum chemistry is concerned with accurately predicting the behavior of molecules and their interactions with other molecules or electromagnetic fields. This is a significant challenge, and the field has developed methods to address this problem, including solving the Schrödinger equation, which describes the quantum mechanical behavior of the electrons and nuclei that make up the molecule (Cramer and Truhlar 1999; Parr 1989).

However, the solution to the Schrödinger equation gives the wave function of the molecule, which describes the probability distribution of finding the molecule in different states (Levine 2013). The wave function is a complex mathematical object that cannot be directly measured or observed. Therefore, while computational quantum chemistry provides us with valuable insight into the behavior of molecules, it is important to remain cognizant of the limitations of our methods and the philosophical implications of our finding (Schwinger 1998; Bensaude-Vincent 2014).

Understanding the behavior of matter in the quantum realm is a continuous and ongoing challenge in the field of chemistry, and it requires a deep understanding of both quantum mechanics and the role of the mind in constructing our understanding of the world. The process of making measurements in quantum mechanics has been a topic of debate and controversy among physicists for many years (Fine 1975). One interpretation of quantum mechanics suggests that the act of measurement creates a "split" in the universe, where different versions of reality exist simultaneously (Everett 1957). This idea has been challenged by many physicists who argue that it is not supported by the evidence (Bacciagaluppi and Valentini 2009).

Principio del formulario

Final del formulario

To extract useful information from the wave function, measurements or observations must be made that correspond to specific properties of the molecule, such as its energy or charge distribution (Jensen 2017). These measurements collapse the wave function into a specific state, thereby giving the molecule definite properties. This process can be understood as the mind imposing a particular category or structure on the molecule, thus conferring it with defined properties. The categories or structures imposed on the molecule depend on the measurements taken and how the results are interpreted.

For instance, consider studying the bonding properties of a molecule. Measurement of electron density distribution provides crucial insights into regions where electron density accumulates along a molecular bond. This analytical approach allows for precise discernment of the nature of the bonds present, enabling the identification of specific types such as covalent or ionic bonds (Szabo and Ostlund 2012). Such analyses are fundamental in characterizing and gaining detailed understanding of chemical interactions in molecular systems, making significant contributions to the field of theoretical and computational chemistry. However, measuring a different property of the molecule, like its magnetic moment, would lead to different conclusions about its properties. This illustrates that the categories and structures imposed on the molecule are not inherent in the molecule itself, but rather depend on the measurements and interpretations. In line with this, Kant's ideas emphasize the importance of unity in science, a notion that aligns with the reductionist concept of a unified theory in physics (Morrison 2008). However, for example, the various definitions of atomic charge intersect with Kantian categories. The ongoing process of unifying these diverse definitions resembles the philosophical endeavor of consolidating Kantian categories.

The researchers involved in this endeavor of unification theories undertake profound analyses of the relationships between all categories, aiming to discern the intricate connections among them. The philosophical approach proposed by Kant emphasizes the critical role of coherence and interaction among categories in achieving a comprehensive understanding. While Kant's categories provide a framework for comprehending the world, it is noteworthy that some aspects of Kantian philosophy can be interpreted as compatible with reductionist approaches (Champagne 2018). However, Kant's categories operate at a higher level of abstraction compared to reductionist explanations, prioritizing the examination of thought and perception structures over detailed analyses of physical or biological systems.

Kant's perspective on the mind's active role in constructing our understanding of the world can also shed light on the counterintuitive phenomena of quantum mechanics, particularly the concept of wave-particle duality (Ishikawa 2011). This idea challenges our intuition that particles should exist as discrete objects with definite properties. However, the application of computational quantum chemistry has allowed us to accurately predict the behavior of molecules and their interactions with other molecules or electromagnetic fields. This is done through solving the Schrödinger equation, which describes the quantum mechanical behavior of the electrons and nuclei that make up the molecule (Cramer and Truhlar 1999; Parr 1989).

Nevertheless, we must not forget the philosophical implications of these advancements. As we gain a deeper understanding of the quantum world, we must remain mindful of the limitations of our methods and the questions they raise about the nature of reality. The use of empirical observation and experimentation is still essential in the pursuit of knowledge, even as we embrace the use of artificial intelligence and machine learning techniques to enhance the accuracy of molecular predictions.

The connection between computational quantum chemistry and Kantian philosophy runs deep, revealing how our understanding of reality is shaped by our cognitive structures and interactions with the world around us. Kant's ideas suggest that our minds impose certain categories and structures on our sensory experience to make it intelligible, and this notion has significant implications in the field of quantum mechanics. In this realm, the act of measurement or observation plays a crucial role in shaping our understanding of reality, as it collapses the wave function into a specific outcome. This can be seen as the mind imposing a particular category or structure on the particle, which emphasizes the importance of the observer in scientific inquiry.

Moreover, other philosophers in the field of the philosophy of chemistry, such as Jaap van Brakel, have highlighted the need to understand chemical phenomena as emergent and non-reducible to physical laws. This perspective acknowledges the complexity of chemical systems and emphasizes the importance of studying chemical phenomena at different levels of organization. Therefore, while computational quantum chemistry offers significant advancements in understanding the behavior of molecules, it is important to recognize the philosophical implications of these advancements and approach knowledge holistically.

In taking a holistic approach to knowledge, including empirical observation, experimentation, and theoretical modeling, we can deepen our understanding of the quantum world and its complexities while remaining mindful of the philosophical implications of our advancements. By considering the role of the observer in scientific inquiry and recognizing the limitations of our knowledge and understanding, we can develop a more comprehensive understanding of the world around us. Ultimately, the connection between computational quantum chemistry and Kantian philosophy highlights the importance of interdisciplinary thinking and the need to approach scientific inquiry from a multi-dimensional perspective.

Although is not central to the main discussion, the author of this article believes that computational chemistry has been successful not only due to its various contributions, both practical and theoretical. This success could also be seen from another perspective. Computational chemistry applications have allowed chemistry to be approached in a more mathematizable manner, reflecting to some extent Kant's initial thoughts when he argued that chemistry could not be considered a science in the same sense as physics in his early writings, due to its lack of mathematization. Computational quantum chemistry seems to fulfill that role today.

Conclusions

A comprehensive understanding of epistemology, philosophy, and technology is crucial for evaluating scientific claims and advancing our knowledge in computational chemistry. Epistemology plays a critical role in evaluating claims to knowledge and assessing the reliability of scientific methods, particularly in the field of quantum chemistry. It is concerned with how we can know about the behavior of atoms and molecules, as well as how we can test and validate our knowledge. The mathematical nature of quantum mechanics heavily influences the epistemology of knowledge in this field, challenging our intuition about the behavior of matter and requiring us to think critically about the nature of scientific knowledge. Kant's philosophy of science can help frame debates and discussions in quantum chemistry, particularly regarding the relationship between empirical observation and theory.

In addition, the use of AI and ML techniques has led to significant advancements in computational chemistry, enabling researchers to design new materials and drugs and gain a deeper understanding of the fundamental properties of matter. However, we must be mindful of the limitations and potential biases of these techniques, and the importance of human interpretation and critical thinking in evaluating scientific claims.

Other philosophers of chemistry, such as Van Brakel and E. Scerri, have emphasized the importance of ontology in understanding chemical phenomena. Ontology concerns the nature of being and existence, and in chemistry, it is concerned with the nature of chemical entities, their properties, and their relationships. By examining the ontological status of chemical entities, we can gain a deeper understanding of their behavior and interactions. (Scerri 2000, 2004, 2011, 2015, 2019, 2022a, b; Van Brakel 2000; Van Fraassen 1980).

To understand computational quantum chemistry and advance our knowledge in this field, a comprehensive understanding of epistemology, philosophy, and technology, including ontological considerations, is essential. This will help us address the pressing challenges in computational chemistry and make further progress in this important area of scientific research. (Rosenfeld 2004)

Funding Open Access funding provided by Colombia Consortium

References

Albert, D.Z.: Quantum Mechanics and Experience. Harvard University Press (1994)

Bacciagaluppi, G., Valentini, A.: Quantum Theory at the Crossroads: Reconsidering the 1927 Solvay Conference. Cambridge University Press. (2009)

Baird, D., Shew, A.: Probing the history of scanning tunneling Microscopy. In: Baird, D., Nordmann, A., Schummer, J. (eds.) Discovering the Nanoscale, pp. 145–156. IOS (2004)

Bensaude-Vincent, B.: Philosophy of Chemistry or Philosophy with Chemistry? HYLE–International J. Philos. Chem. **20**(1), 58–76 (2014)

Boge, F.J.: Quantum reality: A pragmaticized neo-kantian approach. Stud. History Philos. Sci. Part. A. **87**, 101–113 (2021)

Boghossian, P.: Fear of Knowledge: Against Relativism and Constructivism. Oxford University Press (2006)

Bohr, N.: Phil. Mag. **26**(151), 1–25 (1913)

Bohr, N.: The Theory of Spectra and Atomic Constitution. Cambridge University Press (1922)

Cassidy, D.C.: Uncertainty, the Life and Science of Werner Heisenberg. Freeman, New York (1992)

Champagne, M.: Kantian Schemata: A critique consistent with the Critique. Philosophical Investigations. **41**, 10–11 (2018)

Cleland, C.E.: Historical science, experimental science, and the scientific method. Geology. **29**(11), 987–990 (2001)

Cramer, C.J., Truhlar, D.G.: Implicit solvation models: Equilibria, structure, Spectra, and Dynamics. Chem. Rev. **99**(8), 2161–2200 (1999)
Everett, H.: Relative state formulation of quantum mechanics. Rev. Mod. Phys. **29**(3), 454 (1957)
Fine, A.: The Shaky Game: Einstein, Realism, and the Quantum Theory. University of Chicago Press (1975)
Friedman, M.: Causal laws and foundations of Natural Science. In: Guyer, P. (ed.) Cambridge Companion to Kant, pp. 161–199. Cambridge University Press, Cambridge (1992)
Gödel, K.: Über formal unentscheidbare Sätze Der Principia Mathematica und verwandter Systeme, I. Monatshefte für Math. und Physik. **38**, 173–198 (1931)
Gueto, C., Torres, J., Vivas-Reyes, R.: CoMFA, Leap Frog and blind docking studies on sulfonanilide derivatives acting as selective aromatase expression regulators. Eur. J. Med. Chem. **44**(9), 3445–3451 (2009)
Hacking, I.: Representing and Intervening: Introductory Topics in the Philosophy of Natural Science. Cambridge University Press (1983)
Heisenberg, W.: Über den anschaulichen Inhalt Der Quantentheoretischen Kinematik Und Mechanik. Z. für Physik. **43**(3), 172–198 (1927)
Hendry, R.F., Needham, P.: Philosophy of Chemistry: Synthesis of a new Discipline. Springer, Dordrecht, Netherlands (2014)
Ishikawa, S.: A New Interpretation of Quantum mechanics. J. Quantum Inform. Sci. **1**(2), 35–42 (2011)
Jensen, F.: Introduction to Computational Chemistry. Wiley (2017)
Kant, I.: Critique of Pure Reason. Cambridge University Press (2003)
Kuhn, T.S.: The Structure of Scientific Revolutions. University of Chicago Press (2012)
Ladyman, J., Ross, D.: Everything must go: Metaphysics Naturalized. Oxford University Press (2007)
Levine, I.N.: Quantum Chemistry. Prentice Hall (2013)
Morales-Bayuelo, A., Torres, J., Vivas-Reyes, R. H?ckel treatment of pyrrole and pentalene as a function of cyclopentadienyl using local quantum similarity index (LQSI) and the topo-geometrical superposition approach (TGSA). J. Theo. Comput. Chem. **11**(01), 223–239 (2012)
Mercado-Camargo, J., et al.: Homology modeling of Leishmanolysin (gp63) from Leishmania panamensis and molecular docking of flavonoids. ACS Omega. **5**(24), 14741–14749 (2020)
Morales-Bayuelo, A., Vivas-Reyes, R.: Theoretical model for the polarization molecular and Hückel treatment of PhosphoCyclopentadiene in an external electric field: Hirschfeld study. J. Math. Chem. **51**, 1835–1852 (2013)
Morales-Bayuelo, A., Vivas-Reyes, R., et al.: Is quantum chemistry a new science? Teknos Revista científica. **20**(1), 17–22 (2020)
Morrison, M.: Reduction, Unity and the Nature of Science: Kant's Legacy? vol. 63, pp. 37–62. Royal Institute of Philosophy Supplement (2008)
Parr, R.G.: Density-functional Theory of Atoms and Molecules. Oxford University Press (1989)
Rosenfeld, S., Bhushan, N.: How Ab Initio is Ab Initio Quantum Chemistry? Found. Chem. **6**, 93–116 (2004)
Scerri, E.: The new philosophy of chemistry and its relevance to chemical education. Sci. Educ. **9**(1–2), 21–36 (2000)
Scerri, E.: How Ab Initio is Ab Initio Quantum Chemistry? Found. Chem. **6**, 93–116 (2004)
Scerri, E.R.: The Philosophy of Molecular Chemistry. Palgrave Macmillan (2011)
Scerri, E.: The discovery of the periodic table as a case of simultaneous discovery. Philos Trans. A Math. Phys. Eng. Sci. **373**(2037), 20140172 (2015). https://doi.org/10.1098/rsta.2014.0172
Scerri, E.R.: Five ideas in chemical education that must die. Found. Chem. **21**(1), 5–13 (2019)
Scerri, E.R.: Praise of triads. Found. Chem. **24**(2), 285–300 (2022a)
Scerri, E.R.: Hasok Chang on the nature of acids. Found. Chem. **24**(2), 389–404 (2022b)
Scerri, E., McIntyre, L. (eds.): Philosophy of Chemistry: Growth of a New Discipline. Springer (2014)
Schwinger, J.: Quantum Mechanics: Symbolism of Atomic Measurements. Springer (1998)
Sosa, E.: Knowledge in Perspective: Selected Essays in Epistemology. Cambridge University Press (1991)
Szabo, A., Ostlund, N.S.: Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory. Dover (2012)
Torretti, R.: HASOK CHANG. 2012. Is Water H2O? Evidence, Realism and Pluralism. Dordrecht: Springer. THEORIA. Revista de Teoría, Historia y Fundamentos de la Ciencia, 28(2), 331–334. (2013)
Van Brakel, J.: Philosophy of Chemistry: Between the Manifest and the Scientific Image. Leuven University (2000)
Van Fraassen, B.C.: The Scientific Image. Clarendon, Oxford, UK (1980)

Vivas-Reyes, R., et al.: A DFT study of tin-and crown-ether-based host molecules capable of binding anions and cations simultaneously. Eur. J. Inorg. Chem. **20037**, 1315–1324 (2003)
Vivas-Reyes, R., et al.: Theoretical study to evaluate polyfuran electrical conductivity and methylamine, methoxy substituent effects. J. Mol. Struct. (Thoechem). **861**(1–3), 137–141 (2008)
Westphal, K.R.: Kant's transcendental proof of realism. Cambridge University Press (2003)