ABSTRACTS

KEYNOTE LECTURES

The 150th anniversary of Mendeleev’s 1869 article and the work of some lesser known contributors to this discovery

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In a recent book I have argued that science is a unified and collective enterprise [1]. This is not a reference to modern Big Science but a claim for an underlying and organic unity in the development of science. Scientists are correctly seen as competing against each other and there is no denying that such competition serves to advance the growth of science. However, from the point of view of the proposed unified development of science, priority disputes and the need to identify one or other discoverer for any scientific development becomes somewhat futile.

This year we celebrate the 150th anniversary of the discovery of publication of Mendeleev’s first article on chemical periodicity [2]. While conceding that everybody enjoys celebrations and that they serve a worthwhile purpose, this should not detract from the contributions of lesser known contributors. The lecture will involve a review of lesser known precursors to the discovery of chemical periodicity by the likes of Gladstone, Gibbs, Gibbes, Carey Lea, Mercer and others [3].

In addition I will report on some new findings concerning the work of Lothar Meyer, who is generally acknowledged as being Mendeleev’s closest competitor [4]. The aim is not to rehabilitate Meyer and other early contributors but rather to highlight the gradual, and I claim ‘organic’ evolution in the history of ideas concerning the periodic classification of the elements.

[1] E.R. Scerri, *A Tale of Seven Scientists and A New Philosophy of Science,* OUP, New York, 2016.

[2] E.R. Scerri, *The Periodic Table, Its Story and Its Significance*, OUP, New York, 2007;
J.W. Van Spronsen, *The Periodic System of Chemical Elements. A History of the First Hundred Years,* Elsevier, New York, 1969.

[3] G.B. Kauffman, *Journal of Chemical Education,* 46, 128-135, 1969

[4] A. Rocke, Lothar Meyer’s path to periodicity, unpublished paper, submitted for History of Chemistry Conference in Maastricht, 2019.

Ethics of Chemistry

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While philosophy of chemistry is emerging as an independent field of research, ethics, one of the oldest subdisciplines of philosophy, has rarely been applied to chemistry. Public views of chemistry still follow traditional, largely negative stereotypes, often with strong moral judgments, to which chemists have frequently responded by hiding their identity and relabeling their work as “molecular science”, “life sciences”, “materials science”, “nanotechnology”, etc. More recently, some chemists have engaged in developing concepts of “ethics in chemistry”, including the writing of “ethics codes”. They thereby refer, probably by the lack of professional ethicists involved, to the colloquial meaning of “ethics”, the internal rules of behavior within a community. In contrast, ethics, in the academic sense, means the research into the justification of moral rules, values, and virtues that are ideally undisputable on general grounds. In the latter sense, “ethics of chemistry” develops moral guidelines for chemistry that can be derived from, or at least harmonize with, general ethical principles or theories. Only “ethics of chemistry”, rather than “ethics in chemistry”, can harmonize chemical conduct with general morality,

This paper investigates ethical guidelines for chemists on a very general level, in order to provide a framework for further ethical research. Starting from the undisputable moral duty of doing good and the general ethical principle of impartiality, I distinguish between three cases: (1) doing good by not doing harm, (2) doing good by preventing harm, and (3) doing good by improvements, which are each illustrated by examples from the history of chemistry. Chemists have primarily acknowledged (3), which is difficult to achieve, however, because of adverse consequences and disputes on what counts as improvement, whereas (1) and (2) are perhaps more important and uncontroversial but less acknowledged.

In conclusion I argue for the need of ethics courses to be included in chemistry curricula, and suggest a case study approach tailored specifically to chemistry students that I have developed together with Tom Boersen and a large international team of authors [1].

[1] Børsen, T. & Schummer, J. (2016-2019): Ethical Case Studies of Chemistry (A series of special issues of Hyle: International Journal for Philosophy of Chemistry), available online at http://www.hyle.org/journal/issues/special/ethical-cases.html.

Wastes 4.0. Perceptual Alterations of Space and Time

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Living in today's disfigured environment, where nature is but a fragment of an ancient beauty and richness, means living in a global allegory, where humans are forced to dwell in a lunar landscape – a *locus* of rotting trash, made up of all our discarded technological gadgets, where everything is swiftly reduced to "kipple" and "gubble" (P.K. Dick). Because of a strange consumerist schizophrenia, the material universe of waste appears akin to metaphysical evil in the Platonic model: completely disengaged from the immaterial benefits brought by technology (connection speed, ergonomics of smart devices, etc.). To put an end to this strabismus, we need to fully investigate the new 4.0 e-wastes and expose their ontological and circumstantial structure, which deeply affects our concept of space (in terms of geopolitics) and of time (as for the durability of our sensations of wellness).

Primo Levi's Primary Elements

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The International Primo Levi Studies Center (Centro Internazionale di Studi Primo Levi) was founded in April 2008 and is dedicated to acquainting people with Primo Levi. The center is located in Turin, where Primo Levi lived from 1919 to 1987. It aims at collecting the various editions of his works, their translations from all around the world, their critical bibliography and all kinds of written and audiovisual documentation on his figure and on the impact on several disciplinary fields, like chemistry, psychology, philology, etc. It also aims at supporting scholarly research and promoting initiatives aimed at fostering discussions on Levi's favourite topics.

Science, especially chemistry, played a very important role in Primo Levi's life and works. What he loved about chemistry, was its objective method for studying nature as well as its abundance of investigation tools for the world and life itself. To be a chemist also meant to Levi to be able using the extraordinary resources that chemistry made available to him to put order into his memories. Levi never made clear-cut distinctions between his being a writer and a chemist. Indeed, he always stressed the fact that his scientific education offered him original points of view and extraordinary original tools for his job as a writer.

Levi's view of the world has always been influenced by science, which left a profound mark upon his whole work. The International Primo Levi Studies Center strives to develop such interest by involving scholars and researchers from different countries and disciplines (both scientific and humanistic) in its activities.

During this first decade of activity the Center organized several events, many of which were related to science. Every year the Center promotes a *Primo Levi Lecture* closely tied with Levi's experiences and interests; this lecture also encompasses broader perspectives. On the occasion of the ESOF 2010 meeting in Torino, the Center presented *The Mark of the Chemist: A Dialogue with Primo Levi*, a dramatic reading of Levi's scientific writings, based on a selection of texts edited and assembled by Domenico Scarpa, literary critic at the University of Pisa (Italy). This reading was also performed at the Museum of Jewish Heritage in New York. In 2013 the Center and Einaudi (Levi's publishing company) published a limited edition (400 numbered copies) of the *Rapporto sulla organizzazione igienico-sanitaria del campo di concentramento per Ebrei di Monowitz (Auschwitz-Alta Slesia) (Report on the sanitary conditions at the Monowitz concentration camp),* written by Primo Levi and Leonardo De Benedetti in 1945. In 2014 five events where science met literature were promoted, starting off from *Vizio di Forma (Flaw of Form)*, Primo Levi's least known work, a surprising collection of technological fiction stories. Year 2015 saw the realisation of the exhibition "*The worlds of Primo Levi - A strenuous clarity*", organised in six sections aimed at illustrating Levi's multifaceted personality through images and words. More recently *Opere complete* (*The Complete Works)* of Primo Levi have been published by Einaudi: they consist of three volumes gathering all fourteen Levi's books with his interviews. Our efforts are now concentrated in building the index of notable terms related to science throughout Levi's whole opus. The outcomes of this work-in-progress will be soon presented on the Center web site. At present, we have mapped the terms more closely related to Levi's scientific world, starting from the two editions of *If This is a Man*, maybe the less scientific book by Primo Levi that reports his testimony of the *Shoah*. We are now extending this search to his whole literary work. It is a distinguishing way of studying Primo Levi's writings, that gives relevance to the scientific world through his precise use of words. We maintain that it will be a useful tool to students and researchers who aim at acquiring a comprehensive and deeper knowledge about this great man and writer.

Il segno del chimico. Conversazione con Primo Levi, a cura di Domenico Scarpa, Einaudi, Torino 2010, edizione fuori commercio.

Rapporto sulla organizzazione igienico-sanitaria del campo di concentramento per Ebrei di Monowitz (Auschwitz - Alta Slesia), Leonardo De Benedetti e Primo Levi, in «Minerva Medica», XXXVII (24 novembre 1946), n. 47, pp. 535-44; ora in *Primo Levi con Leonardo De Benedetti, Così fu Auschwitz*. Testimonianze 1945-1986, a cura di Fabio Levi e Domenico Scarpa, Einaudi, Torino 2015.

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ORAL PRESENTATIONS

How iconic can be a chemical symbol? A brief semiotic analysis of the images in the lectures of August von Hoffman

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Tensions and confluences between the symbolic and the iconic are widely recorded in the literature, both from theoretical frameworks in semiotics (Merrell, 1997) and in philosophy of chemistry (Harré, 2014). The aim of this paper is to present a brief semiotic analysis of Hoffman's "squares", taken from the period of the German chemist in England. The methodology considers the semiotics of Charles Peirce. Hoffman was neither the first nor the only to use squares to represent atomic volumes. However, its form of use is endowed with an expressive mode that (re) places the mysterious scenario around representative processes in the chemistry of the nineteenth century. For Peirce, the icon is a sign that is inscribed in the conditions of a first, an initial formulation that manifests itself in having aspects of similarity with the object to which it refers. The Symbol in turn is a third, a sign that denotes its object through a legal process, an agreement, a convention or even an arbitrariness situated in a given cultural context. Hoffman's pictorial signs are in an increasing order of complexity, referring to the increase in valence of the central atom, pictured from hydrides: hydrogen chloride, water and ammonia. In water and ammonia the oxygen and nitrogen elements occupy central positions and share segments of the edges of the squares that delimit them. We consider this diagrammatic process of representation as a hatching of hypoiconic forms. For Peirce, "hypoicons may be roughly divided according to the mode of firstness of which they partake. Those which partake of simple qualities, are images; those which represent the relations or so regarded, of the parts of one thing by analogous relations in their own parts, are diagrams; those which represent the representative character of a representing by representing to parallelism in something else, are metaphors " (Peirce, 1998). We argue that there is a relevant cultural inscription that organizes this representative process in chemistry, that is, teaching. Supported by teaching interests there is a region of "freedom" to represent it, where transition between iconic and symbolic is more liquid, with less ties to those found in academic pretensions.

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Nanotechnology as a Type of Hermeneutic Technics: Phenomenological Epistemology and the Manipulation of Nanomaterials

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At the World Summit on Sustainable Development, which was held in August 2002 in Johannesburg, an organization called ETC Group (Erosion, Technology, and Concentration) called for a moratorium on the environmental release and commercial use of nanomaterials. They called for a ban on self-assembling nanomaterials and for a ban on patents for nanoscale technologies. The reason given by ETC Group for this concerns the long-term and, perhaps, irreversible damage that can be caused by releasing engineered nanomaterials into the environment, whether for commercial, medical, or other purposes. A 2004 report commissioned by the European Parliament also recommended that engineered nanoparticles should not be released into the environment. However, concern over the safety of nanomaterials is not limited to their impact on the environment since, due to some of their size-dependent unique properties, nanomaterials are also being used in biomedicine and in a multitude of consumer products. In addition to being concerned over the safety of these materials once they are taken into the world outside of the laboratory in which they are manufactured, one must also be concerned about their safety of handling nanomaterials for the chemical engineers who manipulate them in the laboratory. The ability to handle nanomaterials safely in the laboratory depends upon the ability to control these materials and control depends upon having epistemic access to these materials.

Although quite a bit has been written by philosophers of chemistry about the ontology of nanomaterials, this paper proposes to address the question of epistemic access to nanomaterials. This question will be addressed from the perspective of the phenomenology of technology, since this approach can provide important insights regarding nanotechnology's ability to yield transparent epistemic access to nanomaterials. In fact, I will argue that nanotechnology lends itself to the same sort of phenomenological analysis as other technologies (such as nuclear reactors) in which direct epistemic access to the product of the technology is not possible due to the nature and/or features of that product. To argue this point, I will consider what philosophers of chemistry have proposed regarding the ontology of nanomaterials, since ontological questions affect whether or not transparent epistemic access to nanomaterials is possible at all. I will conclude that, in the case of nanotechnology, direct epistemic access is not possible because of the extremely small scale of nanomaterials, which must therefore be engineered and handled via mediating devices.

I will argue that this 'mediated access' creates a relation between the chemical engineer and the engineered nanomaterials that requires the chemical engineer to infer what is happening at the nanoscale by interpreting the information provided by mediating devices. Because of this interpretive inference, the epistemic relation between the engineer and the engineered product is referred to as a 'hermeneutic intentionality relation'. However, the indirect and interpretive nature of this epistemic relation increases the probability of 'misreading' what is occurring at the nanoscale and of unintended exposure to the nanomaterials being manipulated. Due to the nature of the technology and of the engineered materials, the problem of indirect epistemic access and of possible misinterpretation are problems that are inherent to nanotechnology itself and that persists regardless of how the methods for handling nanoproducts are modified. This analysis will conclude that, from the standpoint of safety, there are serious reasons for concern regarding nanotechnology due to the toxicological and environmental effects that may result from accidental direct or indirect exposure to nanomaterials. These concerns stem from the fact that, among other things, the phenomenological limits of the epistemic access is endemic to nanotechnology itself.

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The electrolysis of water and its implications about pluralism in chemistry

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While some recent work about this topic presents the history of the electrolysis of water as commencing in 1800, this is not the case: the first major paper on the subject was published in 1789.

Van Troostwyck and Deiman (1789) rightly commented on what was still wanting for the experiments which had led to Lavoisier's theory of water to be absolutely decisive: this was an analysis of water which produced both gases at once. They proposed that they could now do this by electrolysis. However, their gases were not produced separately, so their work was not yet decisive. Nicholson and Carlisle (1800) managed to partly separate the gases, and Cruickshank (1800b) took this process further. Davy (1800) managed to produce the gases separately and without impurities, using well-boiled water. Davy (1807) completed the process by showing exhaustively that all proposed constituents of water other than oxygen and hydrogen were impurities. This whole composite process produced an unprecedentedly clear confirmation of Lavoisier's chemistry.

The discovery of the attraction of oxygen and hydrogen to different and separated electrodes by Nicholson and Carlisle (1800) occurred in parallel with this process of confirmation. This gave rise to a "multitude of imaginary hypotheses" (Grotthus 1806). Grotthus proposed a model by which a chain of decomposing and recomposing molecules in the water produced the effect of the appearance of one type of air at each electrode. This proposal was not the same as that of Davy (1807). Davy's experiments had shown that materials were actually passing through water, or what was connecting the water around each of the two poles. Davy was rightly agnostic about the detail of what was happening during the transfer, due to the limits of experimental capability at the time. This was the most accurate answer that was then practicable. Davy noted that nevertheless this seemed to invalidate the conjectures of Ritter.

Cavendish's (1784) phlogistic theory had been abandoned by him by early 1787, both because it was inconsistent, and because his view of nitrous acid was shown to be inaccurate by his own (1785) experiment, as he (1788) accepted. In a roughly similar way, Ritter's theory (e.g. Ritter 1800, Babington 1801) about the elementary nature of water led to inconsistent views of oxygen, when any attempt was made to extend the theory to the decomposition of other materials, as Berzelius and Donovan pointed out, and was thus seen by these authors as being clearly unworkable.

Accordingly, this paper argues that the early history of the electrolysis of water affords no support for the normative ideology that the practice of chemistry should always involve pluralism.

Philosophical Foundations of Chemistry from a Quantum Thermodynamic Engineering Perspective

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In both our philosophical and scientific conception of reality and our place in it, chemistry is in the cat-bird seat, between physics and biology. Chemistry goes beyond Newtonian point-mass physics with the introduction of qualitatively distinguishable substances, material systems with shape, volume and internal energy. Mechanical representations of chemistry are ‘useful’, but the thermodynamic nature of the chemical bond and the evolution of chemical systems transcends (viz. is not reducible to) reversible, mechanical physics.

Evolutionary biologist, Lane (2015), insists that the metabolic behaviour of biological systems ‘transcends’ chemistry and physics (viz. transcends the ‘mechanistic representations’). The new origin of life research program views evolution as a recursively enabling, chemical metabolic process (Russell, Martin, 1999). To understand the behaviour of biological systems one needs a post-mechanical framework, per hypothesis – a thermodynamic framework.

Quantum chemistry emerged with Pauling’s 1925 post-doc year with Bohr and Heisenberg. Yet in 1992 Pauling is still defending against a plethora of misunderstandings he traces to quantum theory. In quantum theory (Bohr, Pauli) Newtonian and Maxwellian mechanics are idealized special cases. Smolin (2010) notes it has become ‘rather Kafkaesque’ that we have made no progress at all in understanding quantum (chemical) reality. The particle-wave representations have obscured the original energy-time complementarity in Planck’s black body research. Planck’s research was an engineering thermodynamic research project, funded by the German electric light industry. Quantum theory is more properly understood as a post-mechanical, thermodynamic theory.

Atkins (1997) notes two historical paths to modern thermodynamics: Carnot’s engineering formulation concerned with power and efficiency, and the Clausius-Boltzmann mechanical formulations. Atkins emphasizes that both formulations are alive and well in the modern milieu, despite being incommensurable. Carroll (2014) argues, that the mechanical representations of thermodynamics have never made sense. Loschmidt was correct, and Boltzmann fails to account for any increases in entropy and the arrow of time. Per hypothesis, engineering thermodynamics is the more general formulation of post-mechanical thermodynamics, subsuming and superseding all possible mechanical formulations as special cases.

The link between engineering thermodynamics and quantum chemistry is surprising– until you see it. Planck saw the link between his quantum of action and Maupertuis’s dualistic, post-mechanical Principle of Least Action (PLA). Maupertuis’s conjugates of action (viz. complementarity) influenced Lazare and Sadi Carnot (Gillispie, 2016) in their engineering thermodynamics. Bugliarello argues modern engineers should be taught that they are natural extensions of the proper narrative understanding of biological evolution. Like Lane and Bugliarello, Lazare insisted that the behaviour and evolution of engineers and engineering practice transcends ‘rational, axiomatizable mechanics’.

Per hypothesis, the structures, functions and evolution of all physical, chemical, biological and engineering systems transcend all possible mechanical accounts. They are better understood in terms of an experimental, exploratory, constructive engineering thermodynamic enterprise.

The philosophy of chemistry and the foundations of chemistry should be based on quantum theory – a quantum theory understood in terms of engineering thermodynamics. Only with the transition to a better understanding of quantum theory will the misunderstandings of quantum chemistry encountered by Pauling (1992) be overcome.

Epistemology in Context: a Linguistic Approach to Primo Levi's *Periodic Table*

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The critical and historical literature devoted to Primo Levi is immense (Scarpa 2019). The universal character of Levi's writings is particularly evidenced by the translations of his works in (at least) 41 different languages (Levi and Soave, 2011). Among these translations, those of *Il sistema periodico* in 18 different languages stand out; this is somehow surprising as this text is difficult to be classified as a literary genre (Moiroux 2003, Thomson 2012). Two English translations of *Il sistema periodico* are currently available, whose (improper) title is *The Periodic Table* (Levi 1984, Levi 2015). In this communication we will refer to the text of Raymond Rosenthal’s translation (Levi 1984) and will designate it with the title’s initials “PT”.

Even the academic chemical community has paid some attention to PT (e.g. Hoveyda 2004), and has been inspired by it (Ghibaudi and Cerruti 2017). According to Domenico Scarpa, the fundamental idea beneath the writing of PT was "the welding of Levi's two inspirations, private, autobiographical memory [...] and the experience of work" (Scarpa 2015, p.285). |Work| is a key word in Primo Levi’s thought (Cerruti 2007), and Levi’s work as industrial chemist is the main character in the narrative of the PT. Hence, the text of PT offers a broad landscape of Levi’s epistemology, that has been barely explored (Cerruti 2018).

The linguistic approach concerns some passages of PT where the text deals with qualitative analysis, quantitative analysis, macro/micro realities, models used by chemists, meta-epistemological comparison between chemistry and physics, laboratory procedures. The linguistic analysis led us to the noteworthy conclusion that Levi’s epistemology is an existentialist epistemology (Richardson 1986, Cannon 1996). Not without emphasis, Anoop Gupta wrote: "The ground of our knowing, where our spade turns, is our bloody lives" (Gupta 1996, p.101).

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Organic Mathematics. Atomic Numbers as the Natural Pre-order for Integer Applications of Peirce-Tarski-Lesniewski Logics to Natural Sorts and Kinds

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Chemical elements form the base for atomic physics. Atoms can be decomposed into subatomic parts and composed into molecules, cells, and the vast arrays of natural sorts and kinds. Astoundingly, the exact mathematical order of counting is manifested in physical data, from the *geometrically* construction of Rutherford and Moseley. Amazingly, arithmetic operations on the atomic numbers (addition and subtraction, multiplication and division, and exponentiation and roots) are used to compose and decompose all relations of natural sorts and kinds. These facts suggest that the Table of Elements form a natural logical pre-order for mathematics. The chemist/philosopher C. S. Peirce (1839-1913) attempted to use organic chemistry as the bedrock for his inquiries into scientific logic (MS (R) 300, 1908) of existential graphs but was not able complete his argument. ((MS (R) 300, 1908, see D. D. Roberts, 1973). Here, by differentiating between the notations used for mathematics, physics, chemistry and genetics, and integrating over the primitive notions of C. S. Peirce (relative logics), A. Tarski (meta-logics), S. Lesniewski (part-whole relations), a sketch of diagrammatic propositional reasoning is constructed from the atomic numbers and perplex mathematical graph theory.

Earlier work has established portions of the argument necessary for the logics of organic mathematics. Mathematically, the atomic numbers were mapped to a bipolar form of graph theory by Coulombic relations (Chandler, 2009). In “Introduction to Chemical Information Theory” (Chandler, 2017), I proposed eleven arguments that support the proposition that atomic numbers are universal units for the logics, quantities, grammars and relations among natural sorts and kinds.

In this talk, I introduce a systematic approach (within organic mathematics) to compose concepts to extend the logic of the “perplex number spine” from scientific notation to scientific notation. First, the relations between perplex integers and quantum theory are formed by abductively and mereologically diagramming the structural graphs of attractive and repulsive Coulombic forces necessary to form a generalized Schrodinger equation. Identities are formed by satisfying a series of abductive propositions that constrain adjacency relations among parts. Secondly, the empirical scientific notations for natural sorts and kinds are composed by associating diagrams for perplex integers heteropathically. The associative propositions uniquely bind the notational terms of Tarskian meta-logics and meta-languages to the Lesniewskian part-whole anatomies. Thus, the anatomical scope of notational terms is mapped to the scales of the parts. The perplex propositions require both copula and predicates to generate sentences that satisfy the notational constraints on relationships.

In summary, compositions of atomic numbers, constrained by Coulombic relations, generate mathematical objects that scale with the notations of the natural sciences, the logical diagrams of natural categories and the scope of natural language descriptions. The theory of parallelism of logical, arithmetical, and diagrammatical representations of natural sorts and kinds opens the possibility for rigorous testing of structural theories of origins, emergences and evolutions of natural sorts and kinds.

The four ways of reasoning within Chemistry: Mendeleev's building his table, chemist's multiverse logical habit and a specific geometry

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In history of science the study-case of Mendeleev's building his Table is exceptional since he reported on the ways of reasoning that he applied [1]. I analyse his report by means of a structure of four ways of reasoning (= WoRs) which I abstracted from various fields of investigation: *i*) the four inference processes theorized and practised by the chemical-physicist C.S. Peirce (incapacities, induction, abduction, deduction), *ii*) the four prime principles of the main physical theories (limitation, extremants, existence of a mathematical object, causality) and *iii*) the four kinds of calculations of Computability Theory (undecidabilities, minimalization, oracle and recursion) [2]. I show that Mendeleev made use of all WoRs [3]; no other scientist building a theory did the same.

At present, Chemistry includes several theories. I establish a correspondence between each of the four WoRs and each of the following four theories: Classical Chemistry, Kinetic Chemistry, Physical-Chemistry and Quantum Chemistry [4]. Each of these theories suggests a WoR on experimental facts which does not exclude the Wors by the others, as instead each physical theory does. This feature of Chemistry appears as its most relevant characteristic with respect to Physics. Thus, whereas physicist's habit of reasoning within a specific theory is to apply mainly a prime principle of reasoning, the habit of a chemist is to apply, as an apparent continuation of Mendeleev's habit of reasoning, all together the representative WoRs of the four main chemical theories. After a century of its birth, at present this logical habit is shared by a theorist of Computability Theory.

While the four WoRs are instantiated by specific mathematical techniques within Chemistry Physics and Computability Theory, their instantiations in Chemistry by means of specific geometries are unknown, notwithstanding the great variety of graphic representations of Mendeleev's table [5]. Rouvray reduced them to four types [6]; which *grosso modo* correspond to the four kinds of geometries recognised by Poincaré as basic (Hyperbolic, Minkowskian, Elliptic and Euclidean) [7]. Arguments based on WoRs are offered for connecting classical Chemistry to those graphic representations of Mendeleev's table which Shemishin classed under the type "Hyperboloid" [8]. Each of them represents both matter and anti-matter without any neutral element. When projected on a plane these representations are all spirals, which Imyanitov claims represent the fundamental ones [9].

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Towards an own ontology for quantum chemistry

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According to Quantum Mechanics the Wave Function (WF) of a molecule is a function in a space of 3N dimensions, where N is the number of particles. This is problem in the philosophy of physics because the WF represents the state of the system. This led some philosophers (Albert 2013) to affirm that the real physical space has actually 3N dimensions. However, this issue does not appear in philosophy of chemistry. The reason is that chemists use the so called orbital approximation (OA), which allows us to write the total WF as a product of mono-electron wave functions (Atkins and de Paula 2006). Under this approximation, the wave function of a given electron evolves in the space of 3 dimensions (Lowe and Peterson 2006).

Our goal is to contribute to the ontology of quantum chemistry on the basis of the analysis of how the OA is used in the chemistry. The name OA suggest that this strategy is a mere approximation. As such, they should be only formal tools designed to obtain approximate solutions of an equation that cannot be solved with complete precision (Norton 2012): they are not even endowed with the novel semantic import carried by idealizations (Frigg and Hartmann 2017). If the practical or formal obstacles to obtain the exact solution were overcome, the approximation could be removed. We will argue that the above characterizations do not apply to the OA. The idea that each electron can be described by its three-dimensional WF is at the very core of the discipline and shapes the quantum-chemical picture of the molecule: a structure given by the geometrical disposition of the nuclei, and with electrons that can be conceived as individuals that “occupy” the orbitals, identified by the wave functions of the hydrogen atom (1s, 2s, etc.). The OA ignores the interaction between the electrons. But even when the interactions are reintroduced, the global wave function of 3N-dimensions is not recovered: the target is still described in terms of monoelectronic wave functions. This quantum chemical picture also plays an essential role in the explanations of the processes that occur in atoms and molecules. We will conclude that the OA offers a clear understanding of many molecular phenomena, and it is at the basis of a conceptual framework specific of quantum chemistry.

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Logic, Formal Languages, Conceptual Analysis and Chemistry

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Logic is used in reasoning from given premises to a conclusion. Logical reasoning is analytic; that is, nothing new is added from beyond the premises. We use formal languages in logic to draw out the logical structure of arguments; we abstract from the content and follow the logic. We make inferences from (presumed to be) known truths to other truths. It is the logic that guarantees that truth, or knowledge, is preserved. A formal logical language is a tool for honing and demonstrating the logic of our reasoning.

Conceptual analysis is a more general activity. When we do conceptual analysis, we meta-reason about the reasoning that is being studied as part of a practice. We meta-reason to find clarity, to give explanations, to gain insights and to better understand a practice. The practice of chemists, *qua* chemists, can be analysed, that is, reasoned about (subjected to meta-reasoning). To hone and demonstrate our meta-reasoning, we can develop and use a formal language.

I present a formal language that helps with conceptual analysis and show how it is different from, but inspired by, several formal languages that were developed for representing logical reasoning. The difference is important because the formal languages used in logic, are inadequate for conceptual analysis in chemistry. The reasons given for the *inadequacy* of each of the formal languages draws on features of the experimental part of the practice of chemistry and in how chemists come to understand chemical processes. This is a reflexive exercise in meta-conceptual analysis.

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Molecular Models and Scientific Realism

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The practice of theoretical research in chemistry largely consists in the construction of models without which experimentation would be impossible. The best-known theoretical models of chemistry are those of the molecular structures of chemical compounds. What is the correspondence between these models and the unobservable entities that they intend to explain? What is the ontological status of molecular models? The anti-realists question the basis of the realists' belief in these entities and the truth of claims regarding them. Ultimately, the realist/anti-realist debate points to the question of the scope of scientific knowledge. In this paper, I shall show that the description of natural entities offered by the contemporary scientific worldview reveals that molecular modelling presupposes a realistic epistemology that recognizes the limits of scientific objectification.

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The Complexity Challenges and the role of the Philosophy of Chemistry

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The journey to discovering the secrets of nature, made so far by humanity, has been punctuated by two revolutionary intellectual events: (I) The birth of philosophy in the ancient Greek colonies, during the 6th century BC, and (II) the use of the experimental method for inquiring nature, proposed by Galileo Galilei and finalized by Isaac Newton in the 17th century AD. These two intellectual revolutions have induced profound and fundamental changes in the human methodology of gaining insights about nature. After more than two thousand years of philosophical inquiry and three hundred years of the rigorous and systematic use of the experiments, the knowledge of the natural laws has significantly grown as proved by the astonishing technological achievements. Nevertheless, we still experience strong limitations on our attempts to exhaustively describe systems such as the climate and the geology of our planet; the living beings; the human brain; the human immune system; the ecosystems on earth; the human societies, and the global economy. These are examples of Complex Systems. We are aware that the traditional scientific methodologies, the available theories, and computational tools are not enough to deeply understand and predict the behaviour of Complex Systems. Therefore, we expect that more efficient algorithms, brand-new computing machines, and probably new methodologies and theories are needed. Do we need to study Complex Systems? Of course, yes. In fact, if we succeed to comprehend Complex Systems, we will surely possess new strategies and effective tools to tackle the Natural Complexity Challenges. The Natural Complexity Challenges are: (I) predicting catastrophic events in our planet (like earthquakes or volcanic eruptions) to save lives; (II) defeating diseases that are still incurable (such as glioblastoma, diabetes, HIV, et cetera); (III) protecting our environment and ecosystems from the climate change and the risk of shrinking biodiversity; (IV) guaranteeing a worldwide sustainable economic growth, primarily by focusing on the energy issue, and (V) ensuring stability in our societies.

For the comprehension of Complex Systems, we need a new revolutionary intellectual event. This third intellectual revolution requires breaking the traditional barriers separating the different disciplines by formulating a new transdisciplinary methodology and theory. A Systemic approach along with the Reductionism is required to investigate Complex Systems, and a new theory, including both the quantity and the quality of Information, is needed to interpret Natural Complexity.

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From chemical to physical-chemical ways of perceiving matter-reality: the case of chromatography in the analytical practice

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The physical-chemical chromatographic cluster of techniques is, since several decades, at the center of the analytical processes. Indeed, it could be safely argued that a great part of the today´s chemistry related laboratory practices –including also in biochemistry and genetics –would not be possible in the first place without the existence of the modern chromatographic instrumentation. The introduction and the eventual success of chromatography, it is argued in this paper, became possible only through a shift in the perception of the chemical community of what constitutes matter-reality, as well as what are the appropriate ways of detecting and identifying it. This shift brought chemistry and physics closer together on an ontological level and paved the way for the modern chemical laboratory practice. Key moments of the history of chromatography are being discussed, and contrasted to analogous cases of – co-temporary to them – neighboring domains, to demonstrate this shift of perception and discuss the reasons for its eventual establishment as the new normality.

Molecular shape: one, no one, one hundred thousand?

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"One, no one, one hundred thousand" is the ironic title of a novel by the Italian writer Luigi Pirandello: in fact, a reflection about Truth and the possibility of knowing the truth of ourselves and the other human beings. Out of metaphor, the expression fits well for the concept of molecular shape, due to the multifaceted aspects of this notion.

Molecular shape is a relevant notion in molecular sciences as, together with the key-concept of molecular structure, it allows interpreting and predicting the behaviour of molecules in a reactive or relational context. Unfortunately, structure and shape are often confused and sometimes taken as synonyms:

> *"This idea of molecular structure (or "molecular shape") has been fundamental to the development of our understanding of the physicochemical properties of matter*." (Wolley 1978)

A glance casted over the history of chemistry shows that molecular structure and shape are deeply entangled notions; their relationship involves also molecular topology. Molecular structure, molecular topology and molecular shape refer to distinct models of representation of the atomic-molecular realm. Each one of these notions bear its own philosophical burden and it is related with peculiar epistemic procedures. Here, I will focus on the notion of molecular shape. Firstly, I will analyse distinct acceptations of |shape|, as they are used in chemistry and chemical education. Secondly, I will comment on the connection between shape, topology and structure. I will argue about the conventional character of the notion of shape and I will sustain that – unlike structure – shape has purely epistemic value, rather than an ontological one (Del Re 1998; Ghibaudi et al. 2019; Ochiai 2017). Molecular shape is not an intrinsic molecular property: it has a conventional character. In fact, a single molecule may exhibit distinct shapes. In addition, molecular shape deals with the relational aspects of molecules. This aspect is especially evident in: i) the identification of similar molecules in the frame of QSAR and the search for pharmacologically active molecules (Todeschini & Consonni 2009); ii) the iconographic representations of the shape of biological macromolecules (Putta 2007). Examples from these two areas will be discussed.

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The QSAR similarity principle in the deep learning era: confirmation or revision?

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Background

Chemical properties can be studied using physical models and simulation. Differently, Quantitative Structure Activity Relationship (QSAR) models are based on the postulate that similar molecules exhibit similar physical and biological activity, opening the road to non-physical predictive models. Chemical data representation has been an issue for a long time. Most of the QSARs use molecular 1D and 2D descriptors, and fingerprints. Fingerprints, that codify the presence/absence of functional subgroups, are not unique, as it is possible that the same fingerprint represents different molecules. Usually QSARs make use of a number of chemical descriptors, apply some method to reduce them to a few, and adopt various computational techniques to build the model that predicts an assay [1]. The parallel approach named Structure Activity Relationship (SAR) is instead based on the idea that specific functional groups in the molecules are responsible for the activity; their presence is used to predict the activity. The two approaches are usually mixed, as many QSAR methods use fingerprints.

Similarity or discontinuity?

To accept (Q)SAR models users want it to be interpretable; for many years, researchers tried to use interpretable descriptors from the beginning, but more recently they tend to make the interpretation a-posteriori, for instance analyzing the presence of functional subgroups. The acceptance is also based on accuracy. The reality is that all models, QSAR included, have some errors, so the point becomes: how to detect when a prediction is wrong? Recently it has been proposed to analyze the activity landscape of the assay, i.e. to represent it in N-dimensional space, each dimension being a descriptor, plus the measured activity. According to the similarity principle the obtained surface should be smooth; evidence shows that instead there are activity cliffs, where the difference in activity of two very similar molecules is large [2].

The most accurate QSAR models working in large chemical spaces use non-linear methods as Neural Networks (NN) that, by construction, make the similarity hypothesis less crucial. NN have a role in solving the *similarity-cliff* dilemma: the universality theorem states that a NN with at least one hidden layer can approximate any continuous or discontinuous function. Moreover, adding layers in the net increases the number of parameters to fit and so allows to better approximate complex functions.

Why adding fully connected layers in NN without considering the properties of the data representation? Let us imagine that chemicals are represented by 2D graphs; they are images. The architecture of the network should take into account the spatial structure of images. For instance, why to treat pixels that are far apart and close together? So, instead of starting with a generic NN multilayer architecture we take advantage of the spatial structure. For images it is accepted that the neighborhood rather than the pixel carries the geometrical interpretation; using this principle C*onvolutional NN (CNN)* adds trainable filters and neighboring local pooling operations, in an alternate sequence.

Deep NN contain simple non-linear processing units, each transforming the representation at one level (starting from the input image) into a representation at a higher level. In practice the network works as a representation learning method, learning from low to high level features, without the need of computing and selecting the relevant chemical descriptors [3]. Another popular architecture, Recurrent NN (RNN), successful in natural language processing, can be used to to classify SMILES according to the activity. We will illustrate a few cases.

And now we have the elements to go back to the initial point: are deep learning models confirming or reformulating the QSAR postulate? Is still similarity necessary to predict the activity? The answer is that similarity depends on the property under study; it is not a universal chemical property.

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Overcoming Equilibrium: The Greatest Challenge in Recreating Life’s Origin

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All living things are in a state of sustained disequilibrium. As an example, on a cellular level this disequilibrium can be seen in processes such as the maintenance of gradients across a cell membrane, preventing the equilibrium state of equal concentrations of materials on either side of the barrier. Equilibrium, being the lowest energetic state for a system, is the natural state of nature. Thus, the sustained disequilibrium seen in living things is often considered a hallmark of life, with some going so far as saying it is the most important differentiating factor between non-life and life. So, when considering creating a nominally living thing from a collection of non-living components, something that must have occurred in the origin of life on Earth, the drive of nature towards the lowest energetic state (equilibrium) must be overcome and the sustained disequilibrium characteristic of life must have been established. This fact has been known and acknowledged in modern scientific work and into history, but remains a challenge in practice.

In modern origin of life theories, there are three prevailing groups of theories stemming from different levels of analysis. For researchers coming from a biological perspective, heredity and genetics are often considered the most important feature of life stemming from the modern discovery of the ribozyme. This discovery was extrapolated backwards to the origin of life, yielding the RNA World theory, where the informational polymer RNA is considered of utmost importance and is thought to have arose first. Often, RNA World theories are coupled with Container-first theories, the second group of theories regarding the origin of life, where the focus is the generation of a container for the first living components. Container-first theories often stem from a physical or chemical perspective. Also stemming from a chemical perspective is the last group, Small Molecule World theories. Here, proponents concentrate on metabolism, dictated by self-propagating, catalysed, chemical reaction networks, as the first and most important feature of life. Ultimately, I will show that these different theories suffer from different problems in the context of establishing sustained disequilibrium. While the RNA World is often credited as being the most popular theory, due to researchers’ success in mimicking signs of living system, the results are often still dictated by thermodynamic equilibrium. In contrast, both container-first and Small Molecule World work are often characterized by their disequilibrium, and yet neither produce systems that are recognizable as living. In this talk, I will analyse a few different prevailing findings from each group in the context of establishing the required sustained disequilibrium for life, comparing and contrasting their success in recreating life’s origin.

Philosophy and the (Mis)use of Chemical Examples: Intimacy vs. Integrity as Orientations Towards Chemical Practice

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This essay critically considers the issue of natural kind essentialism. More specifically, the essay critically probes the philosophical use of chemical examples to support realism about natural kinds. My simple contention is that the natural kind debate can be understood in terms of two different cultures of academic production. These two cultures will be conceptualized using Thomas Kasulis's distinction between intimacy and integrity as cultural orientations. Acknowledging Kasulis's contention that, "What is foreground in one culture may be background in another", it may very well be the case that philosophers writing about chemistry place chemical practice in the background, thereby adopting the orientation of integrity. Chemists and philosophers of chemistry, on the other hand, place chemical practice at the foreground of their work, thereby adopting the orientation of intimacy. Because the intimacy orientation is grounded in chemical practice, it is preferable to the integrity orientation. Regarding the debate about natural kinds, thinkers who use chemical examples to support microstructural essentialism tend to adopt an orientation of integrity towards chemistry, so that they tend to infuse discussions about natural kinds with a priori philosophical assumptions and ignore chemical practice. On the other hand, chemists and philosophers of chemistry express doubts concerning the use of chemical examples to support microstructural essentialism, and they do so precisely because they have an orientation of intimacy towards chemistry that foregrounds chemical practice. Understanding the natural kinds debate from this perspective highlights the fact that its misuse of chemical examples is informed by an orientation of detachment from actual chemical practice. This underscores the importance of an intimate understanding of chemical practice when deploying chemical examples in the context of philosophical discussions about ontology and metaphysics.

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How to Investigate the Underpinnings of SciencesHow to Investigate the Underpinnings of Sciences? The Case of the Element Chlorine

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In recent papers, Harré and Llored (2018a, 2018b) take the role of philosophy of science, not as critical commentary on ways of proposing ontological presuppositions or highest-level theoretical premises, nor as formulating laws of nature and their relations to particular instances of *phenomena*, but as a digging out of the 'hinges', that are the tacit elements of a discipline. In this perspective, the philosophy of chemistry consists, at least partly, in the work of making explicit the hinges on which a particular science turns and examining their origins and logical status. In this paper, we propose to query Harré and Llored's research approach in the case study of the element chlorine. Whereas most early 19th-century textbooks define the element as the endpoint of chemical analysis, the controversy surrounding the element chlorine reveals implicit criteria for elementhood that surpass operational indivisibility. From 1810 onwards, Davy argued that chlorine was a simple substance; yet, even though the substance had been known to be indecomposable using the strongest instruments available, its widespread acceptance as an element took until 1816-18. The main factor that contributed to the resolution of the debate and the acceptance of chlorine was the discovery of iodine, an analogous element which provided new theoretical coherence between explanations of different phenomena (Golinski 1992, Gray et al. 2007, Chabot 2006). Thus, the idea that elements should qualitatively resemble each other is an implicit belief which appears to have been shared by many prominent chemists of the time, despite the fact that it was not stated as part of the definition of the chemical element. Could we assert that this idea was a 'hinge' around which the notion of chemical element revolved? Our talk will answer this question.

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Pluralism and Practice in Chemistry

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The “philosophy of science in practice” shifts attention from theories to actions. Since “an activity cannot correspond to the world”, it may argued that it is necessary to give up the correspondence theory of truth, and to take knowledge to consist not in the accuracy of a theory or fact, but in “the ability to do things as reliably as intended” (Chang 2012). Pluralism recommends “the simultaneous cultivation of a set of systems of practice that are as incommensurable from each other as possible” (ibid.). There is no doubt that a crucial part of the development of chemistry in the eighteenth century was the development of more reliable experimental procedures by Cavendish and Lavoisier. The subsequent success of chemistry owes a great deal the exactitude of their methods of analysis and synthesis. Yet their systems of practice were not strongly incommensurable, they were mutually understandable and had much in common despite their theoretical disagreements. The eventual result was a single account of chemical composition in terms of simple substances that is still taken to be largely correct.

Pluralists reject monism defined as the view that “there is only one world, there is only one truth about it, and only one science should seek it” (ibid.). However, such a strong form of monism is not entailed by the rejection of pluralism, and nor is triumphalism, authoritarianism, elitism, imperialism, dominance and dinosauric hubris, popular rhetoric to the contrary notwithstanding. Pluralism is advertised as promoting epistemic humility, but its defence relies on the very bold normative claim that science should be reformed so that incommensurable systems of practice are cultivated, and the very bold historical claim that the development of chemistry would have gone better if this had been done. This paper argues that once we identify the false dichotomy between “pluralism” and “monism” as defined above, the sensible middle ground between them can be identified. In particular, chemistry always includes some pluralities and some partial unities, but the detailed debates that actually occurred were based on commensurable experimental practices being used to settle theoretical disputes with differing proposals being judged by how well they relate to reality. Furthermore this avoided the vast waste of time for chemists that would have been a consequence of pluralism in practice.

Two kinds of pluralism about the Chemical Revolution: an attempt to reconcile active realism with practical realism

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In a posthumously published article, Rein Vihalemm (2016) critically reviews Hasok Chang's version of pluralism about the phlogiston theory and its possible lessons for contemporary chemistry (Chang 2012). The point of departure in Vihalemm's account of pluralism is Kuhnian history of science interpreted in terms of practical realism. For Vihalemm, Chang's active realism remains trapped in the traditional representationalist philosophy of science, as long as Chang is seen to misinterpret Kuhn's concept of paradigm. Kuhn's paradigms if understood in practical realist way, enable scientists to disagree and to some extent, hold different views. The example of the refutation of phlogiston theory in history of chemistry serves as a valuable illustration of the two competing interpretations of pluralism. In my paper, I am going to examine both Vihalemm's and Chang's accounts of phlogiston theory as well as their versions of pluralism. I claim that both Chang and Vihalemm see pluralism as arising from a practice-based theory of science even though practice is understood slightly differently.

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Quantum chemistry
and the representationalist view of scientific models

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The case of different models of a same target was extensively studied in the literature. Nevertheless, from a representationalist position it can be argued that, although the model was successful in his time, it was left aside when the new model was formulated; this last one is the representative model.

Quantum chemistry shows cases in which a single model embodies *contradictory* elements: the case in which an assumption that contradicts a consequence of the theory on which the model is based (in the orbital approximation); the case of an assumption that contradicts a postulate of the theory on which the model is based, since coming from a different, ontologically incompatible theory (in the Born-Oppenheimer approximation). In this kind of cases, advocating for a representationalist conception of models is more difficult. In other words, the models of quantum chemistry seem to offer a further and stronger challenge to the representationalist view of scientific models.

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Aristotle's Mixt Debt to Plato

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It is odd that philosophers of chemistry have by and large neglected Plato and instead followed Aristotle's terms, concepts and approach with respect to chemistry, given that Aristotle largely follows Plato on all major points—with the crucial exception of the role of mathematics in understanding change. With few exceptions, Plato is excluded from serious discussions of the philosophy of chemistry. Whereas pedantic histories of philosophy present them as opponents, there is a school of interpretation that considers Aristotle as the most innovative, unparalleled exponent of Plato… at least until the advent of Plotinus and the so-called Neoplatonists. It is in Neoplatonism that valuable comparisons of Platonic and Aristotlean understandings of element, matter, bodies and properties may be found. For example, Claghorn [1] and Opsomer [2] draw attention to the fact that many of the examples that Aristotle uses to explain mixts are the same as those that Plato uses in his cosmology, the *Timaeus*. Indeed, a comparison of key passages in Aristotle's *De Generationes et Corruptiones* and *De Caelo* reveal a clear debt to Plato's original examples of the coming to be of elemental bodies, their mixtures and dissolution. It is strange that, whereas quantitative proportions naturally arise from the elegant geometry of Plato's atoms, Needham and Hendry [3] consider Aristotle to be the "father of chemistry," despite the latter's lack of a precise idea of proportions. Stranger still, Needham [4] strains to introduce a formalism for Aristotle's "interplay of contraries" in an effort to compensate for its innumeracy and vagueness, for as Needham says, "we can only guess at what, if anything, he had in mind." (2006, 58)

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The identity of chemistry through the development of physical chemistry

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Traditionally, the issue about the relationship between chemistry and other disciplines has revolved around specifying what is meant by 'reduction'. In this tradition, the question of whether chemistry can be reduced to physics places the subdiscipline of quantum chemistry at the center of the debate. Notably, the historical investigations regarding the relationships with other parts of physics, such as thermodynamics, have had little impact on the discussion about inter-field exchanges. However, in order to elucidate the features that ground the identity of chemistry as an autonomous science, thermodynamics needs to be considered (Vemulapalli 2010). From a historical point of view, the theoretical development followed by Josiah Willard Gibbs's approach to thermodynamics (at the beginning of the 20th century) had no great impact on chemists, partly because thermodynamic concepts seemingly lacked a relevant connection to the notion of substance and to chemical change. On the one hand, the physicists and engineers who developed thermodynamics were unable to grasp chemical notions; on the other hand, the shallow mathematical training that chemists were used to prevented them from accepting thermodynamics (Rocke 1993).

These factors changed during the last two decades of the 20th century, when both chemists and physicists gathered around thermodynamics. Thermodynamics was taken to provide chemistry with explanations about the nature of affinity or equilibrium, with criteria to understand the spontaneous direction of chemical reactions, and also with techniques and measurement procedures for qualitative analysis. In addition, chemistry gained a new way of practicing the discipline and new perspectives to understand chemical changes.

The purpose of this work is to face the questions about how the practitioners of chemistry reacted to the interaction between thermodynamics and chemistry since the beginning of 20th century, and how specializations, such as physical chemistry, arose in chemistry as a consequence of that interaction. A historical reconstruction of the relationships among ionists' theories, Gibbs's thermodynamics, and the synthesis carried out by Lewis will provide the answers to such epistemic and historical questions.

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Phage display: a reductionist approach on the protein-protein interaction

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The phage display methods have been used since the 1990s to select proteins that specifically interact with a particular target substance. It is an excellent example of the use of phage display methods for making recombinant antibodies with high specificity and affinity against disease-associated antigens. In the presentation, I will concentrate on the phage display methods used in antibody engineering. The phage display methods for antibody engineering are based on the interpretation of the reductionist view of protein-protein interactions for the following reasons. The phage display methods are based on the assumption that a single interaction between an antigen and an antibody is the most critical factor in the disease mechanism. That is, interacting with the antigen A, which plays a vital role in inducing disease, to inhibit or exacerbate its function, the disease can be treated. Breast cancer in which the disease progresses due to overexpression of the HER2 gene is consistent with this assumption. However, this is not the case in general. In more cases, there is more than one target protein associated with the disease and the process by which the targets cause the disease also consists of several stages of the mechanism. Besides, the strategy to increase the affinity and specificity of the antibody in the phage display methods is to substitute the amino acid(s) in the specific region of the antigen through site-directed mutagenesis. This is an experimental procedure in which the subject of protein-protein interaction is assumed to be two proteins.

In the presentation, I want to examine the limitations of such a reductionist approach in the phage display method. I also want to see what experimental techniques have been applied to overcome these limitations. Furthermore, I examine the protein-protein interactions in terms of the network view, not the reductionist view, and discuss how this tendency can form a complementary relationship with the phage display method.

Understanding molecular structure requires constructive realism

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An old debate over scientific realism and anti-realism is not agreeable in many respects from a chemical point of view, so it needs to be redefined by taking chemical interests and issues into consideration. Can we be a 100% realist or anti-realist when we argue about molecular structure?

Bhaskar says the generative mechanism of phenomena represented by models may come to be established as real in the course of ongoing activity of science.1) However, models are constructed by analogy with things within experience and real molecules are subject to the laws of quantum mechanics. How do models correspond to reality? Physics-oriented philosophers have tendencies to assume that reality can be represented by a single model. Such might be the case with models of fundamental theories. But such is not applicable to submicroscopic entities: the molecule seems to have definite structure in some cases, and a bank of electron clouds in other cases—they do not fall under what Cartwright calls bad models, either.2)

In view of these, we suggested, at ISPC2018 in Bristol, taking different outcomes of observation of one and the same object not as a contradiction but as different affordances which become realized in different phenomenal fields. Based on this understanding we argue about how and to what extent science tracks truth of the molecule. The point is the relationship between models and reality.

Although the world is an objective reality existing independently of the human mind, what we see depends on how we look. In other words, every scientific theory has its own viewpoint. No single theory or model represents or has a similarity relationship with the molecule. What follows from this observation is that the molecule is best described with a population of models. This type of relationship of models with reality is compared to that of paintings with their objects.

Our view of science is based on Bhaskar's ontological structure of the world and close to Gierre's,3) and different from both in terms of the relationship of models with reality. We give a momentary name 'constructive realism' to this philosophical position, which is in effect counted as a third way attained by sublation (Aufheben) of scientific realism and anti-realism.

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From the principle of least action to the conservation of quantum information in chemistry. Can one generalize the periodic table?

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In fact, the first law of conservation (that of mass) was found in chemistry and generalized to the conservation of energy in physics by means of Einstein's famous "$E=mc^2$". Energy conservation is implied by the principle of least action from a variational viewpoint as in Emmy Noether's theorems (1918): any chemical change in a conservative (i.e. "closed") system can be accomplished only in the way conserving its total energy.

Bohr's innovation to found Mendeleev's periodic table by quantum mechanics implies a certain generalization referring to the quantum leaps as if accomplished in all possible trajectories (e.g. according to Feynman's viewpoint) and therefore generalizing the principle of least action and needing a certain generalization of energy conservation as to any quantum change.

The transition from the first to the second theorem of Emmy Noether represents well the necessary generalization: its chemical meaning is the generalization of any chemical reaction to be accomplished as if any possible course of time rather than in the standard evenly running time (and equivalent to energy conservation according to the first theorem).

The problem: If any quantum change is accomplished in all possible "variations (i.e. "violations) of energy conservation" (by different probabilities), what (if any) is conserved?

An answer: quantum information is what is conserved. Indeed, it can be particularly defined as the counterpart (e.g. in the sense of Emmy Noether's theorems) to the physical quantity of action (e.g. as energy is the counterpart of time in them). It is valid in any course of time rather than in the evenly running one. (An illustration: if observers in arbitrarily accelerated reference frames exchange light signals about the course of a single chemical reaction observed by all of them, the universal viewpoint shareable by all is that of quantum information).

That generalization implies a **generalization of the periodic table** including any continuous and smooth transformation between two chemical elements necessary conserving quantum information rather than energy (valid only to any cell of the table but not as to any transition between them): thus it can be called "alchemical periodic table".

Open questions on periodic systems

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Trying to systematise the chemical knowledge of mid 19th century [1], Mendeleev found that two important relationships among chemical elements were order and resemblance, which constitute the mathematical structure of the system [2]. Compounds provided the necessary means to assess similarity and order. Resemblance was assessed through commonality of composition and order resulted from comparing atomic weights obtained from compounds [3]. Thus, known compounds by mid 19th century were central for devising the periodic system. In this setting, some open questions for studies on the periodic system are: What is the influence of the known chemical compounds upon the structure of the system? Would the periodic system be different if chemists would have come up with compounds in a different order? Why we rely on similarity and order to build up a system? Why not other relationships among the elements? If the structure of the current system is based on order and similarity, which other systems are possible in the chemical domain and even in other domains? The setting of these questions and possible ways to address them will be discussed in this talk.

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Plurality and pluralism of the concepts of element

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Surprisingly, the term ‘element’ is understood in various ways in chemistry. According to the IUPAC definition and contemporary descriptions of the periodic table of chemical elements, ‘element’ refers to a concept defined by its atomic number. ‘Atomic number’ is a physical notion, as this property can be detected in physics laboratories; in chemistry, this notion has a more abstract status. In chemical practice, ‘element’ refers to a simple substance defined by its properties appearing in chemical practices such as synthesis-analysis. We argue that both concepts of element are important, irreducible to each other (particularly, the chemical concept cannot be reduced to the physical one, contrary to what is often assumed), and each have their role due to the practices they are embedded in. Our analysis uses pluralist philosophy of science frameworks (e.g., Bachelard, Chang, van Brakel, Vihalemm) to both argue for pluralism due to plurality in chemistry, as well as to draw conclusions for those philosophical accounts from our case study.

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Dervish Pasha Who Introduce Chemistry to the Ottoman Empire and His Chemistry Book ‘’Usûl-i Kimyâ’’

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The introduction of modern science to the Ottoman Empire was about the end of 18th century. So, modern science education was done by the military schools at the Ottoman Empire at the end of the century. In this sense, military schools became the center of translations from European science and technology to Ottoman Turkish books. Therefore, the inauguration of modern schools and entering of science lessons in curriculum resulted in promoting science in the Ottomans at 19th century. To reach this aim, Encümen-i Daniş institute was established to prepare books that had basic-level and clarified Ottoman Turkish language from Arabic and Persian for the Darülfünun. Its lecturers were selected from state officials, but it wasn’t so long to meet the needs of the Ottomans. Later, because of the lack of governmental institutions, translations from English and French were mainly conducted by the individual efforts of the teachers working at educational institutions. At first half of 19th century, few numbers of books were translated to Ottoman Turkish from many foreign languages. For instance, Başhoca İshak Efendi’s books about modern science and military technical issues (prepared by translating and completing from foreign languages) are seen as the pioneer of modern technical education in Ottomans.

The penetration of chemistry to the curriculum was about 1860s at the Ottomans. Because of this reason, the translated books number had increased, but a nomenclature problem had occurred. The question of creating a new system or adopting the European nomenclature system was an important issue. There were some efforts to constitute a new nomenclature system at the Ottomans, but it had many difficulties such as difference between lexical structure of languages and difference in the symbols of alphabets. In that sense, some chemists like Dervish Mehmet Emin Pasha tried to constitute his own systems. In this respect, it will be clarified the biografy and the original nomenclature system of Dervish Pasha in this study. In 1835, Dervish Pasha went to England and then to French to complete his education. When returning to Istanbul, he worked as physics and chemistry teacher at Mekteb-i Tıbbiye-i Şahane and Mekteb-i Harbiye. The treatise of Dervish Pasha’s is the first chemistry lesson book written at 1848 at the Ottoman Empire. The book consists from 2 volumes but only the first volume could be reached and the book was used as lecture book at the Darülfünun. The book mentioned about the acids, bases and many compounds used for ammunition. This book shows the gap between east and west science at 19th century. Since the first-hand sources of ‘’Usûl-i Kimyâ’’ are French and English, it is nearly reach the west science with a small time gap. Indeed, at this century a small time gap is not so important when compared with today. To understand context of the piece, it is obligatory to solve other systems of nomenclatures conducted before and after ‘’Usûl-i Kimyâ’’. Dervish Pasha’s original drawings has shown elements, compounds, and reactions with his own style. Dervish Pasha’s style looks like Jakob Berzelius’ while writing chemical compounds but piece is a compilation of Dr.Edward Turner’s ‘’Elements of Chemistry’’ (1842) and Louis Jacques Thénard’s ‘’Traité élémentaire de chimie’’ (5 vol. 1834-36).

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Convincing or Correct, Explanations in Chemistry

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Chemistry as the art and science of the properties and changes of complex materials requires the systematically classified and ordered representation of the mess of reproducible individual chemical observations, here abbreviated by the word ‘facts’. There are three levels common in chemistry toward the explanation or rationalization of empirical facts: (i) The description of the apparent empirical structure, systematics or order of ‘what is’. This is what the large group of positivists is comfortable with. (ii) The qualitative, apparently ‘convincing’ classical-traditional or otherwise acceptable arguments within the community, of ‘why’ some circumscribed set of facts is so. This will satisfy most other chemists. (iii) The logically and/or computationally supported explanations, apparently consistent within a larger unified context of physically accepted theories. This is the research program of the few reductionists.

We discuss three examples from the fields of Covalent Bonding, of Atomic Charges, and of the Periodic Table of Elements. Focusing on facts and analyzing opinions are both of interest to science and to philosophy. Steps (i) and (ii) are important for memorizing, teaching and practicing chemistry. Step (iii) is a question of ideology and of ‘activation barrier’.

The Chemical Bond as a Real Pattern

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A central concept which is invoked in chemistry and in quantum chemistry in order to describe the structure of a molecule is the chemical bond. Given this, a pressing philosophical question is whether the chemical bond exists and what sort of thing it is. This question is primarily discussed in the context of Hendry's distinction between the structural and the energetic conception of the chemical bond. The structural conception takes chemical bonds to be 'material parts of the molecule that are responsible for spatially localized submolecular relationships between individual atomic centers' (Hendry 2006: 917). The structural conception is taken as supporting an understanding of chemical bonds as entities. The energetic conception takes 'chemical bonding' to signify 'facts about energy changes between molecular or supermolecular states' (Hendry 2006: 919). The energetic conception remains agnostic as to whether the chemical bond is an entity (or as to whether it even exists) and it is consistent with an understanding of chemical bonds as properties of a molecule. The metaphysical interpretation of each conception allegedly creates a tension between the two conceptions because the former is consistent with an understanding of chemical bonds as entities, whereas the latter is consistent with an understanding of chemical bonds as either fictional entities, or real properties of molecules. I argue that this tension can be resolved in a manner that supports the reality of chemical bonds. Specifically, if one takes the two conceptions as representing distinct yet incomplete intensions of the same referent (i.e. the chemical bond), then both conceptions can be invoked to mutually support an understanding of chemical bonds as patterns within a molecule. Such an understanding of chemical bonds is also supported by how chemistry and quantum chemistry each describe and pictorially represent chemical bonds. Several questions need to be addressed in order to sufficiently support the reality of chemical bonds as patterns. First, if a chemical bond refers to a pattern within molecules, then what is it a pattern of? Secondly, assuming that chemical bonds are patterns, what is the respective 'noise' in the chemical and quantum chemical descriptions of a chemical bond, and what is the role of 'noise' in predicting a molecule's structure? Thirdly, is there sufficient empirical evidence to support that the elements of this pattern are real and not merely apparent? I examine these questions in light of the literature on real patterns and briefly outline the advantages of understanding chemical bonds as real patterns. Examining the nature and reality of chemical bonds in the context of the literature on real patterns provides a novel perspective through which one can understand the nature of the chemical bond, but also through which one can re-evaluate the tenability of structural realist accounts in the philosophy of science.

Hendry R.F., 2006, 'Two Conceptions of the Chemical Bond', *Philosophy of Science*, Vol. 75, No. 5, pp. 909-920

Prediction, Accommodation, and the Periodic Table: A reappraisal

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The story of the diffusion and affirmation of Mendeleev's Periodic Table of elements has proven to be a challenging testbed for contemporary philosophical debates on the role of predictions in science. More than ten years of fruitful literature were tickled by Scerri & Worrall (2001) vs. Maher (1988) and eventually culminated in a key conference on novel predictions in Düsseldorf in 2011 (see *Studies in History and Philosophy of Science*, vol. 45). Maher's (1988) early account – according to which the astounding success of the three major predictions alone was enough to explain the affirmation of the periodic table – can now be replaced by a more balanced and thorough picture.

In fact, a major outcome of such renewed interest in the Periodic Table has been the rediscovery of some previously neglected episodes of its history, e.g. the so-called counter-predictions (Brush 1996, Schindler 2008), the accommodation of argon together with other inert gases (Scerri & Worrall 2001), and the troublesome inclusion of rare earths (Akeroyd 2013). However, a number of methodological and interpretative issues have remained open despite such extensive exploration and discussion. Important but scattered contributions to be integrated include, for instance, Worrall's (2005) attempt to assess the role of the accommodation of known elements in the confirmation of Mendeleev's theory, Schindler's (2014) vs. Barnes's (2014) debate on the relevance of the historical evidence traditionally meant to support a predictivist account of the story, and Scerri's (2007) emphasis on the potential negative impact of failed predictions on the diffusion of the table. Our aim in this contribution is to put together as many pieces of the story as possible, in an effort to explain them coherently in terms of (Lakatosian) internal history. Drawing on Worrall's predictivism as a background and guideline, our rational reconstruction assigns a role to both prediction and accommodation. Indeed, we rely on Mendeleev's case as a unique source of material to articulate the subtle boundaries between different kinds of evidence in the development of chemistry as a modern scientific discipline.

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Sources for Appropriation of Chemistry into Japan by Udagawa Youan (1798-1846)

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Appropriation of chemistry science from Europe to Japan was a major work of the Japanese physician-scholar Udagawa Youan. After studying anatomy and specializing in botany and plant classification following Linnaeus method, Youan realized that studying chemistry is essential for understanding processes in plants and in the human body. Youan's major chemistry book is titled *Seimi Kaiso*, Introduction to Chemistry (1837-1847).

In his book he dealt with topics such as chemical affinity, solution, caloric, alkali, salts, phosphoric acid, ammonia, oxidation and reductions of metals, constituents of plants and more. In the last part of *Seimi Kaiso* Youan analyzed the ingredients of water in hot springs in Japan and he also described chemical ingredients of hot springs in foreign countries.

What were the foreign books that Youan used for his studies? What languages could he read and how did he get the books? In a letter to the botanist Ito Keisuke, his colleague and disciple, Youan wrote that he could not get books in chemistry in Edo, (today's Tokyo), since he could not meet foreigners there.

Many of the European chemists of late 18th century and first half of the 19th century are mentioned in *Seimi Kaiso*. Most famous books were by the English chemist William Henry and the French Antoine Lavoisier. Other books were written by P. J. Kasteleyn, Adolphus Ypei, J. J. Plenck, F. Catz Smallenburg and more. The works of those chemists and their citation in *Seimi Kaiso* will be presented.

International exchange of knowledge in writing and by meetings of scholars in Europe was common, in contrary with the isolation in which Youan performed his studies. Nevertheless, Udagawa Youan accumulated knowledge of chemistry that was further developed in Japan. He created chemical nomenclature; many of the terms he coined are still used today. The insight in choosing specific Chinese-Japanese characters to explain chemicals, chemical tools and processes will be discussed. 化

Ontological Status of Time in Chemistry

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While temporal considerations are of prime importance for chemical reactions, as well as for molecular stability, most chemical concepts (outside of the field of chemical kinetics) are not explicitly formulated on a diachronic basis (Earley, 2012). It will be shown that a process ontology (Earley, 2008) explicitly incorporating temporal and epistemological considerations, eschewing unphysical infinities, enables us to treat chemical reactions and molecules on ontologically equal terms, instead of assigning a more fundamental status to the latter. After all, in collision theory, a molecule is just a collision (a "resonance") that takes too long. How long qualifies as "too long", and "too long" in relation to what, are crucial questions that distinguish molecules from chemical reactions, and reversible reactions from irreversible ones, in the process introducing anthropocentric considerations into these distinctions. Too long for a lab chemist is very different from too long for an astrochemist studying chemical reactions between molecules in inter-stellar space on cosmological timescales. Examining several physical and chemical properties on the basis of which molecules are distinguished from one another, the role of temporal and anthropocentric considerations in defining molecular properties will be emphasized. I will conclude with some observations on the much-debated reduction of chemistry to other disciplines, arguing that such reduction depends on our aesthetic choices as to what kinds of observations demand explanation, and what kinds of explanation are acceptable.

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Precipitation Kinetics at the Physics-Chemistry Interface: The Case of Hydrolysis Species of Post-Transition Metal Compounds

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The identification of many precipitated hydrolysis species of post-transition metals has long remained asymptotically impossible even when subjected to the calculative rigor of computational chemistry and the comprehensive purview of laboratory experimentation. This problem is rendered so difficult due to four primary factors: 1) The most minimal differences in experimental synthesis conditions can lead to unpredictably different hydrolysis species. 2) The is no clear-cut way to differentiate various hydrolysis species from each other. 3) Solutions can contain a mixture of various hydrolysis species. 4) In many instances, a solution can resemble (to identity under observational conditions) a colloidal suspension of highly positively charged particles.

The aim of the present paper is to gauge the effectiveness of chemistry's explanatory armamentum in light of three precipitation kinetic models: Kinetic Monte Carlo (KMC), which originates at the explanatory scale of condensed matter physics, Cluster Dynamic, a mesoscopic interstitial model at the reified "border" of physics and chemistry, and the purely chemical Classical Nucleation Theory: Where and when does condensed matter physics "hand off" to physical chemistry? The four aforementioned ambiguities can be presumed to fall well within the epistemic ken of chemistry, yet they remain unscalable at all three theoretical levels. It is noted that said ambiguities are purely observational and taxonomic in nature, and therefore unamenable to any black-box chaos theoretical explanations. The possibility of a theoretic extension is then examined and discarded in this regard in favor of a prospectus for more "candlepower" in the quest for a truly constitutive/phenomenological theory as a last/best hope.

Quantitative-Structure Activity Relationships (QSAR): Some historical notes and epistemological considerations

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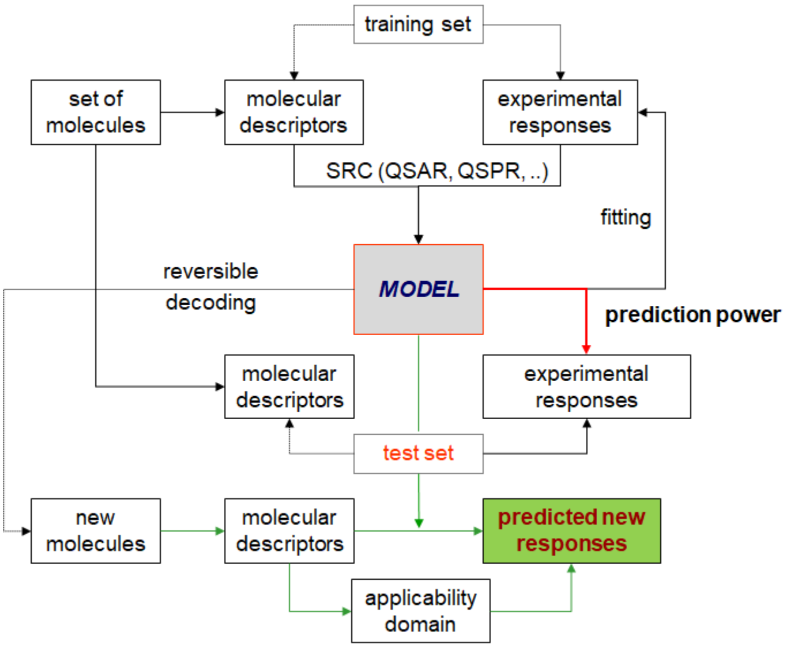
Some historical notes will be presented highlighting the birth of the idea that molecular properties are strongly related to the molecular structure. Starting from the concept of molecular descriptors, the presentation will illustrate the development of QSAR and contemporary chemoinformatics approaches and their epistemological basis.

In particular, the role played by the molecular descriptors [1-2] in the modern QSAR strategy will be discussed, where the set of the best models obtained by the selection of the relevant molecular descriptors becomes a fundamental step: *there is one reality, but several reliable points of view*.



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The *in-vitro*/*in-vivo* problem. Extrapolating chemical knowledge from the laboratory to the biological world

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One of the main epistemological problems of biochemistry is the so-called *in-vitro/in-vivo* problem. Specifically, what kind of knowledge about living systems (*in vivo*) can be obtained by studying chemical systems (*in vitro*) in which biological materials are isolated from their natural environment? Until now, this question has received little attention in the philosophical literature and has been given mainly skeptical answers [4, 6].

In this prospective presentation, the *in-vitro/in-vivo* problem will be addressed as a part of the wider problem of **extrapolation** in biochemical research [1,3]. In this case, the issue can be framed in terms of this wider question: “What can we know about biological nature by studying **artificial experimental systems** in the laboratory?”

Experimental systems (ES) are systems of manipulation consisting of a set of materials (chemical and/or biological), measuring instruments, protocols, data analysis techniques, etc. which are used to produce stable and replicable phenomena in the laboratory [5]. These mostly consist in chemical *in-vitro* systems, but also in model organisms, cellular cultures, etc. Without these artificial systems, any attempt to obtain reliable and reproducible knowledge would be impossible.

In the case of an *in-vitro* ES we have access to an **epistemic object** (like a macromolecule, a cell constituent, a process, etc.) of biological origin by means of some of their physical/chemical properties. If we consider a specific ES, we can distinguish two kinds of properties with respect to their epistemic access: **detection/manipulation properties** (D/MP) and **auxiliary properties** (AP) [2]. D/MPs are properties by means of which we can detect or manipulate the epistemic object; in other words, these are the properties with which a causal chain can be established between them and a detection or manipulation mean in the ES considered. On the contrary, APs are the properties that cannot be detected or used to manipulate the object in the considered ES. An important point is that, given a property, it could be an AP in the context of one ES, but a D/MP in the context of a different ES. On this framework, the most important properties are the ones that could be D/MP in many ESs; these are called **robust properties** [7]. By means of them, we can obtain reliable knowledge about chemical capacities of epistemic objects of biological origin. Basically, if a chemical property resists our interventions in the context of several ESs, it is nonsensical to doubt its existence in nature, and there are also good reasons to postulate its relevance in the mechanistic context of natural biological systems (*in-vivo*) [3].

So, by taking this framework of analysis into account, we can understand how the reliable chemical knowledge produced by means of *in-vitro* ESs can be extrapolated to the biological world. Of course, no extrapolation is definitive and scientists are aware of this fact; however, they have good reasons to justify the knowledge obtained about living things by studying chemical *in-vitro* systems.

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Hierarchies, Complexity, and the Problem of Identity

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The research is focused on the deeper investigation of the idea of identity, and how it can be explained by using the case studies from the philosophy of chemistry. The stronger definition of identity is possible by studying the forms of substance that appear on the different levels of complexity, subatomic, atomic, molecular, or supramolecular.[1] Within such a hierarchy of complexity[2,3] we propose also various levels of identity such as identity of substance, or identity of crystal. It will be demonstrated that the identity depends on the history of growth of particular chemical entity.

In conclusion, we intend to demonstrate how the philosophical idea about hierarchy and identity could be generalized and applied to other fields of science and philosophy of science. The discussion will be extended with the case study about the problem of hylomorphism in chemistry.[4]

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A Tale of Resilience: the Periodic System after Radioactivity and the Discovery of the Neutron

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The Periodic System is probably the most famous icon in contemporary science. Yet since it presented in 1869, the understanding of elements and chemical reactions has tremendously evolved over the last 150 years, as well as the theories on the constitution of matter's building blocks. The resilience of the periodic system to conceptual changes is remarkable, and the explanation as to how this frame of reference was perpetually renegotiated and stabilized by the scientific community is often explained as a result of the underlying atomic structure that turned out to be "true". This however could not have been the perception of the contemporary actors. This paper aims at looking how different scientists have described and used the Periodic System, to shed light on the fine structure of these adaptations.

Among others, the paper focuses on the publications by the physicist Lise Meitner and the chemist Ida Noddack, in *Die Naturwissenschaften* and *Angewandte Chemie* respectively. Written from the perspectives of a nuclear physicist and a chemist experienced in searching for undiscovered elements, they demonstrate how flexible the periodic system was to different communities and usages, yet shared as a common language.

A mechanistic-emergentist view on the relationship between protein composition, structure and function

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One of the foundational problems of biochemistry is conceptualising the relationship between the composition, structure and function of macromolecules like proteins. Notably, the recent philosophical debate is framed in terms that are quite disconnected from biochemical practice (Bartol 2016, Tobin 2010). In order to avert this limitation, this prospective presentation aims to provide a mechanistic framework of analysis (Wimsatt 2007, Bechtel and Richardson 2010).

For a protein to be functional, it must acquire its three-dimensional native structure. The starting point of our analysis stems from the realisation that native structure acquisition is a developmental process. Biochemically speaking, a proper conceptualisation of this process needs to account for each of its relevant stages, from bond formation to protein folding. It is within this developmental process that certain structural features, such as active sites and interfaces, are formed. And it is these features that account for the protein's functional capacities like the catalysis of chemical reactions, the possibility to interact with other proteins or molecules etc. Furthermore, a proper conceptualisation should account for multiple realisability (i.e., the possibility that the same function can be performed by proteins with different composition and/or structure, Alexander et al. 2009) and plasticity (i.e., the possibility that proteins with same composition and/or structure can perform different functions in different cellular contexts, Jeffreys 2017), both problems of significant interest in biochemical practice.

We shall argue that proper reductionist approaches are ultimately committed to an atomistic ontology whereby the structure and function of proteins is accounted for solely in terms of the intrinsic properties of amino acid components as if they were isolated. The fundamental problem of such accounts is that, by relying on on generative atomism (Humphreys 2016), they are forced to tacitly endorse the thesis that all causal capacities of an entity are given at the outset. Anfinsen's "dogma" and many metaphysical accounts detached from biochemical practice (Tahko 2018) can be interpreted as reductionist claims of this kind. We shall instead suggest that a conceptualisation of the relationship between proteins' composition, structure and function consistent with biochemical practice should account for the diachronic emergence of novel causal capacities on the part of proteins within a rich relational context that can be fruitfully analysed in mechanistic terms.

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Molecular structure: a systemic concept

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Molecular structure is probably the most important concept of the molecular world. Its use in today's chemistry is ubiquitous and the introduction of this concept in the XIX century changed completely the nature of chemistry: from a science of analysis to a science of synthesis [1, 2]. Molecular structure is a systemic concept [3] because it conveys information on the internal organization of a molecule. The notion that an atom is modified by its becoming part of a molecule is essential in the systemic frame of ideas; this achievement of modern science is far from the classical concept of atom [4]. Another essential aspect of molecular structure is that it endures small perturbations; its resilience to changes is crucial in defining the boundary that separates a molecule from its environment. Finally, molecular structure is dynamic, it changes with time, and its relationship with quantum dynamics [5] is part of this communication.

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Framing chemical reactivity in reciprocal action

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A *chemical reaction* is every interaction between molecules, ions or radicals in which chemical bonds are generated or broken, giving rise to new molecules. The initial molecules are called “reactants”, and the produced molecules are called “products”. Most reactions occur in solution; hence the characteristics of the solvent molecules and their interactions with the other participating molecules should be taken into account.

Chemical reactions are directed towards the production of a higher relative concentration of the most stable species. It is possible to infer which one the most stable species is by contrasting the forces of the broken bonds and the formed ones, and the energy associated with them. Reactions are represented by means of energy diagrams or reaction profiles, in which the change of the potential energy during the reaction progress is drawn. The “reaction coordinate” represents the degree of progress in which the reactants become products.

Given the standard representation of reactions, it is often considered that they occur in a *causal* way. Since chemical reactions processes are traditionally conceived in terms of a causal framework –the relation involved in chemical reactions is understood as *causality*–, the link between the species is interpreted as *successive*. In fact, such processes are viewed as if, firstly, the reagents interact and, after a while, they *cause* the appearance of the products. It is common to find this simplification in the lexicon of chemists as well as in textbooks. But if we intend to address the issue philosophically, wondering about the very nature of the chemical reactions, we can ask for the reasons for maintaining a causal picture beyond the context of teaching and professional practice. In that direction the causal-interventionist theory has been developed (Statham, 2017),

In opposition to the widely accepted causal interpretation, in this paper we will argue that chemical transformations can be more appropriately elucidated within a framework rooted in the category of *reciprocal action*, inspired in the Kantian notion (Rosenberg, 1998; Torretti, 2013). While causality is marked by succession, reciprocal action must be interpreted in terms of simultaneity. When the mechanisms involved in chemical reactions are analysed, it is necessary to take into account the interactions with the solvent, the formation of intermediary reactants, the productions of parallel reactions and simultaneous reactions, the formation of dynamic equilibrium, and so on. It is also important to bear in mind that all participants (no matter how low their concentration is) are relevant in the kinetics and thermodynamics associated with the reaction. Our main purpose is to discuss whether the Kantian category of reciprocal action is philosophically fertile to account for the nature of chemical reactions.

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POSTER PRESENTATIONS

The parchment in the drawer

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“*I had in a drawer an illuminated parchment on which was written in elegant characters that on Primo Levi, of the Jewish race, had been conferred a degree in Chemistry summa cum laude*.” wrote Primo Levi (1919-1987) in the short story Nickel in *The Periodic Table*.

The idea that the world could be explained through the study of material and therefore of CHEMISTRY, began to enter his mind while he was at high school, attending the Regio Liceo classico Massimo D’Azeglio of Turin and carrying out simple, yet effective chemical experiments in the small laboratory of Crocetta. The young and science enthusiast Primo Levi was a passionate reader: reading was indeed a happy family habit. He was also developing a positive attitude about different languages, at that time Latin and Greek, later on German and English, engaged in scientific translation. Both personal qualities played a pivotal role in his work and life.

After the final exams at the high school the idea took definite shape and Primo Levi enrolled at the Regia Università degli Studi of Turin for a degree in Chemistry. He passed the first years of his course pleasantly between examinations and the lessons and various afternoon laboratories which were to prove fertile source of inspiration for his subsequent literary work. The second and final part of his university experience took place under very different circumstances, when the moral darkness descended on Europe. Levi was busy in the preparation of two sub-theses and the degree thesis, based on a scientific review dedicated to Walden’s work on Inversion. This phenomenon, the inversion of the configuration of asymmetric carbon atoms during the nucleophile substitution reaction identified by the chemist Paul Walden in 1895 was the subject of a detailed and painstaking examination on Levi’s part. His degree thesis puts forward an argument which, within the limits imposed by the scientific knowledge of the period, was to give the great writer a brilliant degree in Chemistry.

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Conservation Science or Heritage Science? Conceptualization of a relative young scientific discipline

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The term conservation science in cultural heritage research has been constantly used in specialized publications contemporaneously to other terminology such as archaeometry, technical art history and most recently heritage science. Even if it might seem that conservation science is already a well established discipline, literature reveals the struggles of many scientists to define in a clear manner the discipline and describe the differences between the "terminology jungle". The problem of defining these new disciplines in the field of cultural heritage is not a mere issue; it is difficult to establish the correct profile of a new specialist and establish the correct criteria and methods that are to be followed in knowledge production. The historical development of the science applied to conservation of cultural heritage illustrates the evolution of the concepts and the complexity of defining the disciplinary boundaries of a multidisciplinary field. The use of "science applied to conservation" started with the early contributions of natural sciences – mainly chemistry – to the study of cultural property in the 18th century [1]. During the second half of the 20th century, modern concepts such as "archaeometry", "conservation science" and later "heritage science" have appeared [2]. Nevertheless, the efforts of specialists to define conservation science as a discipline have shown the complexity of the problem and not complete answers were reached due to controversy, and new terminology less precise, such as heritage science, has gain followers in academic context [3]. An epistemological analysis of the discipline may help to have clearer ideas about the definition of the discipline. The definition of the study object – cultural heritage – to which natural scientists have put little attention and the definition of certain methodological approaches based on theoretical premises such as structure of the objects, not only in material terms but in the complete reality (historical and social importance, sampling methods, and the impact of scientific studies of cultural heritage in their preservation and valorisation). This work presents some thoughts into the problem of the clear definition of conservation science from the theoretical point of view, by analysing the contribution of its specialists, the international projects focused on conservation science, the formation courses and the existing communities on social media, with the aim to call the attention towards the need to clearly define the discipline.

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How to Establish Periodic Law and Periodic System Relation? Inferences in the History and Philosophy of Science for Chemistry Teaching

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The importance of the philosophical and historical perspectives of science has been emphasized in science education (Matthews 2015). More particularly, it is stated that the philosophy of chemistry will contribute to the understanding of the nature of chemical knowledge in chemistry education (Scerri, 2001). The periodic table is stated as one of the most typical examples reflecting the nature of chemical knowledge and it is important in the domain-specific approach to chemistry education (Erduran, 2007). In many chemistry teaching programs around the world, the effective use of periodic table is aimed based on learning outcome. When the studies related to the periodic table are examined in the chemistry education literature, it could be seen that the studies are aimed to provide the learning of the periodic table with its current state. However, the epistemological characteristics of the table could serve to the chemistry education in different dimensions such as; effective use of the table and understanding of the nature of chemical knowledge. The key point here is the periodic law and the periodic system relation. The aim of this study is to draw attention to the epistemological nature of the periodic table in terms of its historical developmental process, which is rarely found in chemistry textbooks, and to open a door to the idea that this nature is an advantage in terms of chemistry education. For this purpose, the historical development and present situation of the periodic table are briefly mentioned, and the concepts of periodic law, periodic system and periodic table are analysed from a philosophical point of view. Afterwards, in the light of the methodological and epistemological aspects of the historical development of the periodic table, periodic law and periodic system relations is discussed in the context of the chemistry education for the effective use of periodic table. In this discussion, the hypothetical-deductive method was pointed that might be compatible for the effective use of the periodic system, and some suggestions for chemistry education have been given.

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Analogies in Chemistry: Risks and Undisclosed Potential

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Analogy is a powerful tool for the rationalization of new, unfamiliar and unknown phenomena. Indeed, an analogy explicates a target domain in terms of a base domain, which is the source of the knowledge. The target is then known mapping the base and exploiting its established understanding. Therefore, analogy allows the interpretation of a new, or relatively unknown, problems or systems in terms of an already known and well understood phenomenon, allowing steep learning curves. Analogical thinking is considered one of the main differences between humans and other primates. For these reasons analogy is extensively employed during developmental age, and, of course, in physical sciences.[1]

The pervasiveness of analogical thinking in physical sciences – and in chemistry – can be highlighted by numerous examples, and its use is even more widespread in teaching and in public understanding of science.[2] Nevertheless, there are limits to the analogical process, because the mapping of the target has a certain amount of arbitrariness and its physical meaning has to be verified. Therefore, the mapping of the target, though convincing and appealing, may be inconsistent. Moreover, the term “analogy” could refer to at least three different cognitive processes: literal similarity, analogy and abstraction. Awareness of these similar – although peculiar – relations between target and base not only helps in avoiding unphysical interpretations of the target, but allows even deeper understanding of both target and base.

In our contribution we will illustrate the power, but also the risks of analogical thinking in chemistry through few examples, namely the extension of the Sabatier principle from catalysis to electrocatalysis,[3] the Drude model for electrical conduction,[4] and the use of the Langmuir-Hinshelwood isotherm to rationalize the results of heterogeneous photocatalysis.[5] Moreover, we will demonstrate how a more aware use of analogical thinking could exploit its potential to a larger extent.

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