BOOK OF ABSTRACTS AND CONFERENCE PROGRAM

INTERNATIONAL SOCIETY FOR THE PHILOSOPHY OF CHEMISTRY

20th ANNUAL SYMPOSIUM

AUGUST 1-4, 2016
BOCA RATON, FLORIDA

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WELCOME

Dear Participants,

Welcome to the 20th annual International Society for the Philosophy of Chemistry summer symposium. This conference is made possible by your presence, by your contribution, and by the support of our sponsors. We would also like to thank Mrs. Sheryl Hulet, Senior Secretary of the philosophy department, for all her work in helping us organize this conference. We hope you will enjoy both the presentations and the beauty of Boca Raton and South Florida.

Marina P. Banchetti Robino, Clevis R. Headley
Organizers, IPSC 2016

PRACTICAL INFORMATION

DATE
August 01-04, 2016

VENUE
House Chambers
Student Activities Center
Florida Atlantic University
777 Glades Road
Boca Raton, Florida – U.S.A.

ACCESS TO THE VENUE
All necessary information and directions are in your conference documents. The Wyndham Boca Raton Hotel will provide complimentary transportation to the conference venue to all participants. The hotel shuttle will take all participants to the conference venue in the morning, and the shuttle will be available during the day to pick up participants from the conference venue to take them back to the hotel. Please inquire with the hotel staff regarding pick up times for the hotel shuttle.

REGISTRATION DESK
The registration desk will be open on Monday, 01 August 2016 from 3:00 to 6:00 p.m. and will be located in the lobby of the Wyndham Boca Raton Hotel so that participants can register after checking into the hotel. For those participants who will arrive on August 02, the registration desk will be located in the lobby of the House Chambers (conference venue) and will be open from 9:00 a.m. to 4:00 p.m. The registration desk will also be open on Wednesday, August 03 from 9:00 a.m. to 4:00 p.m. and on Thursday, August 04 from 9:00 a.m. to 12:00 p.m. to assist you and answer any questions you may have.

NAME BADGES
Upon registering, you will receive a name badge that you are requested to wear for all Symposium activities. Your badge will be your pass for ISPC-SS2016

WELCOME RECEPTION
The welcome reception is complimentary and will be held on Monday, August 01, from 6:30 to 8:30 p.m., on the poolside patio of the Wyndham Boca Raton Hotel. The reception will feature a delicious buffet that will cater to vegans, vegetarians, and non-vegetarians, keeping in mind any food restrictions that were specified in the registration forms.

CONFERENCE DINNER
You will be able to register for the conference dinner at the registration desk on Monday, August 01. The conference dinner will be held on Wednesday, August 03, from 7:30 to 9:30 p.m., at "The Farmer's Table" restaurant of the Wyndham Boca Raton Hotel. "The Famer's Table" is a 'farm to table' restaurant that serves only organic foods, grass-fed beef, free-range chicken, and sustainable seafood. The dinner buffet will feature appetizers, entrees, side dishes, and desserts that will cater to vegans, vegetarians and non-vegetarians, keeping in mind any food restrictions that were specified in the registration forms.

CATERING
All coffee breaks and refreshments will be organized in the lobby of the House Chambers (conference venue). All lunches will be organized in the Atlantic Dining Hall, which is located in the Student Union immediately outside the conference venue. Kindly consult the conference program for the times of the coffee breaks and lunches.

LECTURES
All lectures and presentations will be held in the House Chambers, which is situated on the first floor of the Student Activities Center. A laptop and beamers will be available for all participants making PowerPoint presentations. Two wireless microphones will be available, one for the speaker(s) and one for the session chair. Wireless internet connection will be available to all participants.

LIST OF PARTICIPANTS
A list of participants is provided on p. 6 of this book of abstracts.

CONFERENCE WEBSITE
Please refer to https://sites.google.com/site/ispc2016/ for more information.

EMERGENCY NUMBER
In case of emergency during the conference, please call Marina Banchetti at 561-900-8529

COMMITTEES

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- Eric Scerri – University of California, Los Angeles (U.S.A.)
- Brigitte Van Tiggelen – Chemical Heritage Foundation (U.S.A.) / Mémosciences (Belgium)

THEMES AND SESSIONS

The ISPC Summer Symposium 2016 aims to provide a forum for discussion about foundational, historical, epistemological, methodological and ontological problems of chemistry and its subfields by bringing together leading researchers and young scholars from all over the world.

The issues debated in the philosophy of chemistry have emerged from three communities: The chemists reflecting on the foundations of their science, the philosophers of science investigating the nature and specifics of chemistry, and the historian of chemistry making sense of the pathways to discoveries and the practices of chemistry in the past.

This year we are particularly pleased to feature speakers who address ethical and environmental issues that arise from the practice of chemistry, as well as speakers who address philosophically some of the specific pedagogical issues encountered in the teaching of chemistry.

This year's symposium will feature two keynote speakers, Manuel De Landa and Eric Scerri. The rest of the program of the ISPC Summer Symposium 2016 consists of eight plenary sessions, in order to foster as much in-depth discussion and interaction as possible.

The first day of the conference will be entirely devoted to registration and to the opening reception. The second and third day will consist of two morning and two afternoon sessions. The final day will consist of two morning sessions, followed by the closing of the conference and lunch.

LIST OF PARTICIPANTS

KEYNOTE SPEAKERS

- Manuel De Landa – European Graduate School (Switzerland) / Princeton University (U.S.A.)
- Eric Scerri – University of California, Los Angeles (U.S.A.)

PARTICIPANTS

- Tyler Ahlstrom – University of Pittsburgh (U.S.A.)
- Ann-Sophie Barwich – Columbia University (U.S.A.)
- Conal Boyce – Century College (U.S.A.)
- Grant Fisher – Korea Advanced Institute of Science and Technology (South Korea)
- Sebastian Fortin – CONICET, University of Buenos Aires (Argentina)
- William Hannegan – St. Louis Priory School (U.S.A.)
- Eamonn Healy – St. Edward's University (U.S.A.)
- Liu Hsuan Han – Federal University of Mato Grosso do Sul (Brazil)
- Ceth Lightfield – University of California, Davis (U.S.A.)
- Jean-Pierre Llored – University of Oxford (England) / University of Paris 7 (France)
- Olimpia Lombardi – CONICET, University of Buenos Aires (Argentina)
- Juan Camilo Martínez González – CONICET, University of Buenos Aires (Argentina)
- Hirofumi Ochiai – Nagoya Bunri University (Japan)
- Vasil Penchev – Institute for the Study of Societies and Knowledge, Bulgarian Academy of Science (Bulgaria)
- Robert Prentner – Chair for Philosophy and Laboratory of Physical Chemistry, ETH Zürich (Switzerland)
- Vanessa Seifert – University of Bristol (England)
- Yona Siderer – Edelstein Center for the History and Philosophy of Science, Technology and Medicine, The Hebrew University of Jerusalem (Israel)
- Tami Spector – University of San Francisco (U.S.A.)
- Elijah St. Germain – Department of Chemistry and Biochemistry, Florida Atlantic University (U.S.A.)
- Valery Tsimmerman – Founder and President of ORAH Constructive Technologies (U.S.A.)
- Brigitte Van Tiggelen – Chemical Heritage Foundation (U.S.A.) / Mémoscience (Belgium)
- Alfio Zambon – CONICET, University of Buenos Aires (Argentina)

KEYNOTE ADDRESSES

"NEO-MATERIALIST PHILOSOPHY AND THE HISTORY OF CHEMISTRY"

MANUEL DE LANDA
European Graduate School (Switzerland) / Princeton University (U.S.A.)

Tuesday, August 02, 2016
9:30-10:30 a.m.
(House Chambers)

"A TALE OF SIX SCIENTISTS AND A NEW PHILOSOPHY OF SCIENCE"

ERIC SCERRI
University of California, Los Angeles (U.S.A.)

Wednesday, August 03, 2016
9:00-10:00 a.m.
(House Chambers)

CONFERENCE PROGRAM

MONDAY, AUGUST 01, 2016

3:00-6:00 P.M. – **REGISTRATION** (WYNDHAM BOCA RATON HOTEL LOBBY)

6:30-8:30 P.M. – **WELCOME RECEPTION** (POOLSIDE PATIO, WYNDHAM BOCA RATON HOTEL)

TUESDAY, AUGUST 02, 2016

9:00-9:30 A.M. – **OPENING OF CONFERENCE**

9:30-10:30 A.M. – **KEYNOTE ADDRESS**

- MANUEL DE LANDA
  - "NEO-MATERIALIST PHILOSOPHY AND THE HISTORY OF CHEMISTRY"

10:30-10:45 A.M. – COFFEE AND REFRESHMENTS

11:00 A.M.-12:00 P.M. – **SESSION ONE**

- CHAIR – CLEVIS R. HEADLEY
- 11:00-11:30 A.M. – EAMONN HEALY
  - "STRUCTURAL ONTOLOGY AND CHEMICAL EPISTEMOLOGY: THE CASE OF THE π-COMPLEX"
- 11:30 A.M.-12:00 P.M. – JUAN CAMILO MARTÍNEZ GONZÁLEZ
  - "ELECTRONEGATIVITY AND ITS MULTIPLE FACES: PERSISTENCE AND MEASUREMENT"

12:00-1:30 P.M. – LUNCH

TUESDAY, AUGUST 02, 2016 (CONT.)

1:30-3:00 P.M. – **SESSION TWO**

- CHAIR – MARINA P. BANCHETTI-ROBINO
- 1:30-2:00 P.M. – HIROFUMI OCHIAI
  - "DOES A MOLECULE HAVE STRUCTURE?"
- 2:00-2:30 P.M. – TAMI SPECTOR
  - "THE MOLECULAR ELUSIVE"
- 2:30-3:00 P.M. – TYLER AHLSTROM
  - "QUANTITATIVE CALCULATIONS AND QUALITATIVE ORGANIZATION: THE PRIMARY TENSION WITHIN CHEMICAL CONCEPTS"

3:00-3:15 P.M. – COFFEE AND REFRESHMENTS

3:30-5:00 P.M. – **SESSION THREE**

- CHAIR, ERIC SCERRI
- 3:30-4:00 P.M. – ALFIO ZAMBON
  - "HOW TO HANDLE NANOMATERIALS? THE RE-ENTRY OF INDIVIDUALS INTO THE PHILOSOPHY OF CHEMISTRY"
- 4:00-4:30 P.M. – JEAN-PIERRE LLORED
  - "CHEMISTRY AND ENVIRONMENTAL PRINCIPLES"
- 4:30-5:00 P.M. – CETH LIGHTFIELD
  - "λ-CALCULUS AND ARTIFICIAL CHEMISTRIES"

WEDNESDAY, AUGUST 03, 2016

9:00-10:00 A.M. – **KEYNOTE ADDRESS**

- ERIC SCERRI
  - "A TALE OF SIX SCIENTISTS AND A NEW PHILOSOPHY OF SCIENCE"

10:00-10:15 A.M. – COFFEE AND REFRESHMENTS

WEDNESDAY, AUGUST 03, 2016 (CONT.)

10:30 A.M.-12:00 P.M. – **SESSION FOUR**

- CHAIR – CLEVIS R. HEADLEY
- 10:30-11:00 A.M. – BRIGITTE VAN TIGGELEN
  - "NICOLAS LÉMERY'S (ARTIFICIAL) VOLCANO"
- 11:00-11:30 A.M. – ANN-SOPHIE BARWICH
  - "FASHION FADES, ONLY CHANEL NO. 5 REMAINS THE SAME: A CHEMICAL HISTORY OF STYLE AND TECHNOLOGY"
- 11:30 A.M.-12:00 P.M. – VALERY TSIMMERMAN
  - "DERIVATION OF MATHEMATICAL EXPRESSION OF MENDELEEV'S PERIODIC LAW AND ITS IMPLICATIONS"

12:00-1:30 P.M. – LUNCH

1:30-3:00 P.M. – **SESSION FIVE**

- CHAIR – MARINA P. BANCHETTI
- 1:30-2:00 P.M. – SEBASTIAN FORTIN, JUAN CAMILO MARTÍNEZ GONZÁLEZ, AND OLIMPIA LOMBARDI
  - "BOHM'S *QUANTUM THEORY OF MOTION* FOR QUANTUM CHEMISTRY"
- 2:00-2:30 P.M. – WILLIAM HANNEGAN
  - "THERMODYNAMICS AND STATISTICAL MECHANICS: AN IDENTITY REDUCTION?"
- 2:30-3:00 P.M. – ROBERT PRENTNER
  - "CHEMICAL CONCEPTS FOR MIND-MATTER THEORIES"

3:00-3:15 P.M. – COFFEE AND REFRESHMENTS

3:30-5:00 P.M. – **SESSION SIX**

- CHAIR, ERIC SCERRI
- 3:30-4:00 P.M. – LIU HSUAN HAN
  - "FLOWERS, AESTHETICS IN CHEMISTRY, AND TEACHING MOLECULAR STRUCTURE"
- 4:00-4:30 P.M. – ELIJAH ST. GERMAIN
  - "DEVELOPMENT OF A TEACHING EXPERIMENT TO ELUCIDATE A CATION-π EFFECT IN AN ALKYNE CYCLITIVE ADDITION REACTION AND ILLUSTRATE HYPOTHESIS DRIVEN DESIGN OF EXPERIMENTS"

4:30-5:30 P.M. – **BUSINESS MEETING** (ISPC EXECUTIVE COMMITTEE)

7:30-9:30 P.M. – **CONFERENCE DINNER** ("THE FARMER'S TABLE" RESTAURANT)

THURSDAY, AUGUST 04, 2016

9:00-10:30 A.M. – **SESSION SEVEN**

- CHAIR – OLIMPIA LOMBARDI
- 9:00-9:30 A.M. – JEAN-PIERRE LLORED
  - "CONNECTING THE PHILOSOPHY OF CHEMISTRY AND BIOLOGY: IMPLICATIONS FOR PHILOSOPHERS AND ETHICISTS"
- 9:30-10:00 A.M. – GRANT FISCHER
  - "CONTENT, DESIGN, AND REPRESENTATION IN CHEMISTRY"
- 10:00-10:30 A.M. – YONA SIDERER
  - "UDAGAWA'S YOUAN'S (179801846) TRANSLATION OF *KOUSO SEIMIKA* 光素 舎密加 (1830): AN EXPERIMENT ON THE COMBINATION OF LIGHT ELEMENT AND WARMTH ELEMENT WITH SUBSTANCES"

10:30-10:45 A.M. – COFFEE AND REFRESHMENTS

11:00 A.M.-12:30 P.M. – **SESSION EIGHT**

- CHAIR – MARINA P. BANCHETTI
- 11:00-11:30 A.M. – VASIL PENCHEV
  - "PROBLEM OF THE DIRECT QUANTUM-INFORMATION TRANSFORMATION OF CHEMICAL SUBSTANCES"
- 11:30 A.M -12:00 P.M. – CONAL BOYCE
  - "GIVING THE ATOM ITS DUE AS WE CONSIDER OUR CORPOREAL HUGENESS AND LIBERATE OURSELVES FROM THE DUMBPLEXITY OF 'HIGHER' CHEMISTRIES (AND LIKEWISE THE DUMB THING DOWN THERE SYNDROME IN PHYSICS"
- 12:00-12:30 P.M. – VANESSA ANGELA SEIFERT
  - "EXAMINING KINCAID'S NON-REDUCTIVE UNIFICATION OF THE SCIENCES IN THE CONTEXT OF CHEMISTRY'S RELATION TO QUANTUM MECHANICS"

12:30 P.M. – **CLOSING OF CONFERENCE**

Conference Abstracts

Structural Ontology and Chemical Epistemology: The Case of the π-complex

Eamonn F. Healy

St. Edward's University, Department of Chemistry, Austin, USA
healy@stedwards.edu

In his 1949 book titled "The Electronic Theory of Organic Chemistry" , the Oxford-educated organic chemist Michael J. S. Dewar, declaring as his purpose "…to give as complete an account as possible of organic chemistry in the light of modern quantum theory", presented an ambitious mechanistic re-examination of all major organic reactions in light of "modern theory". Featured prominently throughout are mechanistic schemes involving the generation of a novel π-complex species.

In Dewar's mechanistic framework a model of the potential energy surface (PES) for a reaction is constructed with the π-complex identified as a local minimum. The observed regio- and stereochemical specificities are then used to refine and extend this model. Such a methodology would have been a radical departure from the more accepted approach at the time, which applied the fundamental principles of Robinson and Ingold's arrow notation to obtain a reaction mechanism consistent with the experimental data. Within the first, or constructive theoretical framework, a model of the PES is fashioned by assigning structures for stationary states and saddle points appropriate to their position on the hypersurface. Within the second, or principled theoretical framework, the reaction is described by applying the principles underlying the arrow notation to generate structures for appropriate chemical intermediates subject to the limitations imposed by the rules of valence.

These disparate approaches also highlight competing structural ontologies, a competition that is still in evidence today. While the proposition that the wave function in configuration space does not directly provide information about internal molecular structure was acknowledged even by Schrödinger himself, the approach known as the Quantum Theory of Atoms in Molecules allows for the recovery of classical structure through topology. While many, if not most, chemists today

consign such considerations to the realm of the philosophical, there is much that can be gleaned in this regard from recent experimental results. Specifically time-resolved spectroscopic studies of electrophilic aromatic substitution, and neutron diffraction characterization of dihydrogen complexes are analyzed in light of these ontological perspectives.

Electronegativity and Its Multiple Faces: Persistence and Measurement.

Juan Camilo Martinez[1]; Klaus Ruthenberg[2]

[1]*CONICET, Universidad de Buenos Aires; Argentina*
olimac62@hotmail.com
[2]*Coburg University of Applied Sciences and Arts, Germany; klaus.ruthenberg@hs-coburg.de*

Electronegativity is one of the most relevant concepts in chemistry used to explain many aspects of reactivity. This concept has a long existence in the knowledge of chemists but it was only defined qualitatively with the advent of the theories of bonding as "*the power of an atom in a molecule to attract electrons to itself*" (Pauling 1932). However, the concept itself is far from being precisely determined, and this problem is mainly due to the fact that electronegativity cannot be measured by direct means, and must be inferred on the basis of other properties that can be directly measured. There are two main methods of computing electronegativity: (i) a spectroscopic method, based on the ionization potential I of the isolated atom, and (ii) a thermodynamic method, which uses the enthalpy $\Delta H°$ of formation of the molecule. Although usually presented as two ways of measuring a single property, these two methods lead to different concepts. According to the spectroscopic method, electronegativity is an intrinsic property of the atoms. The thermodynamic method considers the atoms in the context of the molecules and, as a consequence, electronegativity is conceived as a relational property. Although this concept is very successful and widely used, neither a more than intuitive definition nor a generally accepted and standardized quantification model have been developed. Electronegativity is presented and discussed with respect to its main conceptual and operational continuities and discontinuities.

In this paper, we try to analyze the epistemological status of electronegativity, taking the latter as a typical example from the chemical sciences. By "epistemological status" we subsume the following issues: the question of the reference of electronegativity, its historical persistence, and the relation between (empirical) measurement and (theoretical) quantification.

Does a Molecule Have Structure?

Hirofumi Ochiai

Nagoya Bunri University, Japan
Ochiai.hirofumi@nagoya-bunri.ac.jp

The classical model of the molecule assumes that the molecule has a definite shape and structure like a mechanical object in the world of possible experience. The adequacy of the model has been studied and confirmed from the philosophical as well as from the scientific point of view.[1, 2] This study addresses the problem whether a molecule has a shape and structure at all, so as to shed more light on the foundation of the model.

As was pointed out by Woolley, an isolated molecule in a true stationary state cannot have a shape since the theory of space needs to be based on evolution in time. In addition, shape does not appear in a quantum treatment of molecules starting from first principles since the configuration space used in quantum theory is an abstract Hilbert space.[3] However, what if many-body problems can be calculated in the future without recourse to the Born-Oppenheimer approximation? What shape (or 'structure', to state it in the context of organic chemistry) will be revealed?

According to Kant, we cannot cognize objects as they might exist in themselves but only insofar as they appear to us spatiotemporally and in accordance with our concepts of them.[4]

Structure is a concept originating in the visual experience of our daily life. In other words, it is not an attribute of the molecule, but a contribution of the subject. Thus, no matter how sophisticated, a calculation is never able to determine which one among the possible structures is the right one. For molecules to have structure they must be understood by a legitimate application of the concept, and given in sensibility in such a way that they are causally connected with perception.

References

Ochiai, H.: 2013, 'The Logical Structure of Organic Chemistry and the Empirical Adequacy of the Classical Concept of the Molecule', *Hyle: International Journal of Philosophy of Chemistry*, **19**(2), 139-160.

Ochiai, H.: 2015, 'Philosophical Foundations of Stereochemistry', *Hyle: International Journal of Philosophy of Chemistry*, **21**(1), 1-18.

Woolley, R.G.: 1978, 'Must a Molecule Have a Shape?', *Journal of the American Chemical Society*, **100**, 1073-1078.

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The Molecular Elusive

Tami Spector

University of San Francisco, USA
spector@usfca.edu

From Boyle's seventeenth-century corpuscles to modern discussions of the reality of shape as a molecular property, philosophers have debated the ontology of molecules and atoms and the meanings embedded in how we envision them. In the realm of nanotechnology, the discussion has shifted from what we once knew to be invisible to what it means to "see" ultimately unseeable atoms and molecules using complex visualization technologies; a shift that reflects much of the previous cultural debate about the truth-value of photography. This talk focuses on a more neglected aspect of molecular visualization: the ways in which chemists represent the elusive and transient, and the aesthetics of these representations. Chemistry by its very nature is a science of transformation; reactions begin with knowable starting materials and end with tangible products; yet, for chemists it is often the non-isolable molecular species that exist en route from these stable endpoints that are particularly fascinating. These immaterial unstable states can only be imagined through drawn or computationally rendered molecular depictions. How chemists map chemical instability into the legible domain of molecular representations and the associative aesthetics of such representations are my focus. Specifically, I will examine two aspects of the molecular elusive: systems that exist only in extremely constrained circumstances, and once released from those conditions transform into more stable species; and transition states that can only be postulated and never exist as discrete isolable species.

Quantitative Calculation and Qualitative Organization: The Primary Tension Within Chemical Concepts

Tyler Ahlstrom

University of Pittsburgh, U.S.A.
tylerahlstrom@gmail.com

The pursuit of answers to traditional philosophical questions in the context of chemistry cannot be successful without first addressing a more basic question about what theoretical chemists are trying to accomplish with the development of their concepts. Chemical concepts are developed with two functions in mind: the precise quantitative characterization of atoms and molecules, and the organization of these chemical species along qualitative trends. For example, the concept of electronegativity can be used to assign atoms and molecules a quantitative ability to attract electrons, and also to arrange atoms and molecules in terms of their relative ability to attract electrons. While there is a sense in which the second function is a corollary of the first, the two functions often pull concepts in different directions: the more precise the concept is made to be, the less general the qualitative trends become. This tension—between quantitative calculation and qualitative organization—is debated by theoretical chemists and pervades discussions of many chemical concepts, including electronegativity, the chemical bond, aromaticity, and the atom in the molecule. So long as philosophers place value in descriptive adequacy, this poses a problem for those seeking to answer traditional philosophical questions aimed at uncovering the nature of these concepts, including questions about reduction. In particular, the tension prevents the philosopher from looking to the science to obtain a straightforward understanding of the concept, an understanding which is required before pursuing these philosophical questions. In this talk, I focus on the concept of the atom in the molecule, and show that the above mentioned tension precludes the success of attempts to determine whether it has been reduced to physical theories or models.

How to Handle Nanomaterials? The Re-Entry of Individuals into the Philosophy of Chemistry

Mariana Cordoba[1]; Alfio Zambon[2]

[1] *CONICET – Universidad de Buenos Aires, Argentina*
[2] *Universidad Nacional de la Patagonia San Juan Bosco, Argentina*
mariana.cordoba.revah@gmail.com; azambon@infovia.com.ar

The problem about which are the ontological items that chemistry –particularly, macro-chemistry– refers to has been largely discussed in the philosophy of chemistry. In this scenario, the opposition between individuals and stuff has received some attention. In the philosophical literature, the notion of chemical substance has been associated with the philosophical concept of natural kind; but natural kinds were traditionally thought as collections of individuals, given the priority of ontological categories of individual and property in physics. In the context of chemistry, by contrast, substances are more accurately understood when conceived as stuff (Ruthenberg and van Brakel 2008). Schummer (2008) analyses the difference between chemistry and physics in terms of the distinction between matter and form: while physical items are better conceived from the form perspective, the matter or stuff perspective is more suitable for chemistry; nevertheless, matter and form are complementary perspectives and should be combined for a better scientific understanding of reality. Following this line, the problem of the chemical ontology can also be thought as an issue concerning ontological categories (Lewowicz and Lombardi 2012): physical ontology is an individuals-and-properties ontology whereas chemistry deals with stuff.

Although appealing, we think that something is missing in this picture: the treatment of nanomaterials. The specificity of nanomaterials is their longitude scale: their structure is manifest between 1 and 100 nanometers –a scale of molecular order (Whitesides *et al.* 1991, Drexler 1992, Buzea *et al.* 2007). The best known examples of nanomaterials are carbon nanotubes, a stable form of carbon with unexpected properties of traction and temperature resistance, and graphene, an allotrope of carbon formed of atoms arranged in an hexagonal regular pattern similar to graphite,

but in planar sheets which are one atom thick. These materials result from the reduction of particles of a chemical substance till the nanometric scale, in which the material can show properties that are very different from the properties showed by the substance at the macro-level. While macro-substances are continuous and homogeneous, in the nanoscale atoms and their structural relations acquire central importance. The category of stuff, which can be considered appropriated in the realm of macro-chemistry, is not convenient to deal with nanomaterials. Nevertheless, the difficulties of the interpretation of the quantum ontology do not play a relevant role at the nanoscale: the spatial geometrical structure of nanomaterials is essential to their behavior.

The purpose of our presentation is to show why the consideration of nanomaterials leads to the re-entry of the category of individual into chemistry and its philosophy. A nanomaterial must be considered an individual since it is either one or multiple; it is a complete non divisible unity –if divided, different individuals result–; when nanomaterials are grouped because of their properties, some kinds emerge; and given a group of nanomaterials, each member of the group can be re-identified in it.

References

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Chemistry and Environmental Principles

Jean-Pierre Llored

Linacre College (Oxford University, U.K.) &
Laboratory Sphere (University Paris 7, France)
jean-pierre.llored@linacre.ox.ac.uk

Environmental law has always responded to risks posed by industrial society but the new generation of risks have required a new set of environmental principles, emerging from a combination of public fears, science, ethics, and established legal practice. This paper first points out how three of the most important principles of modern environmental law of this new age of ecological risk: the 'polluter pays' principle, the preventive principle and the precautionary principle interact with chemistry at large, green chemistry in particular, and chemical regulation. Conversely, we will scrutinize how green chemistry uses environmental principles in order to gain legitimacy and to widen the scope of its activities.

The second part of the paper will connect the philosophy of chemistry, ethics, and environmental principles in order to further investigate the meaning of chemical risks and hazards from the standpoint of a relational approach of chemical bodies.

To conclude, we will highlight how the notion of chemical risks implies the necessity to renew the reflection upon the meaning of environmental principles in order to address environmental issues, and especially among them, those raised by chemistry. Following this line of reasoning, we will show how mesology, that is the study of human 'milieux,' could provide interesting concepts, such as that of 'mediance' or that of 'ecumene', so as to think about the connections between science, technology, society, and the Earth.

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λ-Calculus and Artificial Chemistries

Ceth Lightfield

University of California, Davis, USA; clightfield@ucdavis.edu

Some of the earliest work in artificial chemistry research was the Algorithmic Chemistry project started by Walter Fontana. Though Fontana's early work based Algorithmic Chemistry on λ-calculus, in later work Fontana and Leo Buss report numerous problems with this approach. In response, they proposed a proof-theoretic alternative in which molecules are modeled as proofs in linear logic. Since their work concluded, many alternative artificial chemistries have been developed, including refinements of those based on λ-calculus. In this paper I address whether those refinements are enough to avoid Fontana and Buss's original criticisms. I then propose a way to move forward with a chemistry-first approach to artificial chemistry development.

Nicolas Lémery's (Artificial) Volcano

Brigitte Van Tiggelen

Chemical Heritage Foundation, Philadelphia, USA/Mémosciences asbl, Belgium
vantiggelen@memosciences.be

In 1700, at a séance de l' Académie Royale des Sciences de Paris, of which he was a member since a year, Nicolas Lémery discussed an experiment performed in his *Cours de Chymie* since a few editions, which became known for several centuries as "Lémery's (artificial) volcano". Observing the reaction of iron fillings with sulfur powder, Lémery conjectures an explanation for the underlying chemistry of volcanic activities. He develops his theory in a Mémoire, which I will examine the status of the "experiment" in Lémery's scientific method, drawing also on different mentions and versions of his displays to reconstitute volcanic eruptions. This research is part of a broader project to re-do the experiment.

Fashion Fades, Only Chanel No. 5 Remains the Same: A Chemical History of Style & Technology

Ann-Sophie Barwich

Columbia University (Center for Science and Society, Departments of Philosophy of the Biological Sciences), USA
ab4221@columbia.edu

Perfume is more than mere personal adornment. It is a chemical record of style and technology. Underlying the story of modern perfumery is a history of chemical discoveries. While perfumery might be one of the two oldest professions in the world, it owns its modern character as a semi-scientific art to the discovery and development of synthetic materials. With the rise of synthetic chemistry at the end of the 19th century, perfumes turned into an object of reproduction. A new era of industrial perfumery was about to start once the "smelling principle" of one of the most fundamental scented materials was discovered: the synthesis of vanillin from coniferyl alcohol by Ferdinand Tiemann and Wilhelm Haarmann in 1874. Since then perfumery has turned into one of the largest parts of our modern socio-economic landscape. To date, in the US alone 25 billion dollars are made annually with the production of fragrant molecules for products such as detergents, shampoos, perfumes, or soaps. Key to modern perfumery is the design of new synthetic odorants (odorous molecules) as well as an understanding of the perceptual and social dimensions of fragrance preferences.

The focus of my paper is to track the history of late 19th and 20th century perfumery as a history of chemical discoveries and a trajectory of benchmark scents. For this I am looking at the fragrant timeline from 1884's *Fougere Royale*, using the newly synthesized coumarin, to the more recent classic of 1988's *Fahrenheit*, incorporating methyl heptyne carboxylate. Blurring the boundary between what counts as natural and artificial in both a material and a perceptual sense, perfumery presents us with a domain that embodies several disciplinary identities: from being a guarded art and craft to turning partly into a techno-science. By using the invention of new chemicals as a

historiographical tool, I analyze the generation of a chemical repertoire and the idea of benchmark scents in an increasingly techno-scientific context as constitutive of the special disciplinary identity of perfumery: a semi-science. I want to understand what characterizes *semi*-scientific practices that may further offer us a renewed perspective on the nature of science and its progression.

Derivation of Mathematical Expression of Mendeleev's Periodic Law and Its Implications

Valery Tsimmerman P.E.

ORAH Constructive Technologies, Inc., U.S.A.
orahct@gmail.com

Numerical relationships between atomic weights of chemical elements paved the way for the discovery of the periodic table and played an important role in its early development. Many numerical relationships have been pointed out by different authors since that time, yet those relationships captured only certain aspects of the periodic system and were unable to describe the system as a whole in mathematically concise manner. A few years ago the author of this article came across yet another mathematical relationship evident in the periodic table which led him to a realization of its tetrahedral nature. This provided him with unique opportunity for deriving algebraic expressions of the sequence of alkaline earth atomic numbers, period lengths and, finally, the algebraic expression of the periodic system as a whole. This system of equations is capable of generating all groups of elements found in traditional periodic table, with only one exception: it places Helium at the beginning of alkaline earth group of elements. The placement of Helium among noble gases has been previously contested by few authors, mostly on a basis of its atomic structure. This new system of equations mathematically describes position of all elements in their respective groups as presented in Janet's Left Step Periodic Table.

Bohm's *Quantum Theory of Motion* for Quantum Chemistry

Sebastian Fortin; Juan Camilo Martínez González;
Olimpia Lombardi

CONICET – Universidad de Buenos Aires, Argentina
sfortin@gmx.net; olimac62@hotmail.com
olimpiafilo@arnet.com.ar

The relationship between chemistry and physics has been one of the most important topics in the recent philosophy of chemistry. In this context, the links between theories coming from both disciplines have been explored with great detail from different perspectives. However, despite this effort, there is still no agreement between specialists with respect to which is the best inter-theoretic relationship for describing the links between chemistry and physics.

According to the orthodox view, it is possible to reduce chemistry to quantum mechanics: the difficulties are only due to the complexity of the equations. For this reason, in practice physicists introduce some approximations to simplify calculations. However, in some cases approximate methods can deform the heart of quantum mechanics, in such a way that the reduction's success is disputed (Woolley 1976, 1978, 1998). Some authors claim that approximations introduce assumptions that are incompatible with quantum mechanics itself (Lombardi and Castagnino 2010, Chang 2015). On the other hand, the description of certain basic elements for chemistry in quantum terms has proven to be problematic. For instance, the concept of molecular structure finds no place in the theoretical framework of quantum mechanics because it appeals to a classical notion as fixed nuclei positions (Woolley 1978). The nature of chemical bond and orbitals seems to be alien to the quantum mechanics perspective (Vemulapalli 2008, Labarca and Lombardi 2010, Llored 2010, Hendry 2012).

Most of the philosophical difficulties mentioned above are consequences of the peculiar features of ordinary quantum mechanics. However there is an alternative quantum formalism proposed by David Bohm in 1952. The Quantum Theory of Motion (Holland 1993) writes the Schrödinger

equation in a different but equivalent way. The result is an equation that is formally identical to the Hamilton-Jacobi equation of classical mechanics, where a classical potential is added to the quantum terms. This novel term is then interpreted as a quantum contribution to the total potential. On the basis of this fact, the Quantum Theory of Motion proposes a new quantum theory in which the classical equations and the classical ontology are maintained, but a new fundamental force is introduced, the quantum force. Thus one obtains a deterministic quantum mechanics in which particles have definite positions and velocities at any given time, i.e. they have well-definite paths.

In this work we propose a perspective different from the traditional one to analyze philosophical problems in quantum chemistry. We claim that the introduction of the Quantum Theory of Motion

may clarify some problems and to dissolve others. The possibility of definite positions for fixed nuclei simplifies the interpretation of the approximations in quantum chemistry. On the other hand this theory allows us to analyze the position of an electron in a chemical bond. In the particular case of the simple H-H covalent bond, computations lead to conclude that the electrons are in the middle of the two nuclei. In this way, we recover the "picture" of the classical chemistry viewpoint.

As a conclusion, we propose to explore the possibility that, from the conceptual point of view, the Quantum Theory of Motion be a more adequate theory for quantum chemistry.

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Thermodynamics and Statistical Mechanics: An Identity Reduction?

William Hannegan

St. Louis Priory School, U.S.A.
whannegan@niu.edu

Statistical mechanics provides an inter-mechanistic explanation for the properties of thermodynamics. Philosophers often take this to mean that thermodynamic properties can be reduced *ontologically* to the properties of microscopic objects, and that this reduction is a straightforward reduction of identity. Philosophers also use this purported reduction to model and motivate other identity reductions—especially the reduction of mental properties to neurological properties in philosophy of mind. I argue, however, that the successful explanation of thermodynamic properties in terms of statistical mechanics does not warrant an ontological reduction of identity. I make this argument by appealing to the causal theory of properties and multiple realizability. I also show that some of the replies to the problem of multiple realizability (the employment of multiply referring expressions, domain-specific reduction, and the disjunctive approach), which may be promising in philosophy of mind, are nevertheless inadequate for preserving the identity reduction of thermodynamic properties.

Chemical Concepts for Mind-Matter Theories

Robert Prentner

ETH Zürich, Chair for Philosophy and Laboratory of Physical Chemistry, Switzerland
robert.prentner@phil.gess.ethz.ch

Recently, some parallels have been drawn between the philosophy of mind and the philosophy of chemistry [1]. In the following contribution I wish to discuss two related premises for future mind-matter theories:

1). In current discussions in the philosophy of mind the notion of emergence figures prominently, either as meaningful concept that might bridge the explanatory gap between mind and matter or as fundamentally mistaken idea. A different approach that undermines the artificial demarcation between a productive (mental) and a non- productive (material) domain would posit an inherently productive natural world to start with. *Nature is necessarily productive.*

2). Scientific theories are formally structured. One such structural feature is embodied in the mereology of a theory. The mereology of chemistry is formally rigorous but at the same time context-dependent and dynamic [2,3], which has important consequences for the discussions regarding the substantiality of things and natural productivity. Still, the question remains whether this should be interpreted in terms of a re-description (or dissolution) of seemingly troubling problems in the philosophy of mind or whether it further emphasizes the problematic: the *ubiquitous and irreducible role of mind and consciousness in science*.

These points shall be illustrated with respect to the recent literature from the philosophy of chemistry using examples and formal models. Future mind-matter theories could seriously profit from insights generated in the philosophy of chemistry. However, there are also some issues that seem to go beyond the scope of the current debates.

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Flowers, Aesthetics in Chemistry and Teaching Molecular Structure

Liu Hsuan Han; Onofre Salgado Siqueira

Federal University of Mato Grosso do Sul – UFMS, Brazil
tensaidota@gmail.com

Aesthetics in chemistry is a theme of several investigations on Philosophy of Chemistry, almost always related with molecular structure or structures of materials [J. Schummer, HYLE, vol. 9 (2003), nº 1, 73-104 for example].

On the other hand, teaching molecular structure concepts at public high schools in the State of Mato Grosso do Sul – Brazil has been shown a difficult problem. That is, the topic of chemistry related with beautifulness for the chemists and very important for the development of this science for the philosophers of chemistry, appears no making senses for the students.

So, we propose a didactic sequence involving the beautifulness of the flowers, related with their structures, to present the importance of to think about the structures of molecules before to initiate the teaching of the VSEPR theory. This was done by a homemade video (30 sec) composed by several imagines of flowers, mailing orchids, that finished with a close view of a drop of water on the petal of the one flower – inside the drop was drawn a molecule of water, to call attention to the theme of the class.

The sequence was applied in two first year classes: the motivation of the students was greatly increased and scores of the tests was higher than the previous one.

Development of a Teaching Experiment to Elucidate a Cation-π Effect in an Alkyne Cyclitive Addition Reaction and Illustrate Hypothesis Driven Design of Experiments

Elijah J. St. Germain; Andrew Horowitz; Dominic Rucco;
Evonne M. Rezler; Salvatore Lepore

Florida Atlantic University, Department of Chemistry and Biochemistry, Boca Raton, USA
estgerma@fau.edu

An organic chemistry experiment is described that is based on recent research to elucidate a novel cation-π interaction between tetraalkyl ammonium cations and propargyl hydrazines. This non-bonded interaction is a key component of the mechanism of ammonium-catalyzed intramolecular cyclitive addition of nitrogen to the terminal carbon of a C-C triple bond of the propargyl substrate. In this teaching experiment, reactions and control experiments are employed to demonstrate the testing of two alternative mechanistic hypotheses via the criterion of falsification. Specifically, cyclization reactions are performed with a soluble base (sodium phenoxide) with and without tetrabutylammonium bromide under homogeneous conditions. Students observe that the added ammonium salt accelerates the reaction. They are then encouraged to develop a testable hypothesis for the role of the ammonium salt in the cyclization mechanism: typical phase transfer or other. IR spectroscopy is then used to directly observe a dose dependent shift of the alkyne stretching mode due to a cation-π interaction. In this experiment, undergraduate researchers are able to practice the scientific method on a contemporary system and see how data are generated and interpreted to adjudicate between rival hypotheses in a way that emulates authentic and current research in a lab setting. This experimental design demonstrates the combination of falsificationism and confirmationism that are typically employed by synthetic organic chemists in making the case for a novel intermolecular interaction.

Connecting the Philosophy of Chemistry and Biology: Implications for Philosophers and Ethicists

Jean-Pierre Llored

Linacre College (Oxford University, U.K.) &
Laboratory Sphere (University Paris 7, France)
jean-pierre.llored@linacre.ox.ac.uk

The paper is about new philosophical perspectives brought to the fore by philosophers of chemistry and biology, and which, according to us, are of importance in order to renew philosophical and ethical perspectives on organisms, emergence, life, disease, and on the relationships between human beings and the Earth understood as a whole.

The starting point of this paper is the scrutiny of current chemistry and biology. Following this line of enquiry, we will point out: (1) the co-definition of chemical relations (transformations) and chemical *relata* (bodies) within chemical activities; (2) the constitutive role of the modes of intervention in the definition, always open and provisional, of 'active' chemical bodies; and (3) the mutual dependence of the levels of organization in chemistry. We will insist on the way chemists tailor *networks of interdependencies* within which chemical bodies and properties are context-sensitive and mutually determine by means of particular chemical operations or transformations. We will then focus our attention on the ways philosophers of immunology investigate biological identity and redefine organisms (Pradeu 2012). We will also highlight the constitutive role of the contexts in the expression of genes in epigenetics, and how neuroscience now describe the brain using complex modelling. Eventually, we will study how biosemiotics refers to the co-definition of a living species and its 'Umwelt.'

Following the aforementioned perspectives, the last part of the paper will propose new developments about the ways of conceiving: (1) individuals, organisms and subjecthood; (2) relational and intrinsic properties; (3) emergence and reduction, and (4) new concepts from which we could develop a new kind of environmental ethics in connection with a new kind of humanism,

that is to say, not an 'abstract humanism' cut off from the whole Earth and the other forms of life, but, by contrast, a humanism thought in mutual dependence with other 'milieux,' be they human or not.

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Content, Design, and Representation in Chemistry

Grant Fisher

Korea Advanced Institute of Science and Technology, South Korea
fisher@kaist.ac.kr

The aim of this paper is to engage with the interplay between *content* and *design* in representation in chemistry and explore its epistemic consequences. By "content" I mean the properties attributed to the representational target. "Design" consists of the tools and media used to convey that content: marks, lines, topological tools, graphs, alphanumeric characters, shading, tones, contrasts, colours, textures, etc., using various media from pencil-and-paper to computer graphics. Representation is selective and this selectivity of representational content can arise in various ways. I argue that designs help us to manipulate selectivity and constraints on representational content in epistemically significant ways.

Representational content can depend on the choice of instrumentation and the material conditions of experimentation. One aim of representation in chemistry is to work around this instrumental selectivity by a kind of abstraction whereby practitioners attempt to represent plural predicative content. Drawing on literature in philosophy of art and as well as philosophy of science, I argue that while practitioners make specific commitments to represent certain properties or to choose to leave them out, sometimes representing a target as possessing a certain property can involuntarily rule out the representation of others. As a result representational occlusions arise, which are a feature of our representational practices. This paper argues that designs are *representational schemes* that not merely convey content but determine the content cognitive agents are capable of representing. The generativity of design practices creates the conditions for manipulating constraints on representational content and hence knowledge of target systems in chemistry.

Udagawa Youan's (1798-1846) Translation of *Kouso Seimika*光素 舎密加 (1830): An Experiment on the Combination of Light Element and Warmth Element with Substances

Yona Siderer

Edelstein Center for the History and Philosophy of Science, Technology and Medicine,
The Hebrew University of Jerusalem, Israel
sideryon@netvision.net.il

Translation of chemistry books from the West started in Japan in early 1800s in order to be able to confront and adapt western civilization. Udagawa Youan (1798-1846) translated the most important book on chemistry, *Seimi Kaiso*, "Introduction to chemistry", published 1837-1847. For the introduction of a new discipline with a different world view, what terms did Udagawa Youan use? Old terms or new ones? The question relates to names of chemical elements, compounds, tools, chemical processes and manufacturing methods. Due to the *Bakufu* regime rulings, mainly books in Dutch were allowed to be introduced into Japan. Thus Dutch translations of books from England, Germany, France, Sweden and Italy were imported. Udagawa Youan used the Dutch translations of more than twenty books from Europe in his studying and writing *Seimi Kaiso* and other botany and chemistry books. Those books that he possessed indirectly emphasize the wide exchange of scientific knowledge among European scholars, in contrast with the work in isolation of the Japanese scholars.

Currently we study Udagawa Youan's book *Kouso Seimika*, "Chemistry of the Element of Light" that is held at Kyo-U archive of Takeda Science Foundation in Osaka. Based on Lavoisier's *Traité Élémentaire de Chimie* Youan wrote "On the combination of light element and heat element with different substances". His translation is studied and will be compared with the French original, its English translation and the Dutch translation by N.C. Fremery, (*Grondbeginselen der Scheikunde*, (1800), the last one Youan used. Youan's chemistry writing, his new terminology, as well as his

own life will be presented. The obstacle in translation some Dutch terms will be shown. Youan's consideration of the term 'God', coming from different faith than Lavoisier, lead him to some changes in the Japanese text. Nevertheless, Youan was the greatest pioneer of introducing natural sciences language and coining new terms for botany and chemistry. It will be shown that some of those terms are in use today.

Problem of the Direct Quantum-Information Transformation of Chemical Substance

Vasil Penchev

Bulgarian Academy of Sciences: Institute for the Study of Societies and Knowledge, Bulgaria
vasildinev@gmail.com

Arthur Clark and Michael Kube–McDowell ("The Triger", 2000) suggested the sci-fi idea about the direct transformation from a chemical substance to another by the action of a newly physical, "Trigger" field. Karl Brohier, a Nobel Prize winner, who is a dramatic persona in the novel, elaborates a new theory, re-reading and re-writing Pauling's "The Nature of the Chemical Bond"; according to whom: "Information organizes and differentiates energy. It regularizes and stabilizes matter. Information propagates through matter-energy and mediates the interactions of matter-energy." Dr Horton, his collaborator in the novel replies: "If the universe consists of energy and information, then the Trigger somehow alters the information envelope of certain substances –". "Alters it, scrambles it, overwhelms it, destabilizes it" Brohier adds.

There is a scientific debate whether or how far chemistry is fundamentally reducible to quantum mechanics. Nevertheless, the fact that many essential chemical properties and reactions are at least partly representable in terms of quantum mechanics is doubtless. For the quantum mechanics itself has been reformulated as a theory of a special kind of information, quantum information, chemistry might be in turn interpreted in the same terms.

Wave function, the fundamental concept of quantum mechanics, can be equivalently defined as a series of qubits, eventually infinite. A qubit, being defined as the normed superposition of the two orthogonal subspaces of the complex Hilbert space, can be interpreted as a generalization of the standard bit of information as to infinite sets or series. All "forces" in the Standard model, which are furthermore essential for chemical transformations, are groups [U(1),SU(2),SU(3)] of the transformations of the complex Hilbert space and thus, of series of qubits.

One can suggest that any chemical substances and changes are fundamentally representable as quantum information and its transformations. If entanglement is interpreted as a physical field, though any group above seems to be unattachable to it, it might be identified as the "Triger field". It might cause a direct transformation of any chemical substance by from a remote distance. Is this possible in principle?

Giving the Atom Its Due as We Reconsider Our Corporeal Hugeness (Schrödinger 1944) and Liberate Ourselves From the Dumbplexity of the 'Higher' Chemistries (and Likewise the Dumb Thing Down There Syndrome in Physics)

Conal Boyce

Century College, U.S.A.
conalboyce@gmail.com

Why is the ATOM so small?' In the annals of science, it is a pivotal moment when Schrödinger turns that tired question around to ask: 'Why are WE so huge?' Granted, the whole train of thought turns out to be a red herring that he disavows in Chapter 2. But that twist needn't concern us here. Rather, what should excite us is that someone, however briefly, *did* invert the question, which might inspire one to push on in this direction: "Instead of asking, 'Why are atoms so FAST?' let's consider, 'Why are we so SLOW?' " From the atomic perspective, contraptions that exist on the macroscopic scale (such as ourselves) might be deemed too absurdly large and slow to count even as coherent entities, much less living ones. Does my argument for the atomic realm as the locus of life sound outré? This might be due in part to certain biases we all hold that are difficult to see. In the essay, I articulate two such biases. The first I call Dumb Thing Down There (DTDT) syndrome. It is the unstated premise of all particle physics: For the rule-bearing 'cue-sticks' of the theoreticians to shine, there must be some maximally dull 'billiard balls' to be pushed about on the table. The second I call *dumbplexity*. When we rush into the 'higher' chemistries without even bidding adieu to the real thing, 'basic' chemistry, that is an example of dumbplexity-awe.

Far from being able to comprehend the blitz of activity at the atomic level, we are not even able to grasp *One Human Minute* (Lem 1986), way up here in the macroscopic realm. Closely related to the fraud of 'world news' (as detailed by Lem), we have also the Information Age to consider (a flat impossibility for us slow-moving simians, yet trumpeted every ten years or so). In concert with

the Information Age, we hear talk often of 'information theory,' a factoid that hitches a ride atop Shannon's *mathematical* theory of *data* communication. (Somewhere in the universe, a *true* information theory has been attempted, or shall be some day, so the term 'information theory' should not be defiled by us as a cheap sound bite.)

Thematic link between [1] my BCCE (*Biennial Conference on Chemical Education*) presentation and [2] the present paper: At the BCCE 2014, I pitted electrons in a wire, moving at a literal snail's pace, against the electromagnetic wave-front traveling near c over the same wire, and showed how the echem mechanism relies almost exclusively on the latter. (Meanwhile, textbooks at all levels persist in their fairy-tale of 'electron flow.') In the present article, I allude to the ten nanoseconds required for an atomic electron to return to ground state, my aim being to stimulate interest in the flip-side of that oft-quoted timing data: Namely, what goes on in the atom during the *other* 999,999,990 billionths of that same second? The common theme is: Speed matters. What to do? Study physical chemistry, the best window we have.

Examining Kincaid's Non-Reductive Unification of the Sciences in the Context of Chemistry's Relation to Quantum Mechanics

Vanessa Angela Seifert

University of Bristol, U.K.
vs14902@bristol.ac.uk

There has been extensive discussion about the relation of chemistry with quantum mechanics. Focusing on chemistry's and quantum mechanics' descriptions of molecular structure, the debate upon the relation of the two sciences unfolds through the development of two opposing views.

On the one hand, reductionists hold that chemistry is reducible to quantum mechanics in such a way that, (1) the vocabulary of the higher-level theory is translatable into the vocabulary of the lower-level theory via the identity relation or the use of bridge laws, (2) the postulations of the higher-level theory are deducible by those of the lower-level theory, (3) the lower-level theory sufficiently explains and predicts all phenomena that the higher-level theory explains and predicts. The reductionist position towards the relation between the two theories has both epistemological and ontological implications. The epistemological ones are that, in principle, quantum mechanics could substitute chemistry in the description, explanation and prediction of chemical phenomena. The ontological implication is that, since chemical theory is reduced to quantum mechanics, higher level entities can either be taken to be eliminated by the lower-level ones, or be vindicated in terms of their existence, by their identification to real lower-level entities.

On the other hand, emergentists hold that chemical theory cannot be reduced to quantum mechanics and that, consequently, the chemical concepts employed to describe chemical phenomena have a distinct ontological status; namely they emerge from the lower level entities, and they possess distinct causal powers with respect to them. This ontological position understands higher-level entities, not only as having distinct existence with respect to the lower- level entities from which they are composed of, but also as having independent causal powers that determine and explain the behaviour of the lower-level entities on which they supervene (i.e. downwards causation).

The paper rejects both of these positions and claims that there is a middle way of understanding this relation through Harold Kincaid's idea of non-reductive unity of the sciences. Kincaid's "unity- without-reducibility model" proposes an alternative view of the relation between chemistry and quantum mechanics that requires the ontological supervenience of chemical entities on quantum mechanical ones, without committing oneself to reduction or emergence. Rather, chemistry and quantum mechanics form an "integrated interleveled theory" that describes, explains and predicts molecular structure through the evidential, explanatory and descriptive contribution of both sciences. Apart from the apparent epistemic implications that this position has to the explanatory, predictive and heuristic dependence of the two theories, there are also interesting ontological implications concerning the reality of chemical entities.

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