

# ISPC PARIS CONFERENCE

## *PHILOSOPHY OF CHEMISTRY*

ORGANIZER: DR. JEAN-PIERRE LLORED

JULY 3-6, 2017

LABORATORY SPHERE  
UNIVERSITY PARIS DIDEROT, PARIS,  
FRANCE

ROOM L. VALENTIN, 454A (LEVEL 4). BUILDING CONDORCET,  
10, RUE ALICE DOMON ET LÉONIE DUQUET, 75013 PARIS

GRAPHIC CONCEPTION: THÉO CHAZAUD



INTERNATIONAL SOCIETY FOR THE  
PHILOSOPHY OF CHEMISTRY



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de paris

SΦHERE  
SCIENCES, PHILOSOPHIE, HISTOIRE  
UMR 7219



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Mélissa Druet's courtesy

## **I. ISPC**

The International Society for the Philosophy of Chemistry (ISPC) is devoted to the international exchange of ideas concerning the philosophical foundations of the chemical sciences and related areas. This exchange fosters discourse between chemists, biochemists, philosophers, historians, sociologists, and educators.

Philosophy of chemistry concerns both internal questions arising from the methods, concepts, and ontology unique to chemistry and chemical research as well as traditional questions in the philosophy of science, addressed from a chemical perspective.

ISPC President: Rom Harré, Georgetown University (USA), Linacre College (Oxford University, UK).

ISPC Executive Committee:

- Michael Akeroyd (Bradford College, United Kingdom).
- Robin Hendry (University of Durham, United Kingdom).
- Olimpia Lombardi (Universidad de Buenos Aires, Argentina).
- Paul Needham (Stockholm University, Sweden).
- Guillermo Restrepo (Universidad de Pamplona, Colombia).
- Klaus Ruthenberg (Hochschule Coburg, Germany).
- Eric Scerri (University of California, USA).
- Brigitte Van Tiggelen (Chemical Heritage Foundation, USA & Mémosciences, Belgium).

## **II. OUR SPONSORS**

The ISPC annual summer symposium will be held on July 3-6, 2017 at the Laboratory Sphère, which belongs to the University Paris 7, in Paris (France).

We gratefully acknowledge the support of our sponsors:

- The International Society for the Philosophy of Chemistry (ISPC).
- The laboratory SPHERE, Mixed Research Unit between the University Paris 7 and the CNRS.
- The department of History and Philosophy of Science at the University Paris 7.
- The Institute of Humanity and Science at the University Paris 7.
- The laboratory LIED, Mixed Research Unit between the University Paris 7 and the CNRS.
- The ‘Fondation de la maison de la chimie’: The Foundation of the House of Chemistry.
- The ‘Société Chimique de France (SCF)’: The French Chemical Society.
- The ‘Commissariat à l’Energie Atomique de Saclay (CEA)’: The French Atomic Energy Commission at Saclay.
- France-Intec Bourbonnais.

We also gratefully acknowledge the intellectual support of:

- The ‘Société Française d’Histoire des Sciences et des Techniques (SFHST)’: The French Society for the History of Science and Technology.
- The French Group for the History of Chemistry (GHC).
- The Circle of the Philosophers of Nature supervised by Miguel Espinoza.

### III. ORGANIZER AND SCIENTIFIC COMMITTEE

The ISPC Paris Conference is organized by Dr. Jean-Pierre LLORED (Laboratory Sphère, University Paris Diderot, France; Linacre College, Oxford University, Oxford, UK). Jean-Pierre Llored was helped by the following scientific committee for determining the programme of the conference:

Marina Banchetti-Robino (Florida Atlantic University, USA).  
José Antonio Chamizo (Universidad Nacional Autónoma de México, Mexico).  
Didier Debaise (Free University of Brussels, Belgium).  
Rémi Franckowiak (Université Lille 1, France).  
Michele Friend (Georgetown University, USA).  
Gabriela García-Zerecero (Universidad Panamericana, Guadalajara campus, Mexico).  
Rom Harré (Linacre College, Oxford University, UK).  
Clevis Headley (Florida Atlantic University, USA).  
Robin Hendry (University of Durham, UK).  
Mehrnaz Katouzian-Safadi (CNRS, Laboratory SPHERE, University Paris 7, France).  
Muriel Le Roux (CNRS, Institut d'histoire moderne et contemporaine, France).  
Jean-Pierre Llored (Laboratory Sphère, University Paris 7 & Linacre College, Oxford, UK).  
Olimpia Lombardi (Universidad de Buenos Aires, Argentina).  
Alfred Nordmann (Technische Universität Darmstadt, Philosophy Department, Germany).  
François Pépin (Institut d'Histoire des Représentations et des Idées dans les Modernités, Ecole Normale Supérieure de Lyon, France).  
Guillermo Restrepo (Universidad de Pamplona, Colombia).  
Pierre Teissier (University of Nantes, France).  
Benoît Timmermans (Free University of Brussels, Belgium).  
Sacha Tomic (Institut d'Histoire Moderne et Contemporaine, Panthéon-Sorbonne University, France).  
Brigitte Van Tiggelen (Chemical Heritage Foundation, USA & Mémosciences, Belgium).

### IV. INVITED SPEAKERS AND PARTICIPANTS

The keynote speakers are:

- Bernadette Bensaude-Vincent (University Paris 1 Sorbonne, France).
- Augustin Berque (*École des hautes études en sciences sociales*, France).
- Hasok Chang (University of Cambridge, UK).
- Ludovic Duhem (University of Lille 3, ESAD Orléans and Valenciennes, France).
- Franck Dumeignil (Chemistry Department, University of Lille 1, France).
- Rom Harré (Linacre College, Oxford University, UK) in collaboration with Jean-Pierre Llored (Laboratory Sphère, University Paris 7, France; Linacre College, Oxford University, Oxford, UK).
- Michel Morange (*École Normale Supérieure de la rue d'ULM*, France; President of the International Society for the History, Philosophy, and Social Studies of Biology)
- Stéphane Sarrade (*Commissariat à l'énergie atomique et aux énergies alternatives de Saclay*, France).
- Eric R. Scerri (University of California, Los Angeles, USA).
- Joachim Schummer (Editor of HYLE: International Journal for Philosophy of Chemistry, Germany).

The participants are:

Yaman Abdin, Saarland University, Germany.

Hernán Accorinti, University of Buenos Aires, Argentina.

Mathieu Arnoux, University Paris 7 & Ecole des Hautes Etudes en Sciences Sociales, France.

Marina Paola Banchetti-Robino, Florida Atlantic University, USA.

Martine Benoit, Maison Européenne des Sciences de l'Homme et de la Société, Lille, France.

Geoffrey Blumenthal, University of Bristol, UK.

Luigi Cerruti, University of Torino, Italy.

José A. Chamizo, Universidad Nacional Autónoma de México, Mexico.

Mariana Córdoba, University of Patagonia San Juan Bosco, Argentina.

Pascal Crozet, CNRS, SPHERE, France.

Sébastien Dutreuil, Max Planck Institute for the History of Science, Germany.

Grant Fisher, Korea Advanced Institute of Science and Technology, Korea.

Sebastián Fortín, CONICET, University of Buenos Aires, Argentina.

Mareike Frevert, University of Kassel, Germany.

Michele Friend, Georgetown University, USA.

Gabriela García Zerecero, Panamericana University, Mexico.

Elena Ghibaudi, University of Torino, Italy.

Clevis R. Headley, Florida Atlantic University, USA.

Sarah Hijmans, University Paris 7, France.

Alexandre Hocquet, University of Lorraine – LHSP Archives Poincaré, France.

Claus Jacob, Saarland University, Germany.

Martín Labarca, CONICET, University of Buenos Aires, Argentina.

Olimpia Lombardi, CONICET, University of Buenos Aires, Argentina.

Juan Camilo Martínez González, University of Buenos Aires, Argentina.

Benjamin J. McFarland, Seattle Pacific University, USA.

Hirofumi Ochiai, Nagoya Bunri University, Japan.

Dominique Pecaud, Ecole polytechnique de l'université de Nantes, France.

François Pépin, IHRIM-ENS de Lyon, France.

Guillermo Restrepo, University of Pamplona, Colombia & Leipzig University, Germany.

Klaus Ruthenberg, Coburg University of Applied Sciences and Arts, Germany.

Vanessa Seifert, University of Bristol, UK.

Yona Siderer, The Hebrew University of Jerusalem, Israel.

Tami Spector, University of San Francisco, USA.

Benoît Timmermans, Free University of Brussels, Belgium.

M.E. Tobin, Independent Scholar, USA.

Sacha Tomic, University Paris 1 Sorbonne-IHMC, France.

Frédéric Wieber, University of Lorraine – LHSP Archives Poincaré, France.

Alfio Zambon, University of Patagonia San Juan Bosco, Argentina.

## V. CONFERENCE PROGRAMME

### MONDAY 3RD, 2017

8:30 Welcome coffee

9:00 Introduction by Pascal Crozet (Dir. of SPHERE) and Jean-Pierre Llored (SPHERE & Linacre College, Oxford University).

#### 9:15-10:15 Plenary lecture

**Eric Scerri (University of California, USA): *An assessment of Woody's thesis on the turn to practice and representations of the periodic table***

10:15-10:30 Coffee break

10:30-12:30 // SESSION 1 // Chair: Eric Scerri (University of California, USA)

- 10:30-11:00 Benjamin J. McFarland (Seattle Pacific University, USA): *Inorganic chemistry, causation, and prediction in natural history*
- 11:00-11:30 Mathieu Arnoux (Paris Diderot University & Ecole des Hautes Etudes en Sciences Sociales, France): *Iron and steel in preindustrial times: words, commodities and chemical element*
- 11:30-12:00 Sarah Hijmans (Paris Diderot University, France): *What are elements? A pragmatic approach to the meaning of a chemical concept*
- 12:00-12:30 Juan Camilo Martínez González & Hernán Accorinti (University of Buenos Aires, Argentina): *Idealized quantum chemistry? Approximations and molecular structure*

12:30-13:30 Lunch

13:30-16:00 // SESSION 2 // Chair: Grant Fisher (Korea Advanced Institute of Science and Technology, Korea)

- 13:30-14:00 Gabriela García Zerecero (Panamericana University, Mexico): *Philosophy of science and ontology*
- 14:00-14:30 Sebastián Fortín, Martín Labarca & Olimpia Lombardi (CONICET, University of Buenos Aires, Argentina): *On the ontological status of molecular structure: is it possible to reconcile molecular chemistry with quantum mechanics?*
- 14:30-15:00 Guillermo Restrepo (University of Pamplona, Colombia & Leipzig University, Germany): *A categorical formalism for classification of chemical substances*
- 15:00-15:30 Vanessa Seifert (University of Bristol, UK): *Downwards causation for the case of molecular structure*
- 15:30-16:00 Alfio Zambon & Mariana Córdoba (University of Patagonia San Juan Bosco, Argentina): *Nanomaterials and intertheoretical relations: macro and nanochemistry as emergent levels*

16:00-16:30 Coffee break

#### 16:30-17:30 Plenary lecture

**Rom Harré, Linacre College, Oxford University) & Jean-Pierre Llored (SPHERE & Linacre College): *Procedures, Products and Pictures***

17:30-18:30 ISPC meeting

## TUESDAY 4TH, 2017

8:30 Welcome coffee

### 9:00-10:00 Plenary lecture

**Bernadette Bensaude-Vincent (University Paris 1 Sorbonne, France):**  
*What carbon teaches to philosophers*

10:00-10:30 Coffee break

10:30-12:00 // SESSION 3 // Chair: Bernadette Bensaude-Vincent (University Paris 1 Sorbonne, France)

- 10:30-11:00 François Pépin (IHRIM-ENS de Lyon, France): *Chemistry and materialism: from matter to materiality*
- 11:00-11:30 Klaus Ruthenberg (Coburg University of Applied Sciences and Arts, Germany): *No analysis without synthesis*
- 11:30-12:00 Yaman Abdin & Claus Jacob (Saarland University, Germany): *The matter of impurities in pharmaceuticals: Substances without a name and how to handle them*

### 12:00-13:00 Plenary lecture

**Augustin Berque (Ecole des Hautes Etudes en Sciences Sociales, France):**  
*Trajective chains in mesology, von Neumann chains in physics, etc. - and chemistry*

13:00-14:00 Lunch

### 14:00-15:00 Plenary lecture

**Stephane Sarrade (CEA of Saclay, France):** *Green chemistry and sustainable development: a survey*

15:00-16:30 // SESSION 4 // Chair: Klaus Ruthenberg (Coburg University of Applied Sciences and Arts, Germany)

- 15:00-15:30 Benoît Timmermans (Free University of Brussels, Belgium): *REACH's impact on the ways of thinking and making chemistry*
- 15:30-16:00 Michele Friend (Georgetown University, USA): *Ecologically sound practice in chemistry*
- 16:00-16:30 Dominique Pecaud (Ecole polytechnique de l'université de Nantes, France): *Investigating the concept of social acceptance from chemistry: the Case of mosquito control*

16:30-17:00 Coffee break

### 17:00-18:00 Plenary lecture

**Franck Dumeignil (University of Lille, France) in collaboration with Martine Benoit (Maison Européenne des Sciences de l'Homme et de la Société, University of Lille, France):**  
*Biosourced chemistry, biorefineries: the origin, the status and the fate of bioeconomy in our civilization*

## WEDNESDAY 5TH, 2017

8:15 Welcome coffee

### 8:45-09:45 Plenary lecture

**Hasok Chang (University of Cambridge, UK): *Pragmatism, technoscience and chemistry***

09:45-10:00 Coffee break

10:00-12:30 // SESSION 5 // Chair: Hasok Chang (University of Cambridge, UK)

- 10:00-10:30 Geoffrey Blumenthal (University of Bristol, UK): *The late phlogiston theories 1791-1813 and the debates concerning pluralisms*
- 10:30-11:00 Clevis R. Headley (Florida Atlantic University, USA): *What can the philosophy of chemistry contribute to critical philosophy of race: the case of phlogiston and race*
- 11:00-11:30 M.E. Tobin (Independent Scholar, USA): *Why are there so many unknowns in chemistry?*
- 11:30-12:00 Luigi Cerruti & Elena Ghibaudi (University of Torino, Italy): *Peirce's semiosis and the representation of protein molecules*
- 12:00-12:30 Marina Paola Banchetti-Robino (Florida Atlantic University, USA): *The explanatory significance of negative-empirical concepts in Daniel Sennert's experimental chymistry*

12:30-13:30 Lunch and poster session

13:30-15:30 // SESSION 6 // Chair: Yona Siderer (The Hebrew University of Jerusalem, Israel)

- 13:30-14:00 Tami Spector (University of San Francisco, USA): *Fugitive form: a close reading of cyclobutadiene*
- 14:00-14:30 José A. Chamizo (Universidad Nacional Autónoma de México, Mexico): *The fourth chemical revolution (1945-1966): From substances to chemical species*
- 14:30-15:00 Sacha Tomic (University Paris 1 Sorbonne-IHMC, Paris): *Toxicology in France in the mid-XIXth Century*
- 15:00-15:30 Sébastien Dutreuil (Max Planck Institute for the History of Science, Germany): *An archeology of the chemical conceptions of the Earth: from chemical geology to Gaia and Earth system science*

16:00-16:30 Coffee break

### 16:30-17:30 Plenary lecture

**Michel Morange (Ecole Normale Supérieure Ulm, Paris; President of the International Society for the History, Philosophy, and Social Studies of Biology): *Biology and chemistry: strong, but ambiguous relations***

19:00-21:00 Conference dinner at the restaurant 'Café Louis Philippe'



## THURSDAY 6TH, 2017

8:30 Welcome coffee

### 9:00-10:00 Plenary lecture

**Ludovic Duhem (University of Lille 3, ESAD Orléans and Valenciennes, France):**  
***Philosophy of Technology: Rethinking the Conditions of Knowledge***

10:00-10:30 Coffee break

10:30-12:00 // SESSION 7 // Chair: Joachim Schummer (Editor-in-Chief of *Hyle*, International Journal for the Philosophy of Chemistry)

- 10:30-11:00 Grant Fisher (Korea Advanced Institute of Science and Technology, Korea):  
*Chemistry and concurrent exploratory science*
- 11:00-11:30 Hirofumi Ochiai (Nagoya Bunri University, Japan): *The role and reach of transdiction in chemical epistemology*
- 11:30-12:00 Alexandre Hocquet & Frédéric Wieber (University of Lorraine – LHSP Archives Poincaré, France): *“Only the initiates will have the secrets revealed”:*  
*computational chemists and the openness of scientific software*

### 12:00-13:00 Closing plenary lecture

**Joachim Schummer (Editor-in-Chief of *Hyle*, International Journal for the Philosophy of Chemistry):** What does the present neglect of ethics of chemistry tell us about the past neglect of philosophy of chemistry, and vice versa?

13:00-14:00 Lunch

14:00 End of the ISPC Paris Conference

## **VI. PRACTICAL INFORMATION**

### **VI.1 Conference**

The ISPC annual summer symposium will be held on July 3-6, 2017 at the Laboratory Sphère, (CNRS-University Paris 7) in the room L. Valentin, 454A (level 4), Building Condorcet, 10, rue Alice Domon et Léonie Duquet, 75013 Paris.

Our keynote speakers and participants will have no fee to pay for attending the conference, as well as no fee to pay for lunches and coffee breaks during the whole conference. Dinners are not included in the conference schedule, except for the conference dinner (please refer to the following page of the present document). Other people who want to attend the lectures will have to lunch outside the building (lunches are reserved for our keynote speakers and participants only). They will have no fee to pay for attending the conference and no fee to pay for coffee breaks too.

Two of my colleagues, members of the staff of SPHERE, namely, Mrs Patricia Philippe and Mr Laurent Lemoine, will be in charge with the supervision of lunches and coffee breaks.

A group of my students in chemistry, past or present, namely, Damien Billaudel, Anaïs Cantin, Théo Chazeaud, Hugo Gérard, Thibault Ranquet and Néal Simerman, and a group of my graduate students in philosophy, namely, Pauline Agator, Sarah Hijmans and Julien Thareau, will help Patricia, Laurent and I to welcome you under good conditions.

### **VI.2 Conference dinner**

The conference dinner will be held on Wednesday 5th June 2017. It take place in the ‘Café Louis Philippe’ from 07:00 pm. The room upstairs, which provides people with a beautiful view over the Seine, has been reserved for welcoming the participants of the conference. Everybody will have to pay individually for the conference dinner once being in the restaurant.

Mailing address of the restaurant:

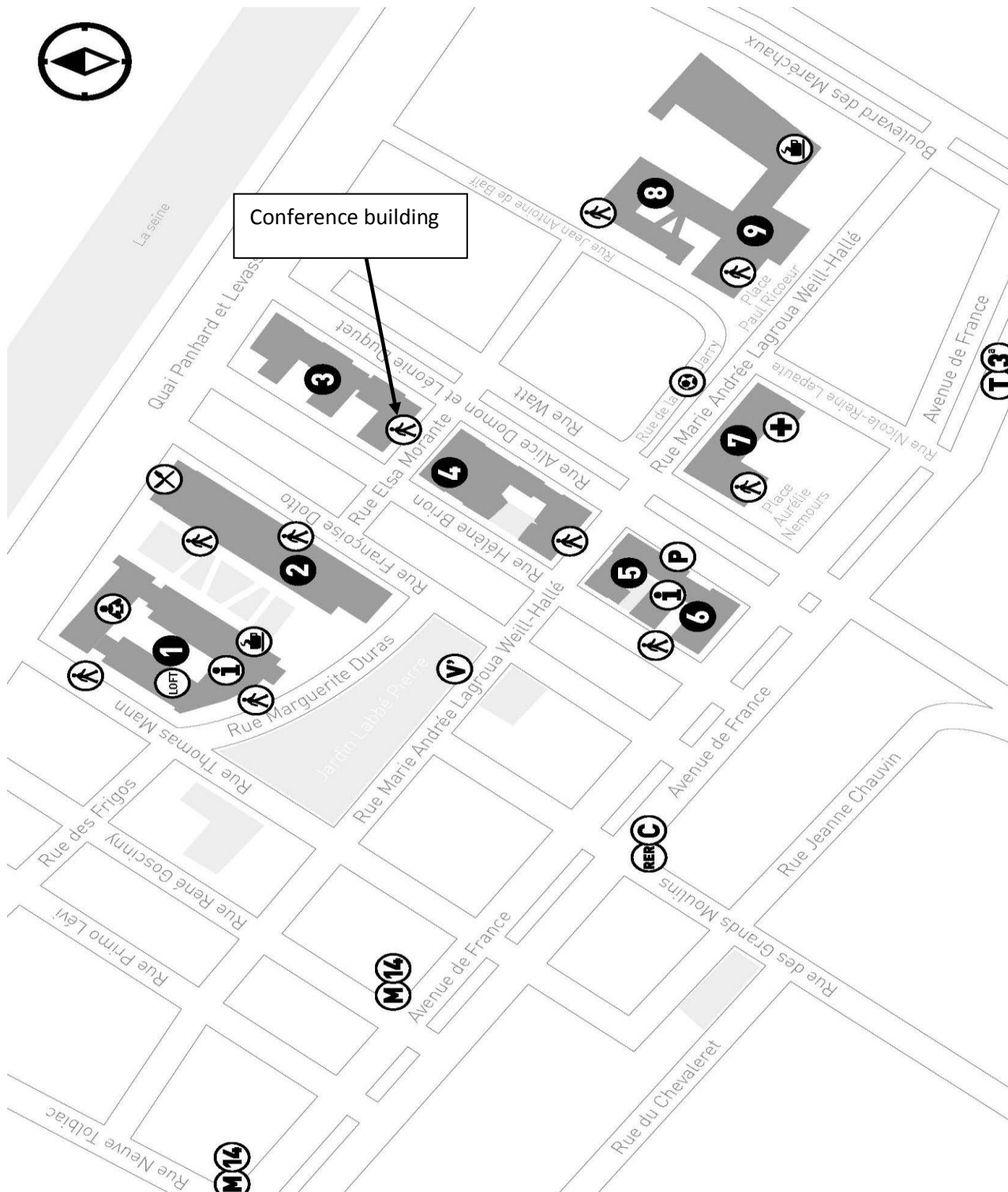
66 Quai de l'Hôtel de ville, 75004 Paris

00 33 1 42 72 29 42

The ‘Café Louis Philippe’ is located close to the Metro Station ‘Saint Paul’ (Metro 1) or to the Metro Station ‘Pont Marie’ (Metro 7).

### **VI.3 Map for coming to the building Condorcet**

The map is available on the page which follows.



#### 1 - Les Grands Moulins

16 rue Marguerite Duras  
BVE - BRI - SAOIP - Service culture  
UFR LCAO - UFR LAC

#### 2 - La Halle aux Farines

Eplanade Pierre Vidal-Naquet  
Amphis - SRIPT - EIDD  
Relais handicap Diderot  
Service social et aide aux étudiants

#### 3 - Condorcet

4 rue Elsa Morante  
UFR Physique

#### 4 - Buffon

4 rue M.A. Lagroua Weill-Hallé  
UFR SDV - Amphibuffon

#### 5 - Lamarck B

35 rue Hélène Brion  
UFR Chimie - UFR STEP  
UFR Sciences du vivant SDV

#### 6 - Lamarck A

39 rue Hélène Brion  
DEU inscriptions

#### 7 - Sophie Germain

Place Aurélie Nemours  
Service des sports  
Locaux syndicaux étudiants  
UFR Mathématiques  
UFR Informatique  
Amphi Turing

#### 8 - Lavoisier

15/17 rue Jean de Baif  
UFR Chimie - MIE LAB013

#### 9 - Olympe de Gouges

Place Paul Ricœur  
CRL - UFR ELA  
UFR Etudes anglophones  
UFR Etudes psychanalytiques  
UFR GHSS - UFR Sciences sociales  
UFR Linguistique

#### Accueils

Bibliothèque

#### Cafétéria

#### Restaurant

#### MEVA

#### Complexe Sportif

#### SIUMPPS

#### BVE - Service culture

## VII. ABSTRACTS OF THE CONFERENCE

### VII.1 Abstracts of the lectures given on Monday 3rd, 2017

#### Plenary lecture (9:15-10:15)

##### An assessment of Woody's thesis on the turn to practice and representations of the periodic table

Eric Scerri

Department of Chemistry & Biochemistry, UCLA, Los Angeles, USA

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The philosopher of chemistry Andrea Woody has recently published a wide-ranging article concerning the turn to practice in the philosophy of science (i). Her primary example consists of the use of different forms of representations that were used by Lothar Meyer and Mendeleev when they presented their views on chemical periodicity. Woody believes that this distinction can cast light on various issues including why Mendeleev was able to make predictions while Lothar Meyer was not. Secondly, she claims that it can clarify the much-debated question concerning the relative values of prediction and accommodation of data in the way that the periodic system was accepted. Thirdly, Woody believes that such differences in the representation of periodicity can be used to argue for the explanatory nature of the periodic table in contrast with the more traditional view that the periodic table is not explanatory.

My lecture will examine each of these claims and will argue that each of them needs to be qualified and in some case rejected. Nevertheless I am in full agreement with the need to concentrate on the practice of chemistry even within theoretical aspects of the subject, although my own turn to practice takes a somewhat different form that I will briefly elaborate (ii).

#### Bibliography:

- (i) Woody, A. (2014). "Chemistry's Periodic Law: Rethinking Representation and Explanation After the Turn to Practice," in *Science After the Practice Turn in Philosophy, History, and Social Science Studies*, edited by L. Soler, S. Zwart, M. Lynch, V. Israel-Jost, (New York and London: Routledge), 123-150.
- (ii) Scerri, E.R. (2016). *A Tale of Seven Scientists and A New Philosophy of Science*, (New York: Oxford University Press, New York).

## **Inorganic Chemistry, Causation, and Prediction in Natural History**

**Benjamin J. McFarland**

Seattle Pacific University, USA

[bjm@spu.edu](mailto:bjm@spu.edu)

The renowned inorganic chemist R.J.P. Williams (1926-2016) helped found the field of bioinorganic chemistry. Late in his career, he described a chemical sequence behind natural history in which the oxidation of the planet changed the bioavailability of redox-sensitive elements and constrained the possibilities for biochemical function. I summarized the evidence supporting Williams's chemical sequence in *A World from Dust: How the Periodic Table Shaped Life*.

Because the elements are universal, this chemical sequence may be universal for aqueous biochemistry -- and therefore predictable. This contrasts with many biologists' view that genetic drift and other random processes make the development of life essentially contingent on chance events and unpredictable. Is the explanatory and predictive power of Williams's sequence significant or trivial, and how should the rules of inorganic chemistry be used for causal explanation?

Joseph Earley and Terrence Deacon have each argued that other modes of Aristotelian causality can describe closed, dissipative sets of interactions such as those found in living organisms, for which efficient causality is regulated and restricted by formal and/or final causality. Deacon theorizes that this may explain how structure, work, and goal-directed behavior emerge from progressive constraint selecting processes from a random substrate, including how coherent consciousness emerges from randomly firing, noisy neurons. When applied to Williams's evolutionary sequence, formal and final causality help explain how non-teleological evolutionary processes based on unpredictable, random genetic drift can be reliably selected by the limited availability, structure, and function of elements in the environment, which can be (and were) predicted by inorganic chemists. Therefore, the general temporal order and biochemical function of the elements used in natural history may be predicted to recur on other Earth-like planets.

### **Bibliography:**

Earley, Joseph E. (2004). "On the Relevance of Repetition, Recurrence, and Reiteration," in Danuta Sobczynska, Pawel Zeidler and Ewa Zielonaka-Lis (eds.), *Chemistry in the Philosophical Melting Pot*, (Frankfurt and Main: Peter Lang), 171-186.

Deacon, Terrence W. (2011). *Incomplete Nature: How Mind Emerged from Matter*. WW Norton & Company.

Ben McFarland is Professor of Biochemistry at Seattle Pacific University. He received his Ph.D. in Biomolecular Structure and Design from the University of Washington in 2001 and was a Postdoctoral Fellow at the Fred Hutchinson Cancer Research Center. His research interests are structural immunology, protein design, and bioinorganic chemistry. In 2016 his book *A World from Dust: How the Periodic Table Shaped Life* was published by Oxford University Press.

## Iron and steel in preindustrial times: words, commodities and chemical element

Mathieu Arnoux

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For more than three millennia, iron has been a major historical agent in the evolution of civilizations. For ancient times, its study is mainly about archaeological findings, chemical analyses and typology of artefacts. For the middle ages, either in western Europe or in China, written sources give evidence that can be combined with material evidence and make it possible to build some hypotheses about the place of iron production and iron produces in the material culture: agrarian, military, architectural. Since the chemical element 26 Fe does not exist alone, but always combined with others elements like oxygen, carbon and many others, it is not easy to understand what kind of produce are meant by words like *ferrum*, *fer*, *iron*, *aciarium*, *chalybs*, *merlaria*, *osmund* (to stay in Western territories).

The intervention will try to make clear that European iron history was about steel produces and when Chinese iron history has been about cast-iron. It will not try to give an encyclopaedic view of the question which remains discussed, but to provide some clue for a better comprehension of a topic which cannot be explained by analytical description of ores and artefacts, but requires a knowledge of the processes of production, trade and use of the iron-based artefacts. A historical and anthropological approach to the history of this element, which is essential, either for our understanding of the natural system of earth and of the evolution of mankind during the last millennium raises the issue of the adequate interdisciplinary dialog necessary for a right assessment of the different functions of some chemical elements in social context.

### Bibliography:

Mathieu, Arnoux. (2014). "European Steel vs Chinese Cast-Iron: From Technological Change to Social and Political Choices (Fourth Century BC to Eighteenth Century AD)," *History of Technology*, 32, 297-312.

Wagner, Donald B. (2008). *Science and civilisation in China*, vol. 5, *Chemistry and chemical technology*, part 11, *Ferrous metallurgy* (Cambridge: Cambridge University Press).

**What Are Elements?**  
**Pragmatic Approach to the Meaning of a Chemical Concept**

*Sarah Hijmans*

*University Paris 7*

[sarahnhijmans@gmail.com](mailto:sarahnhijmans@gmail.com)

There have been many philosophical efforts aimed at finding the meaning of the concept of chemical element by reducing it to an essence. However, even though it is useful to have a nominal essence by which we detect the elements, we should not treat them as universal concepts that exist independently of human scientific inquiry. Instead, we should adopt a pragmatic approach and research the meaning of the concept through its use in chemical practice. This study aims at finding the meaning of the chemical concept of element by asking how it enables the advancement of successful chemical inquiry.

Seeing as the origins of the concept lie in the question of the composition of matter, it might seem as though the main function of the element is the explanation of material properties. However, substances cannot be characterized solely by their elementary composition: the knowledge of the subatomic structure of the elements does not suffice to deduce all properties of compounds, since new properties are created by the interactions between particles in a multi-atomic system. Bachelard called this idea the “reality of synthesis”: the properties of a substance result from its synthesis and can therefore only be attributed to the substance as a whole and not to its constituent parts. Moreover, the same reasoning applies to simple bodies, since they exist in the form of multi-atomic systems as well and their properties are the product of a chemical reaction. In both cases, we are dealing with empirical bodies that surpass the sum of their constituents. Nevertheless, there is an abstract meaning of the element underlying these phenomena, which does not have any intrinsic properties itself, but which acts as a bearer of properties that helps rationalize chemical change. The abstract element can be seen as a reinterpretation of Aristotle’s idea of potential existence: it can be actualized in the form of many different empirical bodies, which each have a different set of properties. Thus, every individual abstract element is attributed dispositional properties based on its empirical reactivity, meaning we should characterize the element by the compounds it can form instead of characterizing compounds based on their elementary composition.

Therefore, the elements constitute the nodes in a network of possible chemical reactions. This is clearly visible in the periodic table: each space on the periodic table is defined by its relation to other elements and cannot be detached from the system. Therefore, the elements are truly Cassirerian concepts because their validity stems from their capacity of forming inter-conceptual connections as parts of a complex theoretical system. In turn, the periodic system is constantly adjusted to new empirical data, thus forming increasingly complicated relations between the elements which add to their individual meanings. This reinforces the idea that they should not be seen as timeless essences but as subject to a historical development and inquiry in Dewey’s sense of a self-corrective process during which concepts evolve according to their use. The fact that the periodic system has survived this process of continuous adjustment means we should cherish the elements as natural kinds, but only according to Chang’s interpretation of natural kinds as effective classificatory concepts. In summary, the element can fulfill its function within chemical theory because it is a classificatory concept that is part of a network of relationships. Therefore, its meaning is the result of a long and complex formation of inter-conceptual relations that cannot be reduced to one essential property.

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### **Idealized quantum chemistry? Approximations and molecular structure**

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The different theoretical tools used in scientific practice to explain or represent a target system have a feature without which they would be extremely ineffective. Given the many variables of the system, both models and laws are designed as deliberate simplifications of something inherently complex, with the purpose of supplying some kind of understanding of it. This process of simplification, although essential for mathematical calculations and predictive inferences, is often related to philosophical controversies about the foundations of representation (e.g. Cartwright 1983). In fact, idealizations and approximations contribute to the distortion of the target system, either by omitting some property or directly by representing it as having some property that in fact doesn't have (Jones 2005; Chuang Liu 2001; Hartmann 1998). On this basis, the literature on the matter (Frigg 2002; Suárez 2003; Morrison 2005) addresses this problem by asking: how is it possible that these so-called “misrepresentations” can be considered a source of knowledge?

But what turns this subject matter into an extremely relevant one is the fact that models succeed in being representative or explanatory, not in spite of those distorting processes, but thanks to them. It could be said that misrepresentations are representative precisely due to the fact of being *false* representations. Consequently, the generally accepted idea that the less idealized a model is, the more realistic or better it will be, cannot always be sustained. In fact, introducing too many variables in the description not only may generate inaccurate results, but may directly override the calculation capacity and, therefore, the inferential capacity with respect to the target system. Therefore, not only “de-idealizing” the model is commonly disadvantageous, but reducing the distance between the model and the system is sometimes impossible.

Moreover, if predictive power is an indicative of some kind of realism, then, contrary to classical ideas, the most idealized models are the most realistic since they allow us to perform better predictions. As a consequence, if we want to maintain certain realistic intuitions, the indispensability of the distorting factors inherent to the modeling process invites us to identify and understand how idealizations operate in actual scientific practice.

In the so-called Galilean idealizations (McMullin 1985; Weisberg 2013), for pragmatic reasons, certain variables are removed in order to perform calculations. Emblematic cases of this type of idealization are: the treatment of sun and planets as homogeneous masses or as geometric figures such as circles (e.g. McMullin 1985); the assumption of the sun at rest in order to derive Kepler's laws; or the treatment of gravity as a constant in the model of an inclined plane. Although these idealizations do not provide consistent information regarding the phenomenon, they nevertheless do not lead to contradictions with the theory from which the models are developed. It is precisely for this reason that it is usually expected that the model can be “de-idealized” by reintroducing the originally removed variables, thus generating more complete models. For instance, if the absolutely frictionless motion of a body is not realistic (friction is pervasive in the real physical world), this idealized situation does not contradict Newtonian mechanics. Our central claim in this work is that, although this type of idealization is appropriate to describe at large extent the dynamics of physics, idealized models in quantum chemistry introduce serious interpretative challenges.

The central element in the quantum description of a molecule is the Born-Oppenheimer approximation (BOA) (Born, M. y Oppenheimer, J. 1927), which allows us to decompose the Hamiltonian of a molecule in its electronic and its nuclear part. This strategy is based on treating the atomic nuclei as classical particles at rest and with a definite position. In the resulting Hamiltonian, the structure of the molecule is described by the positions of the nuclei. However, from the point of view of quantum mechanics, the BOA contradicts one of the formal features of the theory, the Heisenberg's principle of uncertainty, by allowing the nuclei definite values for two observables that do not commute with each other (Hendry 1998, 2010; Woolley y Sutcliffe 1977).



Our purpose here is to explain the reasons why the BOA cannot be typified as a Galilean idealization. On the one hand, not only the BOA contradicts the postulates of quantum mechanics, but also it is impossible to “de-idealize” the model by treating it without approximation. Quantum chemistry is unintelligible without the concept of molecular structure arising from this approximation. In other words, without the BOA, the explanatory capacity of the model completely vanishes. On the other hand, despite its name, the BOA is not an approximation in a literal sense. The usual justification for the clamped nuclei assumption is the idea that the mass of the nuclei is infinitely greater than that of the electrons and, therefore, the nuclei’s relative velocity is approximately zero. But not only this is a classical intuition that does not work in the quantum domain (Wolley 1998), but the difference between zero and approximately zero can give rise to two radically different systems when quantum mechanics is taken into account.

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### Philosophy of science and ontology

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Ontological reductionism is a metaphysical claim that holds that descriptions of physics refer to a true and definitive ontology, whereas chemistry only describes apparent phenomena, studies entities that do not really exist or, at best, a reality of a lower ontological level. In its defense of the ontological autonomy of chemistry, ontological pluralism supports the idea of different coexisting ontologies without metaphysical priorities or privileges, given that all ontology arises from the synthesis between noumenal reality and a conceptual scheme. The aim of this work is to show that the philosophy of science does not need any kind of metaphysical-ontological approach to refute the claim that fundamental physical theories are the only ones that can tell us something about the real world, and therefore, have an ontological priority over other scientific theories such as, for example, chemistry. In other words, the study of the topic of reduction concerns the philosophy of science and has a direct impact on the definition of the ontological status of chemistry and its consolidation as a scientific discipline distinct from physics.

Key words: reductionism, ontology, philosophy of science

Filosofía de la ciencia y ontología.

El reduccionismo ontológico es una tesis metafísica que sostiene que las descripciones de la física se refieren a una ontología verdadera y definitiva, mientras que la química solamente describe fenómenos aparentes, estudia entidades que no existen realmente o, en el mejor de los casos, una realidad de menor nivel ontológico. En su defensa a la autonomía ontológica de la química, el pluralismo ontológico sostiene la idea de puede admitirse la coexistencia de diferentes ontologías sin prioridades ni privilegios metafísicos pues toda ontología surge de la síntesis entre la realidad nouménica y el esquema conceptual. El objetivo de este trabajo es mostrar que la filosofía de la ciencia no necesita de ningún tipo de planteamiento metafísico-ontológico para convencernos de que no hay motivo para creer que las teorías físicas fundamentales son las únicas que pueden decirnos algo acerca del mundo real y, por tanto, tienen prioridad ontológica sobre las otras teorías científicas como, por ejemplo, sobre la química. En otras palabras, el estudio del tema de la reducción concierne a la filosofía de la ciencia y tiene una repercusión directa en la definición del estatus ontológico de la química y en su consolidación como una disciplina científica distinta de la física.

Palabras clave: reduccionismo, ontología, filosofía de la ciencia

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**On the ontological status of molecular structure:  
is it possible to reconcile molecular chemistry with quantum mechanics?**

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It is well-known that the classical concept of molecular structure (namely, a set of atoms with a definite arrangement in space and held together by chemical bonds) is central to modern chemical thought given its predictive power. It is also a very useful concept in chemistry education to rationalize and visualize microscopic phenomena. However, such a concept seems to find no place in the ontology described by quantum mechanics, since it appeals to classical notions such as the position of the atomic nuclei or the individuality of electrons, both ideas strongly challenged in the quantum context. Although this problem has attracted the attention of several authors, the discussion is far from settled: the opinions about the link between quantum concepts and the notion of molecular structure diverge markedly.

Many authors have stressed the conceptual discontinuity between quantum mechanics and molecular chemistry. In fact, a quantum system is a contextual entity, described by its non-separable state vector, and maintaining non-local correlations with other quantum systems. In molecular chemistry, on the contrary, a molecule is an individual entity, with definite properties –as its shape– and without non-local correlations with other molecular entities (*cfr.* e.g. Amman 1992, Primas 1994). In this context, while some authors adopt an explicitly reductionist position and advocate to reconstruct the concept of molecular structure within the framework of the quantum theory of atoms in molecules (Hettema 2012), others appeal to the concept of emergence to understand this notion (Hendry 2010).

The aim of this work is to propose a new line of argumentation to address this problem. Indeed, ontological pluralism (Lombardi and Pérez Ransanz 2012) is a particularly fruitful philosophical framework when the problem is to interpret the relations between ontologies described by scientific theories that are equally successful from an empirical point of view. This perspective allows us to admit the ‘real’ existence of different ontologies, with no reduction or priority relationships among them. In this Kantian-rooted philosophical framework, since any ontology results from the synthesis between the ‘noumenal’ independent reality and the conceptual scheme of a theory, the quantum ontology is not a conceptually independent domain but a realm as constituted as the realm of molecular chemistry. Therefore, the quantum world has no priority over the world of molecular chemistry: chemical entities do not need the support of quantum entities to legitimate their objective existence. From this perspective, it is then possible to state that molecular structure does exist in the ontology of molecular chemistry, in spite of the fact that it does not exist in the quantum world. This ontological pluralism has been fruitfully applied to different problems in the philosophy of the special sciences. In the field of the philosophy of chemistry, it has been appealed to with the purpose to address the general problem of the relationship between chemistry and physics, traditionally interpreted in reductive terms (Lombardi and Labarca 2005), as well as to account for the problem of the ontological status of atomic orbitals (Labarca and Lombardi 2010).

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### **A categorical formalism for classification of chemical substances**

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Classification of substances is an essential part of the cognitive structure of chemistry, which, in the end, is attained by exploring chemical similarity of substances (Schummer 1998). Such a similarity entails the exploration of the network of chemical reactions and there have been some attempts for the exploration (Fialkowski et al. 2005, Leal et al. 2012). However, no formal mathematical framework for the chemical classificatory apparatus has been devised. Here we show that category theory is a suitable mathematical framework for chemical classification based on chemical networks. It is shown how the calculation of kernels of the category of Graphs with morphisms as relations play a central role in the characterisation of substances and how this leads to an ordered system of classes meeting conditions of concepts, in its philosophical sense. The framework is exemplified through the study of a network of chemical elements obtained from binary compounds.

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### Downwards causation for the case of molecular structure

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The paper examines the ontological status of molecular structure and, in particular, the role it plays in supporting the strong emergence of chemistry from quantum mechanics (in the ontological sense of ‘emergence’). The main question raised is whether the quantum mechanical description of molecular structure necessitates the acceptance of downwards causation and, consequently, of strong emergence. The investigation of the question is organised into two main stages.

Firstly, strong emergence and the notion of downwards causation are presented. The paper stresses that strong emergence is defined as an ontological thesis that postulates the existence of distinct higher level causal powers that determine lower level entities, properties etc (i.e. in terms of downwards causation). That is, it does not deal with epistemic accounts of emergence. The main postulates and requirements for strong emergence are presented, as well as the kinds of realist theses that it entails or is compatible with.

Secondly, strong emergence is examined with respect to the case of molecular structure. It presents the empirical evidence drawn from chemistry and quantum mechanics, that allegedly supports the thesis of downwards causation for the case of molecular structure. It challenges this thesis by arguing that the empirical evidence utilized in support of downwards causation, does not necessarily suggest strong emergence of molecular structure.

The essay concludes that, based on the aforementioned investigation, downwards causation, and consequently strong emergence, should be rejected as a tenable philosophical account of the ontological status of molecular structure.

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**Nanomaterials and intertheoretical relations: macro and nanochemistry as emergent levels**

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A very appealing area of philosophical debate have been generated regarding the ontological problems involved in chemistry. Within this area, we have discussed about the ontological nature of nanomaterials (Córdoba and Zambon 2016). We have argued that, given the distinction between the ontology of physics –as an ontology of individuals– and the ontology of chemistry –as an ontology of stuff–, neither of them is sufficient to deal with nanomaterials, since they can be subsumed neither under the category of stuff nor under that of individual.

We proposed a third ontological category to account for them: the category of *nanoindividuals*, which does not arise from a conceptual synthesis between the notion of physical individuals and the notion of chemical stuff, but refers to something different from traditional individuals and from stuff. We asserted that nanoindividuals are neither mathematical nor chemical artifices created in order to deal with some practical problems; that they are not theoretical instrumental constructs, but entities with real existence. The ontological category of nanoindividuals picks up certain existent “things” or items that share some features with traditional individuals and some others with substances subsumed under the category of stuff.

We will go further this result, but within the established frame –assuming that nanomaterials are existing things than can be correctly understood as nanoindividuals. The purpose of our present work is to discuss which relation can be established between molecular chemistry, on the one hand, and macrochemistry and nanochemistry, on the other hand. In order to do this, we will consider molecular chemistry as a fundamental level, and macrochemistry and nanochemistry as *emergent* levels.

Emergence is characterized in very different ways in the philosophical literature, nonetheless we will not discuss here those differences. We will consider synchronic and not diachronic emergence (Rueger 2000, Humphreys 2008), i.e., the idea that there is a hierarchy of levels, where the higher levels emerge from the lower ones; and also ontic emergence (O'Connor and Wong 2015) as a relation between items belonging to different ontic levels, according to which the emergent items (in a higher level) arising from a lower level, are ontically new and exist as objectively as the items of the lower level (Lombardi and Ferreira Ruiz 2017). Finally, we will address a distinction established between inter-domain emergence –a relation between items belonging to a same ontic domain– and intra-domain emergence –a relation between items belonging to different ontic domains (Lombardi and Ferreira Ruiz 2017) in order to elucidate the case of the relation between the subdisciplines of our interest.

It is our purpose to argue that from a fundamental molecular level, macrochemistry and nanochemistry emerge in parallel. If this is the case, therefore macrochemistry and nanochemistry are not “successive” levels, but parallel ones, and they can be thought as autonomous levels, independent from each other, but dependent from molecular level. This discussion will be held –as we have pointed out– from an ontological point of view, i.e., considering the ontological nature of the objects involved in the subdisciplines in question, according to which we have characterized nanochemistry, instead of the classical characterization in terms of scale (Córdoba and Zambon 2016). In this fashion, molecular chemistry can be considered fundamental from an *ontological perspective*.

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## Plenary lecture (16:30-17:30)

### Procedures, Products and Pictures

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Has recent philosophy of chemistry stumbled upon a radically different metaphysics for the practices and discourses of stuff changing activities from the 'atomism' that still underlies much of chemical thinking and practice? Several novel concepts and redirections of attention can be found in the last decade, for example in *Foundations of Chemistry*. Mereology: (Needham); the mereological fallacies (Harré); dissipative individuals (Early); affordances and character of experiments (Harré, Early, Llored); scale (Llored); electrons as constituents of iconic models rather than of stuff (Scerri, Harré); Mullikan's orbitals (Llored); substance (Hendry). We will sketch a coherent (we hope) alternative metaphysical, that is conceptual scheme, encompassing experimental practice and theorizing. The alternative to be presented here makes across-the-board use of dispositions and affordances rather than substances and their occurrent attributes. We will argue that the alternative epistemological and metaphysical system we are presenting retains the 'atomism' that still underlies much of chemical thinking and practice, particularly in organic chemistry, but not as a depiction of the world independent of science and scientists, that is of 'reality', rather as a convenient *model* of the constituents of material substances. We will also insist on the relevance of hinge, milieu, and fungible, as concepts for scrutinizing chemistry.

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## **VII.2 Abstracts of the lectures given on Tuesday 4th, 2017**

**Plenary lecture (09:00-10:00)**

### **What carbon teaches to philosophers**

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Carbon has displayed so many profiles over the course of the centuries that it seems to create various “personae” moving with a momentum of their own and creating new adventures while exhibiting new physical and chemical properties. Diamond, charcoal, graphite, carbon compounds, mephitic air, and CO<sub>2</sub> are among the characters who have played and are still playing significant roles in science and mythology, in industry and economy.

This paper makes the case for a biographical approach to carbon that helps develop metaphysical perspectives on chemistry. Not only is it an antidote to Cartesian metaphysics it opens the way to an ontography of materials.



### Chemistry and materialism: from matter to materiality

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Chemistry seems to be a materialist science. As chemistry deals with material compounds, associates forces and materials, and seems to always work on matter, it can even be said the most materialist science.

I would like to argue that it may be true but is not at all obvious from a historical point of view. That chemistry is necessary materialist or (my hypothesis) tends to a specific kind of materialism is a philosophical statement, not an obvious idea. Moreover, there are several periods and kinds of chemistry that do not seem to be or even to tend to materialism, such as classical alchemy and what has been called 'mechanical chemistry' at the Royal Society and the French Académie Royale des Sciences (during the end of 17th century and the beginning of the 18th century).

Thus, several issues have to be dealt with in order to argue that chemistry tends to materialism. 1) First, a historical perspective is necessary in order to avoid general statements about some dubious 'essence' of chemistry dealing with matter. The history of chemistry and of the philosophy of chemistry (for instance with Berkeley) clearly shows that chemistry can be considered, with strong arguments, as working on bodies and not matter and not being at all a materialist science.

2) Second, one has to compare chemistry and other sciences to show that, in a particular scientific context, chemistry can be said the most (or at least one of the most) materialist sciences. I would like to compare chemistry and physics in the French Enlightenment to show that chemistry offers more materialist effects.

3) Third, chemistry implies to qualify the common idea of materialism as a *theory of matter* explaining everything. Chemistry rather tends to a heterogeneous materialism dealing with *materials*. But as materials can be produced from something else, they cannot simply be considered as ontological elements from a philosophical point of view. And even hypothetic fundamental elements would not be universal matter. But materials permit to consider from a fresh perspective what *materiality* is. I would like to develop this idea thanks to an original concept framed by French 18th chemists and philosophers: 'les matières'. This would conduct me to consider that materiality includes forces and qualitative properties.

To conclude, I would like to underline how chemistry changes the classical view of materialism. A materialism inspired by chemistry has to frame some theory (hard to be materialist without any general theory !), but it will first consider practice, experiments dealing with materials. Thus it is no longer a theory of general matter but rather a theory of materiality and interactions. A chemical materialism may even be a materialism without matter.

### **No analysis without synthesis**

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In 1860, Marcelin Berthelot claimed that “chemistry creates its subject”. In 2006, Joachim Schummer wrote in a similar intention: “Chemical synthesis is, to be sure, the most obvious peculiarity of chemistry, albeit the most neglected one because it is foreign to any received idea of philosophy of science.”

In the chemical sciences, it is a received and unquestioned opinion that analytical techniques are necessary for the validation of synthetic efforts. Hence, the picture of analytical chemistry as the subordinate “kitchen maid” of synthetic chemistry has become strong and seemingly inevitable. Very early, however, the significance of the reverse perspective has been mentioned, for example by Etienne-Francois Geoffroy (1704): “One is never sure, in fact, of having decomposed a mixt into its true principles until one can recompose it from the same principles. This reestablishment is not always possible. When it is not possible, it does not necessarily work against the analysis of the mixt, but when it is successful, the analysis is demonstrated.”

In the present contribution, I shall explore the (admittedly unusual) reverse side of the dialectical relationship between analysis and synthesis in some detail. The main question will be: What exactly is the “Analytic-Synthetic Ideal” Mi Gyung Kim (2014) is referring to? My main claim is that no analytical procedure, qualitative or quantitative, can do without synthetic parts. By “synthetic”, I here mean the making of substances as well as the preparation and purification of standards for calibration. One more obvious case is the electrolysis of water: In order to quantify the composition of that substance, oxygen and hydrogen are prepared (synthesized) and their volumes measured and compared. By following the suggestion of Tony Edmonds (Chemical analysis is purification, synthesis, and comparison; 1999), I will try to support my thesis by a close look at various other intriguing examples, among them the “analysis” of noble gases, acids, and selected organics.

**The matter of impurities in pharmaceuticals:  
Substances without a name and how to handle them**

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Chemical synthesis is a science as well as an art. Rooted in laboratory or large-scale industrial manufacture, it inevitably results in side products which eventually may contaminate the final product. Such “impurities” usually occur in small amounts and - within chemistry itself - often are of little concern. Here, indications such as “technical grade”, “ACS grade”, “puriss”, “purum” or >95% inform the expert of what to expect. In pharmacy, however, the biological activity which may be associated with these impurities raises the spectre of toxicity, side effects and serious implications for human health and the environment. The pharmaceutical industry has therefore developed an eloquent regulatory and strategic system to minimize the (chemical) presence or (biological) impact of such substances. Here, we witness an evolution of pharmaceuticals from crude and impure to more defined materials as part of a complex socio-technological system that evolves according to specific rules and regulations at the edge of chaos.

Yet is this issue really just a matter of synthesis, of methodology, or of risk management as is suggested by such regulations? Or are we faced with a more eloquent philosophical issue that cuts at the roots of our understanding of what “chemicals” are? No doubt, the crux of impurities is that we know that they are present, for instance from the mass balance or a chromatographic trace, yet we often do not know what they are. In some cases, we are dealing with known compounds: Substances such as technical grade allyldisulfide - which is rich in some mono- and trisulfide - contain small amounts of undesired yet known contaminants. Yet others contain molecules which at the time we have no notion of at all. Here, the example of Agent Orange springs to mind, a herbicide that was used on a large scale during the Vietnam War and that eventually was found to be contaminated with a dioxin, a compound unknown at the time Agent Orange was first employed. In essence, such unknown impurities exist yet we do not know them. Or, in more philosophical terms: we are, paradoxically, dealing with chemicals in an ontological sense, which, strictly speaking, are not chemicals in an epistemological sense as they reside outside the realm of chemistry as a science at that time.

We will refer to such substances that are not, epistemologically speaking, “chemicals” as “unidentified impurities” or Xpurities. It is obvious that the presence of such Xpurities, which is surprisingly common, is also a major issue in pharmaceutical research and practice. These impurities may be side-products of a chemical synthesis. They may also be “natural”, for instance as companions of an active ingredient in an herbal extract. Knowing this unknown is a challenge that brings together science, manufacture, risk assessment and epistemology, and as mentioned at the beginning, is a science as well as an art.

**Plenary lecture (12:00-13:00)**

**Trajective chains in mesology, von Neumann chains in physics, etc. - and chemistry**

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The leading idea of mesology (the study of milieux) originates in Plato's *Timaeus*, with the paradoxical relationship of *chôra* (milieu) and *genesis* (relative being), which are posed as both an imprint and a matrix of each other. Though foreboded, the idea of milieu was locked out by Plato's rationalism, because it infringes the principle of the excluded middle: A (an imprint) cannot be non-A (a matrix), and there is no third term, both A and non-A. After Uexküll, who proved experimentally that an animal and its proper milieu (*Umwelt*, not to be confused with the general data of the environment, *Umgebung*) are precisely in such a relation, and after Watsuji, who, as for the human, named this relationship *fûdosei* (mediance) and defined it as the structural moment of human existence, mesology has logically and ontologically formulated empirical reality *r* (that of concrete milieux) in the following way :  $r = S/P$ , which reads "reality *r* is the subject *S* as the predicate *P*". Reality is neither *S* (the Real in itself) nor *P* (a subjective representation), but emerges in a process called *trajective chain* by dint of which, indefinitely, *S* is assumed as *P*, producing *S/P*, which in its turn is hypostasized into *S'* by *P'*, and so on in the following way :  $((S/P)/P')/P''/P'''...$  and so on. Homologous chains have been observed also in physics, and named "Neumann chains". Then what about chemistry?

## Plenary lecture (14:00-15:00)

### Green chemistry and sustainable development: a survey

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85,000 chemicals are marketed worldwide each year and 7,000 are produced in a massive way. From now on, Humanity must be able to face five strategic challenges. For future generations and ourselves, research activities achieved by chemists are already contributing to tangible solutions to the five major strategic questions for our survival and development:

- **Food Production:** Since the end of the 20<sup>th</sup> century, the production of food, that is to say agriculture, livestock and processing through the agro-food industries, is a patent problem. So fertilizers and pesticides remain at the heart of the debates on food production, essential if we plan to feed 9 billion people in 2050. Feeding the planet requires also the availability of uncontaminated agricultural land protected from all pollution.

- **Contribution to protection of human health:** The important demographic development we are facing, coupled with a continuous increase in life span in industrialized countries, leads us to completely rethink the preservation of human health and also the production of active ingredients for human health. The challenge is also to develop relevant systems for the detection of toxic molecules as close as possible to the generation of pollution, either in water and in air or in manufactured products.

- **Water production and preservation:** About two million people die every year because of limited or insufficient access to safe drinking water. Some areas of the world are experiencing water stress and they are paying a heavy toll in child mortality. The major problem is that water supplies for human consumption or agriculture are unevenly distributed on the surface of the planet, and here too demographic change can aggravate locally precarious situations.

- **Energy production and saving:** The production of carbon-free energy is at the heart of the citizens' concerns. This concerns our habitat, our transportation, but also our industry. The level of access of a population to energy conditions the life expectancy of this population and the expected increase of demography requires us to think about sustainable and efficient production systems.

- **Environment Protection:** This last area is obviously transverse and its taking into account seems recent. Our planet has finite resources of water, fossil energy, raw materials of all kinds. Since its creation, the chemical industry has been led in theory to reflect on the impact of its activities on the preservation of our environment, in terms of depletion of fossil resources and production of industrial discharges, but also now on Climate Change. The planet and humanity will only be sustainable if we are able to produce ever more by protecting our environment. It means that we have to mobilize as low as possible raw materials, then producing less industrial wastes and greenhouse gases.

In all these fields, chemistry is also going to have a decisive role to play, which is why it was structured at the end of the last century, in order to become green and sustainable. At that time, Paul Anastas and his colleagues from the United States Environmental Protection Agency (EPA) laid the foundation for the 12 principles of Green Chemistry. From a practical point of view, these principles have generated four major research axes for green chemical engineers:

- **Better Use of Raw Materials:** The challenge is to maximize the incorporation of all materials used in the process into the final product and then preserving resources and limiting by-products.

- **Cleaner and safer solvents:** The aim is to develop alternative organic solvents with no toxicity to human health and the environment.

- **Better Use of Energy:** For Renewable and Nuclear Carbon Free Energies, the main goals are to improve efficiency, saving and waste management in competitive and safe conditions.

- **More efficient waste management:** The idea is to achieve a lower production of ultimate waste in a convenient phase (solid, liquid or gaseous), avoiding dissemination and enhancing recycling, in order to produce new raw materials.

This contribution will give you a large overview of scientific research conducted in these areas and will take distance from it in order to reflect upon the evolution that remains to be done for implementing a green and sustainable chemistry.

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## REACH's impact on the ways of thinking and making chemistry

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The European regulation on chemicals REACH has been widely discussed in the debates that preceded its entry into force in 2007 and shaped, to some extent, its present form. However, the issue of the dynamics initiated by this new regulation since its implementation has been little questioned on a global or philosophical level. With REACH, chemistry is at the centre of a series of processes that concern political, social, economic and legislative domains as well as the objects and professions of chemistry itself.

After a brief summary of both REACH's functioning and of its main quantitative results, I would like to discuss, with supporting examples, the dynamics of conciliation, adaptation and development initiated or stimulated by REACH. Three axes will be distinguished. First, principles and modalities of REACH's consultation and evaluation procedures vary widely depending on the context (evaluation, authorization, restriction) in which they operate. Secondly, REACH encounters a number of difficulties caused by new forms of toxicity (e.g. endocrine disruptors), or by the nature of the substances to be considered (e.g. nanosubstances). Thirdly, incentives to create substitute products exceed the scope of the REACH procedures (for example with the Innochem, Subsport or SIN List projects). On a philosophical or societal level, these three axes invite us to ask which dynamics and incentives are activated by a new general regulation drawing care and attention to things? How to think the extension of chains, not only of information but also of debate and accountability, initiated by REACH? Are there limits to the free interpretation, by ECHA or by the European Commission, of the rules governing the operation of this new regulation, in particular in relation to the emergence of new substances? Should we consider a "reframing" or "redefinition" of the "environmental principles" on which REACH claims to be based (the precautionary principle seeming here to give way to the principle of active prevention)?

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### **Ecologically sound practice in chemistry**

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I present a comparative and holistic method for *qualitatively* ‘measuring’ sound ecological practice in chemistry. I consider chemicals from cradle to grave, that, is from the moment some are extracted from the earth, water or air, to their transportation, experimentation in a laboratory to waste products. We divide the locations of the ‘life’ of the chemical into four spatio-temporal areas accordingly. We then use the ‘policy compass’ method to determine a qualitative reading of the soundness of the ecological practice. The reading will take the form of an arrow on a trisected circle; where the thirds represent very general ecological and scientific qualities: ecological integrity, scientific value, ecological risks and dangers.

We can then use the policy compass method to produce several readings, of the ‘same’ experiment performed in different places, or at different times (using different equipment or processes), or we can use the readings of several experiments to compare one to the other. The latter is important, for example for funding bodies who have to allocate money towards experiments. Similarly, it can be used for applications for funding. It can also be used to evaluate the performance of a laboratory over time or in comparison with other laboratories.

The method can be extended to the qualitatively measure the industrial development of chemicals for commercial or national/medical reasons.

## Investigating the concept of social acceptance from chemistry: the Case of mosquito control

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If REACH and Green Chemistry require the protection of the environment, what we really want to protect is not always clearly defined. The concept of environment is too loose and multifarious, and does not refer to a 'fixed reality', but, by contrast, to a 'time-evolving reality'. Here is a great opportunity for interaction between society and science; *all the citizens*, among them are scientists, defining what they want to be protected and how much they are willing to pay for it — weighing the costs of either use or non-use of a chemical/product — while science and technology provide solutions. It is also a matter for all the citizens to define political, cultural, and economic priorities and values. In this lecture, we will investigate the concept of social acceptance of a technical device using the example of chemical strategies designed for mosquito control. This case study will enable us to query the relevance of the sociological models currently used in order to explain why and how a chemical or a technological device is socially accepted or not?

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**Biosourced chemistry, biorefineries: the origin, the status and the fate of bioeconomy in our civilization**

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With the contribution of Martine Benoit<sup>2</sup>, Full Professor, MESHS Director, Lille University

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Within a future sustainable society, biomass is expected to become one of the major renewable resources for producing food, cattle feed, materials, fine chemicals, fuel, power, and heat. To meet this challenge, a combined coherent package of measures is necessary: an increase in the overall energy efficiency, a reduced consumption of raw materials, reduced impacts on health and environment, increased durability and a decrease in the goods' costs, while offering the framework for enabling the large-scale transition from a petro-sourced to a bio-based sustainable economy. Such a switch would also provide our production system a greater independence from the current oil producers while bringing a larger degree of freedom from (geo-)political, economic or financial tensions. The transition toward a bio-based economy with the implementation of sustainable bio-sourced raw materials requires completely new approaches in research and development (R&D). On the one hand, biological (the so-called 'biotechs') and chemical sciences will play a leading role in the construction of the future industries of the 21<sup>st</sup> century. On the other hand, new synergies between agronomical, biological, physical, chemical and engineering must be elaborated and established. This will be combined with logistics, media and information technology, and with new inputs from the economic, health, environmental, political, and social sciences. Specific constraints will be imposed on both the industry and R&D sides with regard to raw materials and product line efficiency and sustainability. The development of substance-converting basic product systems, the so-called biorefineries at the core of which many new chemical transformations must be implemented, is the key to initiate this new approach in R&D and will enable access to an integrated production of chemicals, materials, goods, and fuels of the future, as a strong base of a robust bioeconomy.<sup>1</sup>

It is now crucial to go beyond a vertical bioeconomy design, where all the disciplines work in parallel before integration/fitting of the results, by intimately gathering various skills and know-how to assess, explore and develop interfaces in bioeconomy in a multidimensional, *i.e.*, multidisciplinary approach. This effort will yield clear breakthroughs in the field by shifting the bioeconomy concept from a juxtaposition of expertise, which is necessary in a first approach already largely underway, to a real integration of scientific and technical fields so as to create, optimize and promote interdisciplinarity. Such interdisciplinarity should interrogate the global ecological mutation and its ethical, socio-political and socio-economical aspects, as well as solving scientific and societal hurdles, for yielding full efficiency of the approach. Hard Sciences alone as well as SSH alone cannot efficiently address this issue, but their strong integration is expected to yield major breakthroughs in the field.

During this conference, after a global introduction contextualizing the role of bioeconomy and especially of its "chemistry" dimension through an original perspective, some important definitions and concepts will be recalled. The speaker will briefly describe some major programs developed at various levels of maturity in Lille in the field of Chemistry, Biorefineries and Bioeconomy. He will insist on ethical, historical and societal aspects that must definitely be seriously integrated in the global research effort as an essential part, in synergy with the so-called "hard sciences". This is essential if one really desires to reach the goal and achieve the promises of bioeconomy for our civilization.

### **Acknowledgements**

The authors would like to thank all their colleagues of the Region Hauts-de-France for having participated to the definition and the refinement of the bioeconomy multidisciplinary concept at the base of the present paper.

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<sup>1</sup> F. Dumeignil. (2012). "A New Concept of Biorefinery Comes into Operation", Chapter 1 of 'Biorefinery': From Biomass to Chemicals and Fuels," De Gruyter, Michele Aresta, Angela Dibenedetto, Franck Dumeignil (Eds.), p. 1-17.

## **VII.3 Abstracts of the lectures given on Wednesday 5th, 2017**

### **Plenary lecture (08:45-09:45)**

#### **Pragmatism, technoscience and chemistry**

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Analytic epistemology has been unnecessarily constrained by its commitment to the propositional view of knowledge, treating knowledge as solely consisting of belief in propositions. I advocate a more capacious view, which takes knowledge as the ability to do things. Knowledge-as-ability (or, active knowledge) incorporates and uses other types of knowledge, including propositional knowledge, knowledge by acquaintance, and others besides. A number of philosophers including Michael Polanyi, Gilbert Ryle and Marjorie Grene have in fact drawn attention to active dimensions of knowledge, although their insights have largely been rejected by Anglophone epistemologists. In this presentation, I want to highlight three traditions that encourage and facilitate the notion of active knowledge. First, pragmatists have always emphasized the need to understand and assess knowledge in the context of action and in terms of problem-solving; I draw from the work of John Dewey most of all. Second, many scholars in science and technology studies, including Bruno Latour and Michel Callon, have emphasized the inseparability of science and technology; there are important epistemological implications of taking technoscience seriously, which analytic philosophers have ignored. Third, the philosophy of chemistry as such should be (and has been) an important influence, as the nature of chemistry (the “impure science” as Bernadette Bensaude-Vincent and Jonathan Simon have called it) has long been technoscientific, as Ursula Klein has also argued.

### **The late phlogiston theories 1791-1813 and the debates concerning pluralisms**

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In this presentation I will look at a sample of the material that will be incorporated in the paper in the proceedings. In general in the philosophy and history of science we are not just trying to put forward personal views, but are trying to state what is and has been the case in reality. We need methods for doing this, and my own is to put forward generalisations which are grounded as firmly as possible in explicit references to a wide range of the primary literature from a period. That is, instead of applying modern philosophical concepts (such as the underdetermination of theories by evidence) to a historical period, I investigate what philosophical concepts are appropriate relative to the primary literature. The primary literature on the period already contains many divergent views, which prefigure most of the different views in the secondary literature on the period. In such cases Whiggism can best be avoided by keeping the discussion to the primary literature, which is what I will do today.

I will put forward three main theses. The first is that the new chemistry “raised the bar” for competing theories, by unprecedentedly increasing the difficulty of formulating one that was equally good overall. The presentation in 1787 and 1789 of the new chemistry demonstrated that it was coherent, wide-ranging, and as testable as was practicable at the time, while in general it corresponded well to the range of available experimental findings. None of the late phlogistic theories came anywhere near to matching the full set of these qualities, and in aggregate the late phlogistic theories demonstrate that to produce a general match for the new chemistry was now virtually impracticable. This has been demonstrated for the period before 1791 in a pair of papers by myself and James Ladyman that has been accepted for *Foundations of Chemistry*. I will now illustrate this in the cases of the work of Gren and Westrumb. The result was that by 1813 proliferation had almost ceased on topics covered by the core of the new chemistry, and had moved on to topics where it was still required and still practicable.

The second is that, even though none of the late phlogistic theories managed to achieve more than transient acceptance even by other phlogisticians, the phlogisticians had the common cause of maintaining a phlogistic theory despite the existence of the new chemistry. This is why several phlogisticians attempted to gain support among their peers by personalising the situation and arguing that Lavoisier and his colleagues were being authoritarian, or inattentive, or elitist, and so on, despite the lack of any supporting evidence concerning these claims, and even though the actual difficulty was posed by the new chemistry itself. Professions of libertarianism from the phlogisticians were transient rhetorical tactics which occurred at an even later stage in the decline of phlogistic theories, which had no beneficial effect on the problems in chemistry that these theories were not solving, and which were rapidly superseded by other tactics, including the participants abandoning their theories or retreating into other activities.

The full paper will contribute to supporting the argument that the usefulness of types of plurality varies depending on topics such as experimental practices, the development of theories, types of strategy in theories, the presentation of theories, styles of argument, theory comparison, theory choice, the ontology of substances, and policies concerning naming substances, and on the stage the subject has reached. The third thesis today is that there were multiple benefits from the type and degree of unity that was achieved by the core of the new chemistry, but this did not detract from the usefulness or potential usefulness of several pluralities in chemistry.

**What can the philosophy of chemistry contribute to critical philosophy of race:  
the case of phlogiston and race**

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This paper will focus primarily on the relation between concepts and reference. Contrary to the view that one must first articulate an a priori theory of reference before engaging in scientific practice and inquiry, I contend that a philosophy of chemistry that is appropriately informed by the history of chemical practice can provide important insights in our efforts to critically engage with particular philosophical problems. We should also note that, in their efforts to deliver pure theories of reference that are free from ‘empirical contamination’ by the history of scientific practice, philosophers have often invoked chemical metaphors and analogies. In investigating the issue of reference, this essay will draw an analogy between the chemical notion of phlogiston and the concept of race. Like other scholars, philosophers believe that the history of chemistry provides a great example for dealing with non-referring terms, that is, such terms should be ontologically eliminated. Hence it is argued that, just as chemists have eliminated the term ‘phlogiston’ because no such substance exists, we should also eliminate the term “race” because there is no such natural kind in the world. Ashley Montagu has famously stated that “The probabilities are high that the concept [of race] will be afforded a status similar to that now occupied by the nonexistent substance known as “phlogiston”. Race is the phlogiston of our time.”<sup>[1]</sup> The analogy is clear: Terms that fail to refer to existing substances or to natural kinds enjoy the dubious honor of being considered analogous to the term ‘phlogiston’.

David Ludwig describes this approach to dealing with non-referring terms as the “‘phlogiston model’ of ontological elimination.” Ludwig fleshes out this model as follows:

The first and most obvious assumption of the phlogiston model is that an eliminated entity *x* is postulated by some theory T1 but its existence is rejected by an ontologically incompatible competitor theory T2. In order for T1 and T2 to be ontologically incompatible, it is not sufficient that the term *x* is not part of T2 but also necessary that *x* can neither be reduced to nor identified with any entity in T2.<sup>[2]</sup>

In rejecting the phlogiston model of ontological elimination, this essay will turn to Hasok Chang’s<sup>[3]</sup> recent problematization of the standard historical narrative regarding the fate of phlogiston in the 18<sup>th</sup> century. Chang’s work is revolutionary in the sense that he favors critical interaction between the history of science and the philosophy of science. Accordingly, Chang is inclined toward pluralistic, as opposed to one-dimensional, explanations. Informed by the history and historiography of the Chemical Revolution, he argues that phlogiston can serve as a counter model for reference, rather than as the model for a naïve but failed attempt at reference. Following on Chang’s critique of this standard narrative and on his argument for pluralistic explanations, this essay argues for a radically different perspective on the issue of reference, particularly as it applies to the concept of ‘race’. Thus, determining the referent of the term ‘race’ is not transacted simply as a one-dimensional and vertical relation between terms and natural kinds but is construed, instead, as a complex horizontal relation between language, practice, agency, and history.

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### Why are there so many unknowns in chemistry?

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A survey of the literature of Chemistry reveals myriad epistemic lacunae in regard to structure and process that exceed those of Physics. This is readily demonstrable in the results of a basic, *ad hoc* search of the entry-level textual treatment of both subjects. Brady and Senese's *Chemistry: Matter and its Changes*, a well-regarded introductory text, is examined alongside.

Halliday and Resnick's *Fundamentals of Physics*, a standard work of similarly high quality. Instances of the appearance of such conditional qualifiers as: "not yet known," "undetermined," "possible structure of...", "not fully identified," "formulation is only approximate," etc are noted and contextualized in the Chemistry text. The relative paucity of such terms is observed in the Physics text. It is observed/asserted that, in the case of chemistry, these tropes are generally not references to quantum phenomena, but mechanistic and nano-structural. Contrapuntally, in the physics text, references to such unknowns are observed to be almost exclusively in regard to General Relativity or quanta (which receive cursory attention at this level). It is concluded that the epistemic lacunae described in elementary treatments of Chemistry result from: 1) Ephemeral and/or excessively complex instances of fleeting/occult molecular structure. 2) Computationally prohibitive kinetic processes, and 3) A gap between *in situ* experimentation and laboratory work. The possibility of an "Epistemic Horizon Problem" in Chemistry's current Research Programme is postulated.

Seven epistemic lacunae from the general body of Chemical Literature are then described: 1) The lack of explanatory power in the tenets/postulates of contemporary Theory of Adhesion. 2) The inscrutability of an optical colour source in Amethyst (We don't know where the purple comes from.). 3) The inadequacy of current Theories of General Anesthesia. 4) The lack of definitive understanding concerning the mechanism of bleaching of Hydrogen Peroxide. 5) The inability to formulate an adequate definition of Electronegativity. 6) The absence of a definitive theoretical description of the kinetics of secondary mineral formation in soils. and 7) The unknown structure of Humic Acid.

It is concluded, in each of the aforementioned cases, that such unintelligibly stems from 1) A variable surfeit and 2) An inadequate etiological and/or metaphysical conception of "Mechanism." The concomitant limitations of contemporary Computational Chemistry and experimental observation are then discussed in the context of an over-arching boundary problem in Chemistry: In the realm of the Macro/Nano, the experimenter can never be *in situ* enough, given that there is no black-box recourse to a quantum wave function collapse analogue.

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### Peirce's semiosis and the representation of protein molecules

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In their disciplinary communication chemists use natural, formal and iconographic languages. In this paper, we discuss some aspects of the iconographic communication, with particular reference to the representation of the molecules of proteins and in the light of the semiotics of Charles S. Pierce [1]. Peirce's semiotics is a widely debated issue in contemporary philosophy. In the context of an applied research in epistemology we have taken only some of the many proposals of the American philosopher, chosen for their actual applicability and used as interpreted by Floyd Merrell [2].

Peirce's semiotics is based on two triads. For Peirce, a sign consists of three inter-related parts: a *representamen*, an *interpretant*, an *object* (CP 2.228). These three parts are not separable, in fact semiosis is a process that involves all of these parts (CP 5.484) and continues until the conceptual part of the sign, the interpretant, stabilizes and becomes a *habit*, i.e. "A general law of action" (CP 2.148). The second well known triad consists of three classes of signs: *icon*, *index*, *symbol* (CP 2.247-2.249). The three classes are not mutually exclusive because each sign has a mixed character; as Peirce writes, "[A] symbol, if sufficiently complete, always involves an index, just as an index sufficiently complete involves an icon" [3].

The semiotic analysis of any iconographic representation of a protein immediately highlights that it is very poor if not devoid of indexical character. The indexicality is generally entrusted to a caption, the function of which comprises the *ancre* [4] to a specific interpretation of the sign. The symbolic aspect is very rich and consists of the numerous conventions that regulate the use in the image of shapes, lines, shadows, colors. The iconic aspect is the more surprising, not only because it makes 'visible' what is inherently invisible, but because it lends itself to a pragmatics of the sign [5] of great interest. The researchers represent the molecular systems projecting in the atomic-molecular world 'forms' that belong to their/our ontological level (balls, ribbons, corridors, tunnels, pockets, etc.). The images that result from this semiosis become heuristic tools, which often allow the researcher to better interpret the experiments and/or to design new ones. The formation of the images and their use in research qualify their epistemic status as that of conjecture (CP 6552, CP 2430).

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**The explanatory significance of negative-empirical concepts in Daniel Sennert's experimental chymistry**

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This paper examines the way in which the chymical philosophy of Daniel Sennert (1572-1637) mediates between the strictly Aristotelian and the strictly Democritean theories of matter by modifying the notion of substantial form and by employing an operational definition of substances as the limits attained by the analytical method of the laboratory. Sennert appropriates this 'negative-empirical concept', as Bernadette Bensaude-Vincent and Isabelle Stengers have called it, from the tradition of Scholastic alchemy. This negative-empirical concept acquires particular explanatory significance in the context of one of Sennert's most influential experimental procedures, the reduction to the pristine state. Sennert's explanation of the observable results of this experiment shows the interplay between structural and substantial explanations, since he appeals both to microstructure and to chymical properties that originate in the substantial form of corpuscles. Sennert's work is influential in many important ways. First of all, it clearly belongs to the transitional phase between the theory of substantial form and the purely mechanistic corpuscular theory of matter. Secondly, his work anticipates the important role that the notion of structure and the idea of negative-empirical concepts would play in later early modern chemistry. Finally, the 'reduction to the pristine state' would later be used by early modern chemists to accommodate the mechanistic theory of matter to the notion of chemical properties. The paper concludes by examining some of the limitations of Sennert's approach such as, for example, the difficulty of sustaining the notion of substantial form within genuinely chemical explanations.

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### Fugitive form: a close reading of cyclobutadiene

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Since the late 19<sup>th</sup> century cyclobutadiene (CBD) has been of keen interest to chemists, generating hundreds of papers, the majority theoretical. A review of the literature reveals a focus on CBD's status as the prototype of anti-aromaticity – a still contested status; its use as an intermediate in synthesis; its autoisomerization; and its shape and ephemeral existence. My presentation focuses on the ways these latter characteristics inflect chemists' apprehension of this fascinating molecule. I will begin with a brief overview of how CBD's computationally generated potential energy surfaces/diagrams articulate an explicit transient temporality; subsequently, I will close-read schema from four key experimental papers to reveal the ways in which the coalescence of form and time intersect in CBD's static images. I will apply Le Poidevin's concept of the specious instant [1] as a framework for understanding how time is articulated by the molecular images of trapped, buttressed, captured and confined CBD as found in Masamune *et al.*'s "Cyclobutadiene is not Square," [2] Maier *et al.*'s "Tetra-*tert*-butyltetrahedrane," [3] Cram *et al.*'s "The Taming of Cyclobutadiene" [4], and Barboiu *et al.*'s controversial "Single X-ray Structure of 1,3-dimethylcyclobutadiene by Confinement in a Crystalline Matrix". [5]

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### **The fourth chemical revolution (1945-1966): From substances to chemical species**

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The explanation of science's change and development over time has been the subject of various proposals both historically and philosophically. Of all stands that of Thomas Kuhn, whose book *The Structure of Scientific Revolutions* is a milestone for those interested in the construction of scientific knowledge. Following what was discussed at previous papers (Chamizo 2014), here I will develop what I have called the Fourth Chemical Revolution, using exemplars instead of paradigms. It means considering also the incorporation of new instruments and the emergence of new sub-disciplines within chemistry as the way to recognize a scientific revolution.

The fourth chemical revolution is fundamentally characterized by the incorporation of new instruments in chemical practices (Morris 2002). With this, chemical laboratories changed more than in the previous 300 years. Instruments such as visible-UV, IR, EPR and NMR spectrometers changed dramatically chemist's thinking about substances. It means that the short spatio-temporal approach to substances made it possible to recognize the complexity that that name alone encompassed (Needham 2010). The old conception of substance, which by definition was out of time, could no longer be maintained. Then gradually the narrow and macroscopic concept of chemical substance was progressively being replaced by the broader and microscopic of chemical species as IUPAC's definition shows today:

*An ensemble of chemical identical molecular entities that can explore the same set of molecular energy levels on the time scale of the experiment...*

With the passage of substances to species the field of study of chemistry grew and became considerably complicated (Ruthenberg, 2002). Many of the reaction intermediaries were nothing more than chemical species. Several of the most important instruments for its study are those that have to do with the spin, the entity of this revolution. Besides instrumental chemistry, quantum chemistry and molecular biology appeared as subdisciplines.

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### Toxicology in France in the mid-XIXth Century

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**Résumé en français** - Plusieurs études récentes se sont penchées sur le « moment Orfila » et la « nouvelle toxicologie » qui émerge en France dans la première moitié du XIX<sup>e</sup> siècle. Ces travaux soulignent le rôle essentiel de la diffusion des connaissances et de l'expertise dans la promotion de la toxicologie. Il n'existe cependant aucune vue d'ensemble sur cette nouvelle "discipline" au cœur de la gestion du risque chimique.

Ma communication a pour but de présenter un panorama de la place de la toxicologie au sein des disciplines académiques à travers le long XIX<sup>e</sup> siècle. Le caractère interdisciplinaire de son émergence et de son développement n'est pas sans rappeler celui de la chimie organique qui croise les mêmes champs de savoirs et de savoir-faire avec cependant des poids relatifs différents (chimie, pharmacie, médecine et industrie en particuliers). Le caractère polémique de la toxicologie issue de sa médiatisation (plus ou moins voulue et/ou maîtrisée) ajoute une dimension sociale et politique qui complexifie ce processus.

Ma communication sera axée sur les aspects matériels et sur l'organisation de l'enseignement de la toxicologie à travers les différentes chaires de l'enseignement supérieur. Les manuels sont représentatifs de l'existence d'une « science normale » au sens de Thomas Kuhn. J'examinerai en particulier une littérature très peu étudiée, les thèses consacrées à un sujet de toxicologie. Enfin, je m'interrogerai sur l'existence d'une "communauté des toxicologues" et sur le statut de « toxicologiste » au XIX<sup>e</sup> siècle.

**English summary** - Several recent studies dealt with the "Orfila moment" and the "new toxicology" which emerges in France in the first half of the XIXth century. These works emphasize the essential role of knowledge dissemination and expertise in the promotion of toxicology. There is however no overview on this new "discipline" which is at the heart of chemical risk management.

My communication aims at presenting an overview of the place of toxicology within the academic disciplines throughout the long XIXth century. The interdisciplinary character of its emergence and of its development is comparable to that of organic chemistry which crosses the same fields of knowledge and know-how, with different relative weights however (chemistry, pharmacy, medicine and industry in particular). The polemical character of toxicology stemming from its mediatization (more or less wanted and/or controlled) adds social and political dimensions which complicate this process.

My communication will be centred on the material aspects and organization of toxicology teaching through the various chairs of the higher education. Textbooks are representative of the existence of a "normal science" in Thomas Kuhn's sense. I will examine in particular a little studied literature, the theses devoted to a toxicological subject. Finally, I will question the existence of a "community of toxicologists" and the status of "toxicologist" in XIXth century.

**An archeology of the chemical conceptions of the Earth:  
from chemical geology to Gaia and Earth system science**

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Historians and philosophers of science have traced and analyzed the history of the institutions and ontologies underpinning our contemporary conceptions of the Earth and the environment. The emphasis has been placed upon the *physical* conceptions of the globe – from the theories of the Earth of the 18<sup>th</sup> century (e.g. Rudwick 2005) to the development of geophysics (climatology, sismology) during and after the Cold War period (e.g. Oreskes & Fleming 2000; Turchetti & Roberts 2014; Aykut & Dahan 2015) – and on the importance of *ecology* to give birth to a new conception of nature and the environment (e.g. Worster 1982; Deléage 1991; Drouin, 199 ; Mahrane et al. 2012).

By comparison, *chemical* conceptions of the Earth have been vastly overlooked. Yet they underpin the most influent contemporary framework in the sciences of the Earth and the environment: the so-called “Earth system science”, which emerged in the 1980’s and within which the concept of the anthropocene arose in 2000.

The aim of this communication is to trace the archeology of the chemical conceptions of the Earth at the core of Earth system science. It will thus shed light on the *longue durée* history of the chemical conceptions of the Earth, from the chemical geology (and agricultural chemistry) of the 19<sup>th</sup> century to the contemporary conceptions of the “Earth system” going through the constitution of geochemistry in the mid-20<sup>th</sup> century and the elaboration of the Gaia hypothesis.

More specifically, I will first show that the ontological concepts at the heart of Earth system science – global chemical equilibrium, global cycles, interconnexion –, commonly associated with the “*ecological thought*”, are anything but new: they are deeply rooted in the emergence of the chemical studies of living beings’ metabolism, volcanoes’ exhalation, and chemistry of soils and rocks in the 19<sup>th</sup> century.

Drawing on my previous work (Dutreuil 2016), I will then show the historical importance of the Gaia hypothesis, elaborated in the second part of the 20<sup>th</sup> century by a chemical engineer and a microbiologist (Lovelock & Margulis), to bring to the fore the chemical (and biological) ontology of the Earth at the heart of ‘Earth system science’.

Finally, I will propose a philosophical interpretation of the core differences between the physical, chemical and ecological ontologies of the Earth.

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## Plenary lecture (16:30-17:30)

### Biology and chemistry: strong, but ambiguous relations

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Chemistry is everywhere in extant biology, but often invisible. It is a sign of the ambiguous relations of biologists to chemistry. I will provide a brief historical description of these relations in my lecture.

The first part will be devoted to the increasing place that chemistry had in biology from Lavoisier to the development of biochemistry in the first part of the 20<sup>th</sup> century. A research program, aimed at characterizing the chemical components of organisms, and at determining their structures, grew progressively, and remains active in the first decades of the 21<sup>st</sup> century. It did not prevent the most eminent physiologists to recurrently argue during the 19<sup>th</sup> century that the chemistry of life is different from the chemistry done by the chemists.

The rise of molecular biology was also a time of ambiguities. Genetics, that rapidly developed in the 20<sup>th</sup> century, in parallel with biochemistry, was often considered as the dominant subdiscipline of biology, although it described the gene in an abstract way - the chemical nature of the gene not being seriously looked for. The description of macromolecules, proteins and DNA, was an important part of the rise of molecular biology, but the details of these structures were often neglected. The ribbon representation of proteins, elaborated by Jane Richardson at the beginning of the 1980s, focused on the secondary structures of proteins, and opened the way to the comparison of proteins with nanomachines. Arrows representing the transfer of information progressively replaced those representing chemical reactions. The development of genetic engineering led to the production of « kits », the use of which no longer requires any chemical knowledge from the part of biologists.

The conceptual landscape is presently moving fast in biology, but it remains difficult to know in which direction. On one side, more attention is given to the organization of molecules and macromolecules in systems and networks. On the other side, a new representation of proteins has emerged from the combined progress made in chemistry (NMR) and in computing (molecular dynamics) that appears as the abandonment of the chemical representations that were dominant in molecular biology during the last sixty years.

## VII.4 Abstracts of the lectures given on Thursday 6th, 2017

### Plenary lecture (09:00-10:00)

#### Philosophy of Technology: Rethinking the Conditions of Knowledge

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In the context of the generalisation of technoscience, NBIC convergence, and Anthropocene debates, the aim of this lecture is to introduce some concepts, methods and perspectives about an important issue to clarify: What is technology? And more precisely: what is the relationship between science and technology?

We would explain how and why current definitions are insufficient, and even problematical, as soon as technology is defined as an industrial domain, or as an application of science, or even as the science of technics. In fact, and this is our hypothesis, technology is the *condition of knowledge* and, more generally speaking, the condition of thought understood as a reflective practice which depends on a singular 'associated milieu'. To understand that, we need: (1) to study the assumptions upon which these definitions rely and the limits of their applications; (2) to analyse the composition and the interactions of the technical condition of thought (tools, instruments, and embodied technical schemes); and (3) to propose another definition of « technology », that is to say, to define a *philosophical* technology which would enable us to rethink the great series of metaphysical oppositions between subject and object, matter and form, imagination and realization, theory and practice, discover and invention, and science and technics, without referring to functionalism or to utilitarianism.

If some of great modern and contemporary thinkers have paved the way for a philosophical technology (by following or criticizing Marx and Heidegger), the French contemporary philosopher Gilbert Simondon is certainly the main protagonist of this renewal. This lecture will try to present Simondon's theory of technology as a processual, relational and normative theory, whose different forms (his inductive study of technical objects (*science of technics*); his systematisation and universalisation of technical schemes in order to coordinate sciences (*general technology*), his abstract methodology to rationalise the organisation of technics (*rational technology*), and his overall theory of the reciprocity relationship between technics and science (*reflective technology*)), could turn out to be very useful for philosophers of chemistry, and especially in order to understand the epistemological role of the laboratory system in the advance of knowledge, without falling into a material or sociological reductionism.

Beyond this instrumental realism of the knowledge, the philosophical technology of Simondon plays its full role in the creation of a new encyclopedism. This new encyclopedism, which could be defined as a *technological* encyclopedism, is elaborated in response to the main cause of contemporary alienation, *i. e.*, the ignorance of the signification of technics and, in particular, of the machines working with information and interconnected by networks. Aiming at overcoming the humanism and technicism alternative, this new encyclopedism is also the condition of the future reorganization of technics and culture, with the view to framing a general ecology.

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### Chemistry and concurrent exploratory science

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This paper is an attempt to motivate the idea that exploration in chemistry is worthy of philosophical attention. A recent systematic account of the plural functions of scientific models in general philosophy of science isolates four activities associated with scientific exploration: starting points for inquiry; proof of principle demonstrations; potential explanations; and assessing the suitability of the target (Gelfert 2015). While these exploratory functions of models are often realized in the special sciences, the present paper attempts to highlight some distinctive characteristics of exploration in chemistry. It can consist in a kind of chemical cartography directed to the exploration of molecular ephemera such as transition states and is concurrent with more traditional epistemic activities like representation and explanation.

Chemists use potential energy surfaces to study the relationship between molecular energy and geometry and it is a central tool for the study of molecular transformations. The discourse of physical chemistry is at times reminiscent of physical geography: reference to potential energy “surfaces”, “landscapes” and “cartography” have arisen as chemists compute and envisage the relationship between changes in potential energy as a molecule or group of molecules depart from a low energy equilibrium on a “journey” to an endpoint such as the dissociation of bonds in a molecule or the generation of new products in a chemical reaction. Transition states are the most ephemeral of stationary points on a potential energy surface whose transitory status is of distinct aesthetic significance (Spector, forthcoming). It will be argued that a cartography of molecular ephemera is of exploratory epistemic significance because chemists’ maps create opportunities to epistemically access elusive target systems as well as the computational tools used to create those maps.

The importance of exploratory chemistry can be illustrated by the ways in which it contributes to the engagement between different explanatory activities within and across institutional settings. It has been recently argued that synthetic organic chemistry and quantum chemistry are based on different kinds of scientific understanding and engage in different, although complementary, explanatory agendas (Goodwin 2009; 2013). This paper will argue that exploration comes to the fore in interactions between organic chemistry and quantum chemistry. Perhaps, just like plural uses maps can be put to by different groups of actor, the codification of potential energy surface in maps and graphs can be thought of as “boundary objects” (Star & Griesemer 1989). Exploratory science can occupy complementary but sometimes contested regions of disciplinary legitimacy and identity. As such, potential energy maps and graphs seem to be exploratory in an institutional and social epistemic sense because they create an exploratory space for interaction between organic and computational chemistry with the attendant disciplinary advantages and disadvantages boundary objects can bring.

This suggests that “exploration” is not merely a placeholder for scientific “discovery” because exploratory science can be concurrent with scientific inquiry after at least moderate consensus has been established. In computational chemistry, for example, a considerable amount of exploratory modelling engages with various approximation methods used to construct computational quantum chemical models of canonical organic reactions such as the Diels-Alder reaction. Exploratory modeling in computational chemistry can be characterized by the development of “controllable” models used to underwrite the construction of potential energy surfaces and this in turn can underwrite explanations in organic chemistry.

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### The role and reach of transdiction in chemical epistemology

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Transdiction is to use data in such a way as to not only to be able to move back and forth within experience, but also to be able to say something meaningful and true about what lies beyond the boundaries of possible experience.<sup>1)</sup> It underlies most of the chemical knowledge concerned with the molecule and molecular events. Newton advocates transdiction in Principia and tried to justify it by resting on the uniformity of nature, although the latter is a hypothesis which has never been demonstrated to be true. On the other hand, Kant says it is illegitimate to apply any concepts whatsoever to objects beyond the bounds of sense, because the transcendent use of concepts produces transcendental illusory appearances and leads to mistaking a subjective representation for an objective cognition.<sup>2)</sup> Whether or not chemical concepts such as molecular structure can be justified despite Kant's arguments is an unresolved issue, and the main thesis of this paper.<sup>3)</sup> Transdiction will be discussed in light of the positive role of the transcendental idea, and from a critical realist point of view, as well. My points are 1) transdiction is an example of the regulative employment of reason, and 2) what is referred to in transdiction is not a noumenon, but a scientific model. The latter is a transcendental being which provides the systematic unity of empirical cognition. One consequence of this view of transdiction is that the contents of our knowledge are created by the model. Another consequence is concerned with the nature of chemical knowledge. Chemistry is a science based on the creation-oriented understanding of nature. And creation is a motive for modelling molecular phenomena, which determines the nature of our knowledge. That is to say, chemical knowledge is of a practical nature, and hence, it has room for analysis from an ethical point of view. Thus, this study suggests that chemistry is worth critical investigation with practical reason.

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**“Only the initiates will have the secrets revealed”:  
computational chemists and the openness of scientific software**

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In Computational Chemistry, various ways of modeling molecules, associated with distinct “epistemic cultures” (from the reductionist perspective of quantum chemistry (Gavroglu & Simões, 2011) to the pragmatic perspective of “molecular mechanics” (Wieber, 2012)), have been developed. The implementation of these methods of modeling into software has been linked to epistemic concerns such as for example the Sisyphean task of “parameterization”. Our study aims to analyze the difficult relationships between these various modeling methods and the software implementing them throughout the nineties. Developing, using, licensing and distributing software led to multiple tensions among and between the scientists in intertwined academic and industrial contexts. In order to understand these tensions, we explore the Computational Chemistry List (Labanowski, 2007). We analyze in detail two flame wars which exemplify these tensions and show how issues of theories, methods of modeling, parametrization, code, reproducibility of results, epistemic transparency, intellectual property, and the commercialization of software are articulated.

Finally, our study is more generally an example of the complex relationship between scientific practices and software. It addresses the more general issue of “openness” (Tkacz, 2015). Openness, in this particular scientific context, includes concerns regarding models and their parameterization, scientific collaboration, accessibility of results and publications. These concerns relate to the technical, industrial, commercial and legal aspects of software in scientific activity (Kelty, 2011).

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**Plenary lecture (12:00-13:00)**

**What does the present neglect of ethics of chemistry tell us about the past neglect of philosophy of chemistry, and vice versa?**

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It has been a standard procedure to introduce papers and books on the philosophy of chemistry by referring to the longstanding neglect of chemistry by philosophers of science. Various explanations have been offered and even more can be said on that. Yet while complaining about that, philosophers of chemistry have themselves similarly neglected the ethical issues of their discipline, unlike for instance philosophers of biology or technology. That is more than surprising because ethical issues of chemistry have been publicly debated ever since, and because ethics is after all one of the major subdisciplines of philosophy. It is also puzzling because various national and international organizations recommend or require ethics components in the teaching of chemistry, which is already mandatory in many countries. Who else than philosophers of chemistry should do that?

The main part of the paper goes through various explanations of the past neglect of chemistry and draws parallels to the current neglect of ethics in philosophy of chemistry. In conclusion I will argue: If you want to know why philosophers have neglected chemistry in the past, you can easily find most of the answers by asking yourself: Why am I reluctant to work on ethics of chemistry?

Finally I present a project by Tom Børsen (Aalborg University, Denmark) and myself which develops a canonical set of “Ethical Case Studies of Chemistry” suitable for undergraduate teaching and available in *HYLE: International Journal for Philosophy of Chemistry* (<http://www.hyle.org/journal/issues/22-1/index.html>, <http://www.hyle.org/journal/issues/23-1/index.html>).

## **VIII. POSTER SESSION**

A poster session is organized during the lunch on Wednesday 5th, 2017. Two researchers will share their work with us:

Mareike Frevert (University of Kassel, Germany) will introduce her research in chemical education, and especially her scrutiny of the philosophical concepts being used in chemistry teaching.

Yona Siderer (The Hebrew University of Jerusalem, Israel) will introduce her historical research, and especially about chemistry in Japan.