



ANNUAL REPORT

2016

Instituts Internationaux
de Physique et de Chimie
fondés par Ernest Solvay, asbl

Internationale Instituten
voor Fysica en Chemie
gesticht door Ernest Solvay, vzw

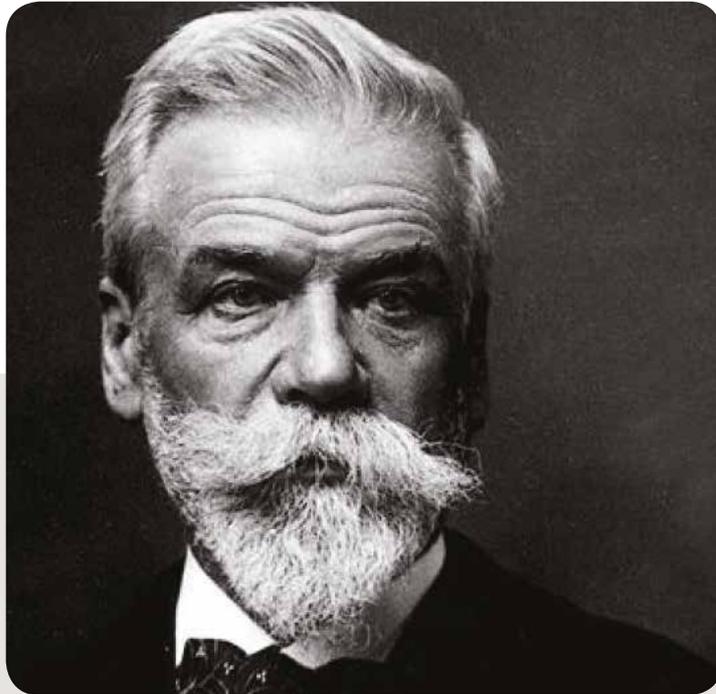


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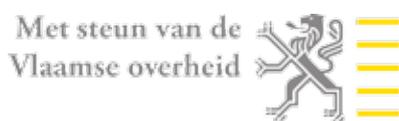
There are no limits
to what science can explore

Ernest Solvay



The International Solvay Institutes for Physics and Chemistry, founded by Ernest Solvay, acknowledge with gratitude the generous support of

The Solvay Family



FONDATION
DAVID ET ALICE
VAN BUUREN



The Belgian National Lottery and the International Solvay Institutes: a long-term partnership



The Belgian National Lottery is one of the main philanthropic organizations in Belgium, which has consistently supported the activities of the International Solvay Institutes for decades. We gratefully acknowledge all those who make this support possible.

This support contributes to the international visibility of Belgium. Most of the greatest chemists and physicists of the 20th and 21st century have come to Brussels to participate in the prestigious “Solvay Congresses”, the pictures of which are known worldwide and have become a symbol of excellence. The Solvay Conferences have put Brussels on the scientific world map.

The support of the National Lottery also paves the way to the future of our society. Investment in scientific knowledge and brainpower is more crucial than ever. Specific activities of the Institutes targeted to inspire the young generations towards science as well as to develop training-through-research (Colloquia, open Workshops, Public Event) directly benefit from the support of the National Lottery.



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In Memoriam



It is with immense sadness and deep emotion that the International Solvay Institutes recall the memory of their former director **Baron André Jaumotte**, who passed away on December 18, 2016.

Professor at the Faculty of Applied Sciences/Engineering School of the Université Libre de Bruxelles, Rector and then President of the Board of that same university, André Jaumotte relentlessly supported the International Solvay Institutes for more than half a century.

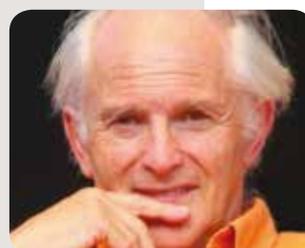
Instrumental in the establishment of the Institutes as an independent “Association sans but lucratif - Vereniging zonder winstoogmerk” after the creation of the Vrije Universiteit Brussel in 1970 - a measure that gave them a new start -, he brought his full talent and energy to overcome the difficult transition period that followed the death of Professor Ilya Prigogine in 2003. Not only did he hold the position of Director from June 2003 through December 2003, but he also contributed, in coordination with Professor Irina Veretennicoff, to define rules and goals for the Institutes that helped them develop successfully new ambitious programs.

Member of the Board of Directors of the Institutes, his sharp comments and incisive advices played a crucial role in many of the important decisions adopted by the Board.

Man of a great culture with an unusual curiosity in all aspects of human creativity, André Jaumotte had in particular a profound interest for science and fundamental research. The International Solvay Institutes will keep a grateful remembrance of his attentive action.

The year 2016 has also been marked by the death of two personalities close to the Institutes, **Professors Harold Kroto** (Chemistry Nobel Laureate 1996) and **Ahmed Zewail** (Chemistry Nobel Laureate 1999). Both were members of the International Solvay Committee for Chemistry, in charge of the Chemistry Conferences.

We will deeply miss them.



A word from the President

I will remember the year 2016 for 2 significant events:

The first one was to see the highest scientific recognition being bestowed onto our friends and participants of the 2007 Solvay Chemistry conference, Ben Feringa, Jean-Pierre Sauvage and Fraser Stoddard. We were thrilled to learn this news from Stockholm, just days before the start of our 24th Chemistry conference, on October 18th. This was especially joyful because Ben Feringa is a distinguished member of our Advisory Committee and was not only participating in this year's Chemistry Conference but he was also scheduled to be one of the keynote speakers of our public event that concluded the conference.

We congratulate our friend Ben for this outstanding acknowledgment.

The second event was the celebration of the 50th anniversary of the meetings "Les rencontres de Moriond" at the International Center for Interdisciplinary Science and Education in Qui Nohn, Vietnam. These meetings, founded by Jean Tran Thanh Van, are a tribute to the spirit of informal and focused scientific conversations. This celebration and the presence of the outstanding people that gathered in Qui Nohn are a statement to the importance of fundamental science as a shared understanding of the world that surrounds us. Curiosity driven research has the amazing ability to bring people together, no matter their origin on this planet, to tackle the most compelling questions and find solutions to humankind's most difficult challenges.

We thank Jean Tran Thanh Van and his wife Kim for the opportunity to support such an outstanding event.

Lastly, as I look onto the list of the events organized or supported by the Institutes during the year 2016, I cannot but be impressed by the diversity of the participations and the quality of the collaborations with other research and academic institution in Belgium and abroad. For this, I thank, the director, his team and the members of the local committees in physics and in chemistry who together offer these activities to our community of young scientists.

I extend my special thanks to the back-office team composed of Dominique, Isabelle and Chantal that make all this possible.



A handwritten signature in blue ink, which appears to be "JMS".

Jean-Marie Solvay
President

A word from the Director

The year 2016 was again an intense scientific year for the International Solvay Institutes.

The major event was the organization of the 24th Solvay Conference on chemistry (“24^e Conseil de Chimie Solvay”) in the Hotel Métropole from 19-22 October 2016. Devoted to “Catalysis in Chemistry and Biology”, the meeting attracted in Brussels about 50 leading scientists from all over the world who confronted their views on subjects as diverse as “Homogeneous Catalysis”, “Catalysis by Microporous Materials”, “Catalysis under Extreme Conditions: Studies at High Pressure and High Temperatures – Relations with Processes in Nature” and “Catalysis by Ribozymes in Molecular Machines”. The conference was a great scientific success. The International Solvay Institutes are most grateful to the conference chairs, Nobel laureates Kurt Wüthrich and Robert Grubbs, for the remarkable preparation work that went into the organization of the scientific program.

As it is the tradition, the 24th Solvay Conference on Chemistry was followed by a public event on October 23, whose theme was “Chemistry for the World of Tomorrow”. Nobel Laureates Robert Grubbs and Ben Feringa delivered popular lectures on the translation of academic research into industrial applications, and on molecular machines, respectively. The event was remarkably successful. The lecture hall was fully packed by participants from all generations. We thank the two lecturers for their very inspiring talks.

Many distinguished scientists connected with the Institutes were awarded important Prizes in 2016. Let us mention the two most notable Awards.

- Professor Ben Feringa, member of our Advisory Board, received the 2016 Nobel Prize in Chemistry for “the design and synthesis of molecular machines”. This scientific distinction – the highest among the international prizes – recognizes his pioneering and imaginative work in a field that holds remarkable promises. The 2016 Nobel Prize in Chemistry was shared with Professors Jean-Pierre Sauvage and Sir J. Fraser Stoddart. All three of them participated in the 2007 Solvay Conference on Chemistry, of which Professor Sauvage was actually the chair. It is for us a great source of honor and pride to warmly congratulate them for their exceptional achievements. Professor Ben Feringa will be the holder of the 2018 International Solvay Chair in Chemistry.
- Professors Stephen Hawking and Viatcheslav Mukhanov, holder of the Jacques Solvay Chair in 2014, received the 2015 BBVA Foundation Frontiers of Knowledge Award (attributed in 2016) for “discovering that the galaxies were born from quantum fluctuations”. Their bold prediction on the quantum origin of the large scale structure of our universe was impressively confirmed by space telescope observations. Professors Hawking and Mukhanov are both regular participants in Solvay activities. All our congratulations go to them too.

The report that follows reviews in detail the activities organized or supported by the International Solvay Institutes during the year 2016. These activities (2 chairs, 9 workshops, 11 colloquia, 1 graduate school in theoretical physics) attracted to Brussels hundreds of scientists and covered a wide spectrum of developments at the frontiers of physics and chemistry.

I will just briefly mention in this introductory section the annual international Solvay Chairs in Physics and Chemistry, respectively created in 2006 and 2008. The 2016 Solvay Professor in Chemistry was Professor Raymond Kapral, from the University of Toronto (Canada). The 2016 Jacques Solvay Chair in Physics was held by Professor Dam Thanh Son from the University of Chicago (USA). Both chair holders gave brilliant opening lectures explaining the most pressing challenges in their respective fields of investigation: “Molecular Machines and Synthetic Motors: Active Motion on the Nanoscale” and “Fluid viscosity: from Maxwell to black holes”. These opening lectures were attended by many students and researchers from the ULB, the VUB and other Belgian universities.

This activity report also describes the research carried in the groups of the Director, of the deputy-Directors, and of the Scientific Secretaries of the International Scientific Committee for Chemistry and the International Scientific Committee for Physics. The research highlights of other researchers connected with the Institutes are also outlined.

The research of the group of the Director benefited from the direct and most precious

support of the Solvay family and the Solvay group, as well as from generous gifts from Messrs. Collen, de Selliers de Moranville and Jaumotte.

I heartily thank them.

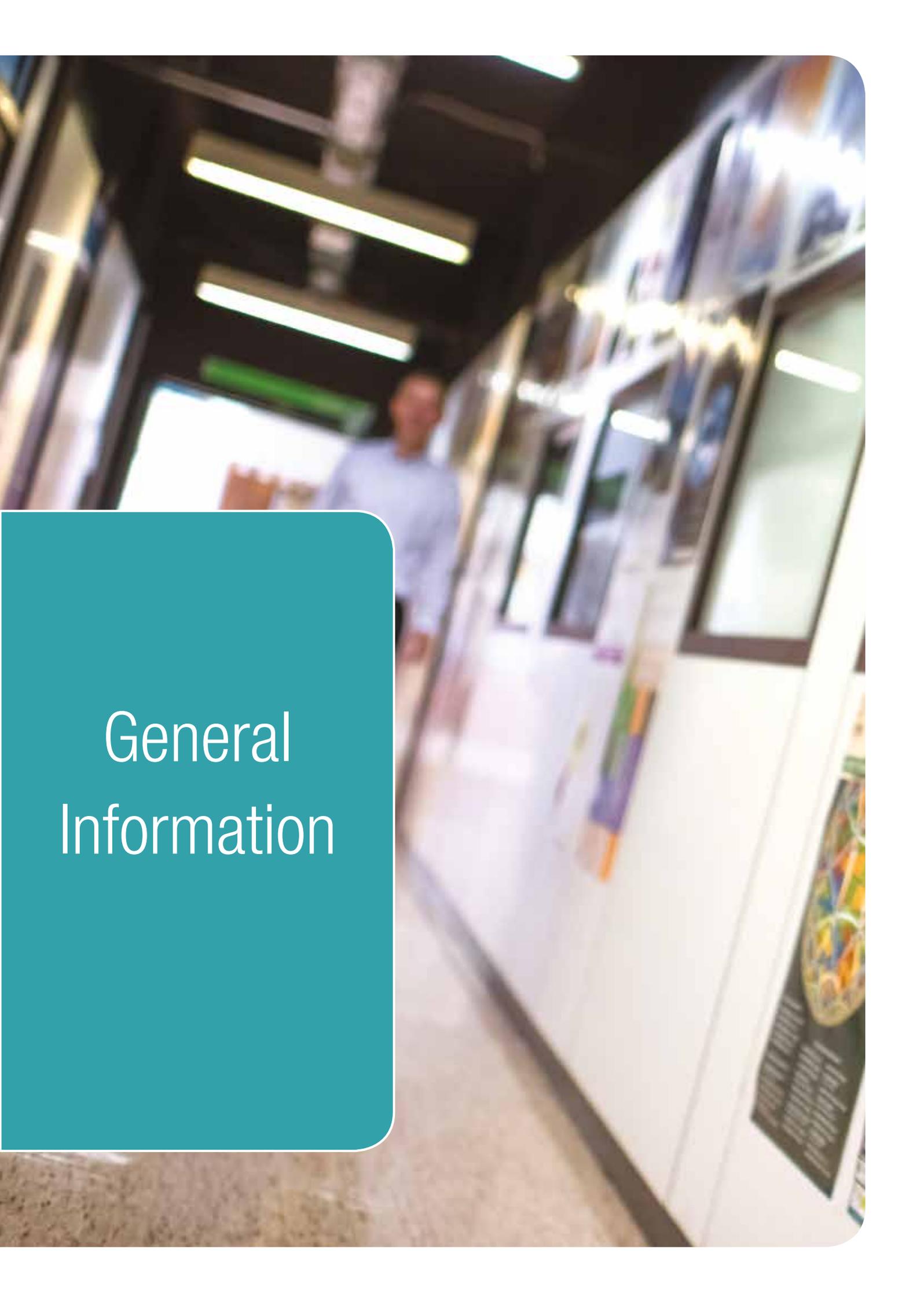
The activities described in this report would not have been possible without the help of the sponsors of the International Solvay Institutes, to whom I would like to express our gratitude. These are the Université Libre de Bruxelles, the Vrije Universiteit Brussel, the Solvay Company, the Belgian National Lottery, the Brussels Region, the Fédération Wallonie-Bruxelles, the Vlaamse Regering, the David & Alice Van Buuren Foundation, the Hôtel Métropole and last but not least – and as recalled above –, the Solvay family: Mme Solvay, Anne-Christine Solvay, Carole Solvay, Marina Solvay and Jean-Marie Solvay who continue with the same conviction a more than a century-old tradition of support to fundamental research.

The remarkable efficiency and dedicated commitment of Dominique Bogaerts and Isabelle Van Geet in the management of the activities of the Institutes, is again gratefully acknowledged.



A handwritten signature in blue ink that reads "M. Henneaux". The signature is stylized with a long horizontal stroke at the end.

Marc Henneaux
Director



General Information

Board of Directors | Members



Jean-Marie Solvay | *President*



Paul Geerlings | *Vice-President & Treasurer*
Professor VUB



Nicolas Boël | *Chairman of
the Board of Directors of the Solvay Group*



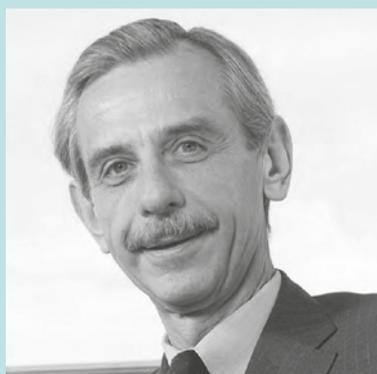
Gino Baron | *Secretary*
Emeritus Professor VUB



Eric De Keuleneer | *Chairman of
the Board of Directors of the ULB*



Daniel Janssen | Former Chairman of the Board of Directors of the Solvay Group



Eric Boyer de la Giroday | Chairman of the Board of Directors ING Belgium sa/nv



Philippe Busquin
Minister of State



Eddy Van Gelder | Chairman of the Board of Directors of the VUB

Board of Directors | Honorary Members

Franz Bingen | Emeritus Professor VUB
Former Vice president and Treasurer of the Solvay Institutes

† **André Jaumotte** | Honorary Rector and Honorary President
of the ULB
Honorary Director of the Solvay Institutes

Jean-Louis Vanherweghem | Former Chairman of the Board
of Directors of the ULB

Irina Veretennicoff | Emeritus Professor VUB

Board of Directors | Guests Members

Anne De Wit | Professor ULB
Scientific Secretary of the International Committee for Chemistry

Freddy Dumortier | Secretary of the Royal Flemish Academy for
Science and the Arts of Belgium

Hervé Hasquin | Secretary of the Royal Academy for Science and
the Arts of Belgium

Marc Henneaux | Professor ULB
Director

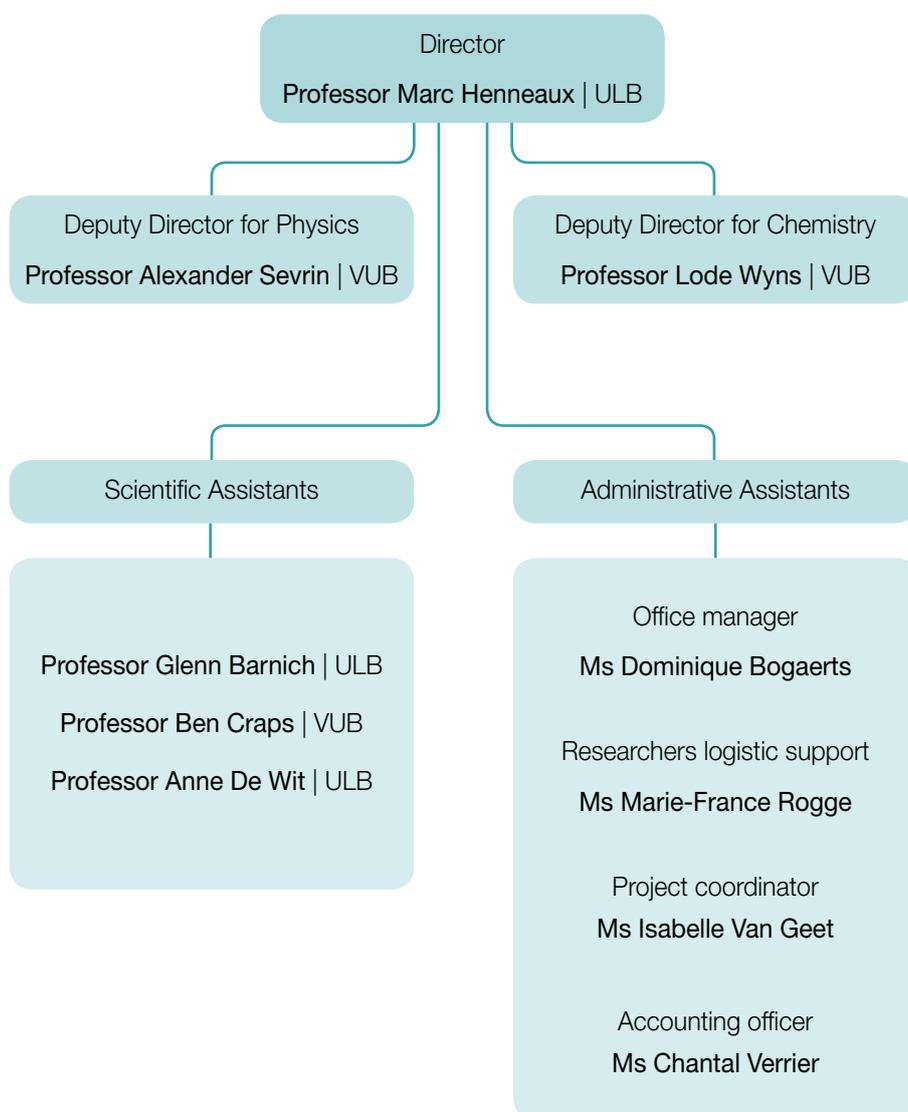
Franklin Lambert | Emeritus Professor VUB

Alexander Sevrin | Professor VUB
Deputy Director for Physics and Scientific Secretary of the
International Committee for Physics

Marina Solvay

Lode Wyns | Former Vice-rector for Research VUB
Deputy Director for Chemistry

Management and Staff



The Director is assisted in his scientific tasks by:

- The International Scientific Committees for Physics and Chemistry, who are fully responsible for the scientific organization of the “Conseils Solvay”.
- The Scientific Assistants to the Director and the Local Scientific Committees, who help him for the organization of all the other activities (workshops, colloquia, chairs).

International Scientific Committee for Physics

Chair

Professor David Gross

2004 Nobel Laureate
Kavli Institute for Theoretical Physics
Santa Barbara, USA

Scientific Secretary

Professor Alexander Sevrin

Vrije Universiteit Brussel, Belgium

Members

Professor Roger Blandford

Stanford University, USA

Professor Steven Chu

1997 Nobel Laureate
Stanford University, USA

Professor Robbert Dijkgraaf

IAS Princeton, USA

Professor Bertrand Halperin

Harvard University, USA

Professor Gerard 't Hooft

1999 Nobel Laureate
Spinoza Instituut, Utrecht, The Netherlands

Professor Giorgio Parisi

Università La Sapienza, Roma, Italy

Professor Pierre Ramond

University of Florida, Gainesville, USA

Professor Klaus Von Klitzing

1985 Nobel Laureate
Max-Planck-Institut, Stuttgart, Germany

Professor Peter Zoller

University of Innsbruck, Austria

The International Scientific Committees for Physics and Chemistry are responsible for the scientific organization of the “Conseils Solvay”.

They are in charge of defining the general theme of the conferences and of selecting a chair person.

Members are appointed for a 6-year period term, renewable once.

International Scientific Committee for Chemistry

Chair

Professor Kurt Wüthrich

2002 Nobel Laureate
Scripps Research Institute, La Jolla, USA
and ETH-Zurich, Switzerland

Scientific Secretary

Professor Anne De Wit

Université Libre de Bruxelles, Belgium

Members

Professor Gerhard Ertl

2007 Nobel Laureate
Fritz-Haber-Institut der Max-Planck-Gesellschaft
Berlin, Germany

Professor Graham Fleming

University of Berkeley, USA

Professor Robert H. Grubbs

2005 Nobel Laureate
California Institute of Technology, Pasadena, USA

Professor Roger Kornberg

2006 Nobel Laureate
Stanford University, USA

† **Professor Harold W. Kroto**

1996 Nobel Laureate
University of Sussex, Brighton, UK

Professor Henk N.W. Lekkerkerker

Utrecht Universiteit, The Netherlands

Professor K.C. Nicolaou

Rice University, USA

Professor JoAnne Stubbe

Massachusetts Institute of Technology, Cambridge, USA

Professor George M. Whitesides

Harvard University, Cambridge, USA

† **Professor Ahmed Zewail**

1999 Nobel Laureate
California Institute of Technology, Pasadena, USA

International Advisory Committee

Chair

Professor Lars Brink

Chalmers University of Technology
Göteborg, Sweden

Members

Professor Leticia Cugliandolo

Université Pierre et Marie Curie – Paris VI, France

Professor Ben Feringa

2016 Nobel Laureate in Chemistry

University of Groningen, The Netherlands

Professor Karen I. Goldberg

University of Washington, USA

Professor Hermann Nicolai

Max-Planck-Institut für Gravitationsphysik,
Golm, Germany

Professor Hirosi Ooguri

California Institute of Technology, Pasadena, USA

Professor Jacques Prost

Ecole Supérieure de Physique et de Chimie
Industrielles (ESPCI), Paris, France

Professor Gunnar von Heijne

Stockholm University, Sweden

In 2008, the Board of Directors of the International Solvay Institutes decided to set up an International Advisory Committee. The International Advisory Committee of the Solvay Institutes is composed of distinguished scientists who have the task of periodically evaluating all the scientific activities of the Solvay Institutes (outside the Solvay Conferences which are run by the respective Scientific Committees), report to the Board of Directors and provide advice for future developments.

Members are appointed for a 6-year period term, renewable once.

Local Scientific Committees for Physics and Chemistry

Local Scientific Committee for Physics

Chair

Professor Marc Henneaux

ULB, Brussels

Local Scientific Committee for Chemistry

Chair

Professor Lode Wyns

VUB, Brussels

Members

Professor Conny Aerts | KU Leuven
Professor Nicolas Boulanger | UMONS
Professor Ben Craps | VUB, Brussels
Professor Jan Danckaert | VUB, Brussels
Professor Pierre Gaspard | ULB, Brussels
Professor Jean-Marc Gérard | UCL, Louvain
Professor Joseph Indekeu | KU Leuven
Professor Philippe Lambin | FUNDP, Namur
Professor Dirk Ryckbosch | UGent
Professor Alexander Sevrin | VUB, Brussels
Professor Jacques Tempere | UAntwerp
Professor Petr Tinyakov | ULB, Brussels
Professor Christian Van den Broeck | UHasselt
Professor Sophie Van Eck | ULB, Brussels
Professor Nicolas Vandewalle | ULg, Liège

Members

Professor Annemie Bogaerts | UAntwerp
Professor Benoît Champagne | FUNDP, Namur
Professor Pierre-François Coheur | ULB, Brussels
Professor Gert Desmet | VUB, Brussels
Professor Anne De Wit | ULB, Brussels
Professor Paul Geerlings | VUB, Brussels
Professor Yves Geerts | ULB, Brussels
Professor Jeremy Harvey | KU Leuven
Professor Sophie Hermans | UCL, Louvain
Professor Roberto Lazzaroni | UMONS
Professor Luc Moens | UGent
Professor Jean-Christophe Monbaliu | ULg, Liège
Professor Han Remaut | VUB, Brussels
Professor Marlies Van Bael | UHasselt

Observer

Professor Anne De Wit

ULB, Brussels

Observers

Professor Pierre Gaspard | ULB, Brussels

Professor Marc Henneaux | ULB, Brussels

The Local Scientific Committees help the Director for the organization of the Workshops, Colloquia, Chairs and Doctoral School.

Members are appointed for a 3-year period term.

Honorary Members

Professor Fortunato Tito Arecchi
Università di Firenze and INOA, Italy

Professor Claudio Bunster
Centro de Estudios Científicos, Valdivia, Chile

Professor Claude Cohen-Tannoudji
1997 Nobel Laureate
Ecole Normale Supérieure, Paris, France

Professor Manfred Eigen
1967 Nobel Laureate
Max-Planck Institut, Göttingen, Germany

Professor François Englert
2013 Nobel Laureate
Université Libre de Bruxelles, Belgium

Professor Ludwig Faddeev
V.A. Steklov Mathematical Institute
St Petersburg, Russia

Professor Stephen Hawking
Cambridge University, UK

Christian Jourquin
Former CEO Solvay Group, Belgium

Professor I.M. Khalatnikov
Landau Institute of Theoretical Physics
Moscow, Russia

Professor Jean-Marie Lehn
1987 Nobel Laureate
Collège de France, Paris, France

Professor Mario J. Molina
1995 Nobel Laureate
Massachusetts Institute of Technology
Cambridge, USA

Professor Victor P. Maslov
Moscow State University, Russia

Professor Stuart Rice
University of Chicago, USA

Professor Victor A. Sadovnichy
Moscow State University, Russia

Professor Roald Sagdeev
University of Maryland
College Park, USA

Madame Solvay de la Hulpe, Belgium

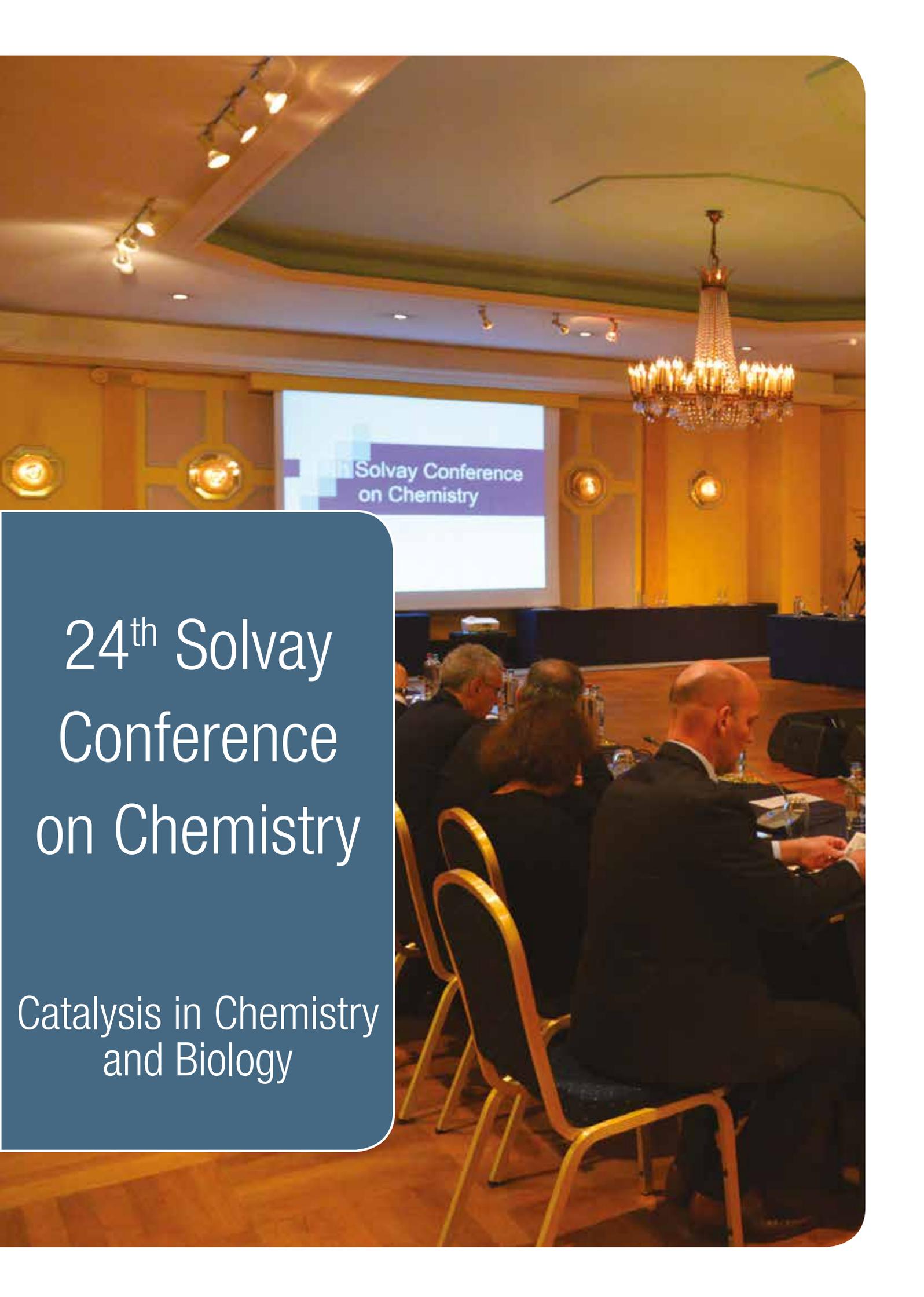
Professor E.C.G. Sudarshan
University of Texas, Austin, USA

Professor Chen Ning Yang,
1957 Nobel Laureate
Chinese University Hong Kong &
Tsinghua University, Beijing, China

Members of the General Assembly

Antoniou Ioannis	Levy-Morelle Jacques
Barnich Glenn	de Maret Pierre
Baron Gino	Misonne Jean-François
Bingen Franz	Monard Elisabeth
Boël Nicolas	Nicolis Grégoire
Boyer de la Giroday Eric	Piret Jean-Marie
Bonnefous Thierry	Querton Alain
Busquin Philippe	Rolin Patrick
Craps Ben	Sanglier Michèle
De Keuleneer Eric	de Selliers de Moranville Jacques
De Knop Paul	Sevrin Alexander
De Vos Gabrielle	Madame Solvay de La Hulpe
De Wit Anne	Solvay Anne-Christine
Dumortier Freddy	Solvay Carole
Gaspard Pierre	Solvay Denis
Geerlings Paul	Solvay Jean-Marie
Geerts Yves	Solvay Marina
Goldbeter Albert	Van Camp Benjamin
Halloin Véronique	Van den Broeck Christian
Hasquin Hervé	Van Gelder Eddy
Henneaux Marc	Vanherweghem Jean-Louis
Janssen Daniel	Veretennicoff Irina
Janssen Emmanuel	Viviers Didiers
Jaumotte André	Wyns Lode
Jolly Baudouin	Wielemans Patrick
Jourquin Christian	Willox Ralph
Lambert Franklin	





24th Solvay Conference on Chemistry

Catalysis in Chemistry
and Biology

24th Solvay Conference on Chemistry

Catalysis in Chemistry and Biology

19 - 22 October 2016

Catalysts are ubiquitous in chemical industry as more than 80% of chemicals have come into contact with at least one catalyst material during their manufacturing process. Similarly, natural life and many chemical processes in nature are simply impossible without the interplay of many enzymes often working in an intimate cascade-type manner.

The 24th Solvay Conference was devoted to this extremely active and challenging field. Its central goal was to bring together leading chemists from different horizons to summarize the progress in their own area, give their perspectives on the challenges lying ahead of their discipline and search for general concepts underlying catalysis in chemistry and biology. The theme of the conference was chosen by the International Solvay Scientific Committee for Chemistry chaired by Nobel laureate Professor Kurt Wüthrich, from the Scripps Research Institute and the ETH.



Professor Kurt Wüthrich

The Conference took place at the hotel Metropole in Brussels from October 19 through October 22, 2016. It was chaired by Nobel laureate Professor Kurt Wüthrich and co-chaired by Nobel laureate Professor Robert Grubbs (Caltech). Together with the chairs of the various sessions, they put up a splendid program. The International Solvay Institutes express their deepest thanks to all of them for the remarkable success of the 24th Solvay Conference on Chemistry.



Professor Robert Grubbs

“[...] It was a real feast of catalysis. I enjoyed every minute and it certainly served the purpose to bring communities together, broaden our horizons and set the stage for the next big steps. [...]”

Ben Feringa, 2016 Nobel Laureate in Chemistry



The inaugural session of the Conference was graced with the presence of King Philippe, who met the participants during the coffee break that followed. (Photo: discussion with Professors Feringa and Wüthrich).

The International Solvay Institutes are fortunate to benefit from the benevolent support of the Royal Family and acknowledge with respectful gratitude the continuation of a centenary-old tradition.



Scientific themes and Program

The 24th Solvay Conference addressed at length many frontier themes:

1. Homogeneous catalysis
2. Heterogeneous Catalysis and Characterization of Catalyst Surfaces
3. Catalysis by Microporous Materials
4. Catalysis under Extreme Conditions: Studies at High Pressure and High Temperatures – Relations with Processes in Nature
5. Catalysis by Protein Enzymes
6. Catalysis by Ribozymes in Molecular Machines

leading to the very challenging following program:

Wednesday 19 October 2016

Inaugural session in the presence of His Majesty the King of the Belgians

- 9:00 – 9:15 Welcome addresses by Marc Henneaux, Director of the Solvay Institutes and by Kurt Wüthrich, Chair of the Scientific Committee for Chemistry of the International Solvay Institutes
- 9:15 – 9:35 *Catalysis in Nature and in Chemical Laboratories and Industries* by Kurt Wüthrich, Chair of the Conference and Robert Grubbs, Co-chair of the Conference
- 9:35 – 10:10 Coffee Break with His Majesty the King

Session 1: Homogeneous Catalysis

Auditors - Gwilherm Evano & Sophie Hermans

- 10:10 – 12:00 Introductory statement by chair Robert Grubbs
Statements: S. Buchwald, M. Sanford, K. Goldberg,
K. A. Jørgensen, E. Carreira, B. Feringa, M. Albrecht, K. Nozaki,
B. List
- 12:00 – 12:30 Discussion among the panel members
- 12:30 – 12:45 Coffee break
- 12:45 – 13:45 General Discussion

Session 2: Heterogeneous Catalysis and Characterization of Catalyst Surfaces

Auditors - Yannick De Decker & Thierry Visart de Bocarmé

- 14:40 – 16:00 Introductory statement by chair Gerhard Ertl
 Statements: G.A. Somorjai, J. K. Norskov, H. J. Freund, J. Sauer,
 G. Hutchings, A. Corma
- 16:00 – 16:30 Discussion among the panel members
- 16:30 – 17:00 Coffee break
- 17:00 – 18:00 General Discussion

Thursday 20 October 2016

Session 3: Catalysis by Microporous Materials

Auditors - Eric Gaigneaux & Cédric Gomme

- 9:00 – 10:20 Introductory statement by chair Mark E. Davis
 Statements: R. van Santen, E. Iglesia, T. Tatsumi, G. Bellussi,
 J. Casci, C. Jones
- 10:20 – 10:50 Discussion among the panel members
- 10:50 – 11:20 Coffee break
- 11:20 – 12:20 General Discussion

Session 4: Catalysis under Extreme Conditions: Studies at High Pressure and High Temperatures – Relations with Processes in Nature

Auditors - Frank De Proft & Pierre Gaspard

- 14:00 – 15:20 Introductory statement by chair Henk N. W. Lekkerkerker
 Statements: S. Helveg, B. Weckhuysen, X. Bao, M. Koper
 R. Nakamura, C. Coperet
- 15:20 – 15:50 Discussion among the panel members
- 15:50 – 16:20 Coffee break
- 16:20 – 17:20 General Discussion

Friday 21 October 2016

Session 5: Catalysis by Protein Enzymes

Auditor - Wim Versées & Gilles Bruylants

- 9:00 – 10:30 Introductory statement by chair JoAnne Stubbe
 Statements: D. Hilvert, S. Boxer, M. Havenith-Newen,
 R. Marcus, F. Neese, B. Dyer, J. Klinman
- 10:30 – 11:00 Discussion among the panel members
- 11:00 – 11:30 Coffee break
- 11:30 – 12:30 General Discussion



His Majesty The King discussing with Professor Joachim Sauer

Saturday 22 October 2016

Session 6: Catalysis by Ribozymes in Molecular Machines

Auditors - Remy Loris & Lode Wyns

- 9:00 – 10:20 Introductory statement by chair David Lilley
 Statements: D. York, P. Bevilacqua, R. Breaker, J. Christodoulou,
 M. Rodnina, D. Herschlag
- 10:20 – 10:50 Discussion among the panel members
- 10:50 – 11:20 Coffee break
- 11:20 – 12:20 General Discussion



Jean-Marie Solvay, Professor Marc Henneaux, Marina Solvay, Professor Rudolph Marcus, Madame Solvay de la Hulpe, Professor Ben Feringa, His Majesty the King of the Belgians, Professor Kurt Wüthrich, Professor Robert Grubbs and Professor Gerhard Ertl

Participants

The Solvay conferences are elitist conferences by invitation-only, with a limited number of participants. Discussions play a central role.

- Albrecht Martin | University of Bern, Switzerland
- Bao Xinhe | Dalian Institute for Chemical Physics, China
- Bellussi Giuseppe | Eni SpA, Italy
- Bevilacqua Philip C. | Penn State University, USA
- Boxer Steven | Stanford University, USA
- Breaker Ron | Yale University, USA
- Buchwald Stephen | MIT, USA
- Carreira Erick | ETH Zurich, Switzerland
- Casci John | Johnson Matthey Techn. Centre, UK
- Christodoulou John | University of London, UK
- Coperet Christophe | ETH Zurich, Switzerland
- Corma Avelino | University of Valencia, Spain
- Davis Mark E. | Caltech, USA
- De Wit Anne | ULB & Solvay Institutes, Belgium
- Dyer Brian | Emory University, USA
- Ertl Gerhard | Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany
- Feringa Ben | University of Groningen, The Netherlands
- Fleming Graham | University of California, Berkeley, USA
- Freund Hans-Joachim | Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany
- Goldberg Karen | University of Washington, USA
- Grubbs Robert | Caltech, USA
- Havenith-Newen Martina | Ruhr University, Bochum, Germany
- Helveg Stig | Haldor Topsøe, Denmark
- Herschlag Dan | Stanford University, USA
- Hilvert Donald | ETH Zurich, Switzerland
- Hutchings Graham | Cardiff University, UK
- Iglesia Enrique | UC Berkeley, USA
- Jones Christopher | Georgia Institute of Technology, USA
- Jørgensen Karl Anker | Aarhus University, Denmark
- Klinman Judith P. | UC Berkeley, USA
- Koper Marc | Leiden University, The Netherlands
- Lekkerkerker Henk N.W. | Utrecht University, The Netherlands
- Lilley David | University of Dundee, UK
- List Benjamin | MPI für Kohlenforschung, Mülheim an der Ruhr, Germany
- Marcus Rudolph A. | Caltech, USA
- Nakamura Ryuhei | RIKEN, Japan
- Neese Frank | MPI for Chemical Energy Conversion, Germany
- Norskov Jens | Stanford University, USA
- Nozaki Kyoko | University of Tokyo, Japan
- Rodnina Marina | MPI für Biophysikalische Chemie, Göttingen, Germany
- Sanford Melanie | University of Michigan, USA
- Sauer Joachim | Humboldt University of Berlin, Germany
- Somorjai Gabor A. | UC Berkeley, USA
- Stubbe JoAnne | MIT, USA
- Tatsumi Takashi | Tokyo Institute of Technology, Japan
- van Santen Rutger | Eindhoven University of Technology, The Netherlands
- Weckhuysen Bert | Utrecht University, The Netherlands
- Wüthrich Kurt | ETH Zurich, Switzerland - The Scripps Research Institute, La Jolla, USA
- York Darrin M. | Rutgers University, USA

Auditors

The Conference was also attended by auditors from various Belgian universities. Auditors play an essential role in the transcription of the discussions into a publishable text.

The International Solvay Institutes are grateful to the editorial team and in particular to Professors Anne De Wit (Scientific Secretary of the International Solvay Scientific Committee for Chemistry) and Thierry Visart de Bocarmé for their efficient handling of this difficult task.

Bartik Kristin | ULB

Bruylants Gilles | ULB

Buess Claudine | ULB

De Decker Yannick | ULB

De Proft Frank | VUB

De Vos Dirk | KU Leuven

De Wit Anne | ULB

Debecker Damien | UCL

Denayer Joeri | VUB

Detavernier Christophe | UGent

Evano Gwilherm | ULB

Gaigneaux Eric | UCL

Garcia-Pino Abel | ULB

Gaspard Pierre | ULB

Geerlings Paul | VUB

Gommes Cédric | ULg

Govaerts Cedric | ULB

Heinrichs Benoit | ULg

Hermans Sophie | UCL

Hofkens Johan | KU Leuven

Licini Giulia | Padoue

Loris Remy | VUB

Maes Bert | UAntwerp

Martens Johan | KU Leuven

Riant Olivier | UAntwerp

Soumillon Patrice | UCL

Su Bao-Lian | UNamur

Van der Voort Pascal | UGent

Van Speybroeck Veronique | UGent

Versées Wim | VUB

Visart Thierry | ULB

Wyns Lode | VUB

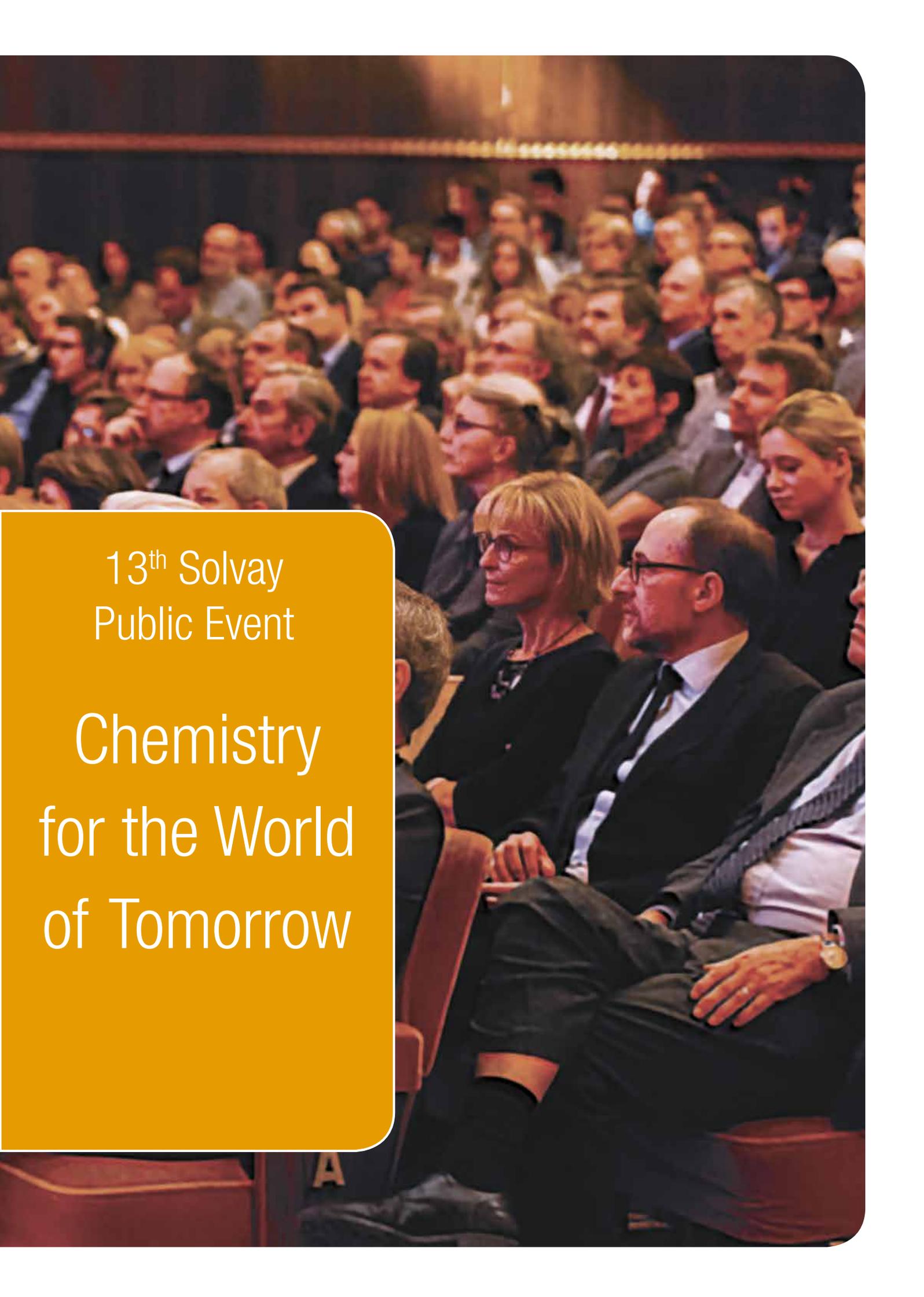




*P. Bevilacqua, G. Bellussi, M. Albrecht, R. Nakamura, J. Sauer, K. A. Jorgensen
B. Dyer, M. Sanford, E. Iglesia, J. Casci, D. Hilvert, M. Havenith
T. Visart, D. Herschlag, S. Helveg, G. Somorjai, R. Breaker, S. Buchwald
A. De Wit, D. Lilley, J. Stubbe, R. Marcus, B. Feringa, K. Wüthrich*



*F. Neese, B. List, E. Carreira, J. Klinman, M. Koper, J. Christodoulou, T. Tatsumi
A. Corma, K. Nozaki, C. Jones, M. Rodnina, R. van Santen, S. Boxer, D. York
H-J. Freund, G. Hutchings, J. K. Norskov, X. Bao, B. Weckhuysen, C. Copéret
R. Grubbs, G. Ertl, M. Davis, K. Goldberg, H. Lekkerkerker, G. Fleming*



13th Solvay
Public Event

Chemistry
for the World
of Tomorrow

13th Solvay Public Event

Chemistry for the World of Tomorrow

23 October 2016

On the day following the 24th Solvay Conference on Chemistry, the International Solvay Institutes organized their traditional annual public event, on the theme “**Chemistry for the World of Tomorrow**”.

The theme of the event intended to convey a very strong message. Too often, chemistry is associated with pollution, deterioration of the environment, excessive energy consumption, and catastrophes. This negative image is unfair because it ignores the spectacular improvements brought by chemistry to our standards of living and life expectancy.

It is true that development can have many excesses with negative impact if it is not controlled. But it is by doing more chemistry rather than less chemistry – it is by doing more science rather than less science - that our environmental problems will be solved. Developing green chemistry, finding new materials with better properties, finding new energy-friendly production methods, will pave the way to a sustainable development.

We need chemistry more than ever!

A tradition that goes back to 2005

In 2005, the International Solvay Institutes initiated the tradition of organizing an annual public event during which distinguished scientists deliver lectures on the state-of-the-art in their field of research with an overview of the most pressing current issues. Organized jointly with the ULB, the VUB and the Solvay Group, this event popularizes science and aims at making it more attractive to the younger generations. The talks are given in English but simultaneous interpretations in Dutch and French are provided. The event closes with a drink offered to all the participants, which allows the public to interact more closely with the invited scientists. The event is free.

The potential of chemistry and its future were central themes in the talks delivered by the two lecturers, as well as in the following panel discussion, which also addressed questions raised by the public.

The event attracted more than 800 participants fascinated by the brilliant lectures on “Translation of Academic Science into the Commercial” and “The Art of Building Small”. It is a great satisfaction to see that the Solvay annual public lectures are so well attended. The event closed with a drink offered to all the participants, during which the public could interact more with the speakers and the panel members.

The International Solvay Institutes are extremely grateful to the two lecturers as well as to the panel members who made this event a big success.

Lecturers

Both speakers received the Nobel Prize in Chemistry for their exceptional scientific contributions.

Professor Grubbs is an expert in catalysis and a member of the International Scientific Committee for Chemistry, which is in charge of organizing the famous "Conseils Solvay" on Chemistry. He was awarded the Nobel prize in 2005.



Professor Grubbs

Professor Grubbs is the Victor and Elisabeth Atkins Professor of Chemistry at Caltech's Division of Chemistry and Chemical Engineering. His research focuses on the organometallic chemistry (materials that accelerate chemical reactions and direct the formation of the desired product) that is required for the design and synthesis of catalysts. His work on catalysis in organic chemistry has led to a variety of applications in biomedicine and industry. It has been recognized by a Nobel Prize in 2005.

Professor Ben Feringa

Professor Feringa is the Jacobus van 't Hoff distinguished Professor of molecular sciences at the University of Groningen. As synthetic organic chemist he has specialized in molecular nanotechnology and homogeneous catalysis.

Professor Feringa received the 2016 Nobel Prize in chemistry, together with Sir Fraser Stoddart and Jean-Pierre Sauvage, for the design and synthesis of molecular machines.

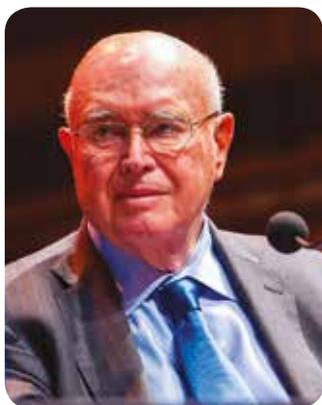
He also obtained the 2015 "Chemistry for the Future Solvay Prize" for his research on molecular motors.



Professor Ben Feringa is an expert on molecular machines and a member of the International Advisory Committee of the International Solvay Institutes. He received the Nobel prize in 2016, less than three weeks before the public event! This was a fantastic news, that filled us with joy!



Panel members



Professor Somorjai

Professor Somorjai is Professor of Chemistry at the University of California in Berkeley and a leading researcher in the field of surface chemistry and catalysis, especially regarding the catalytic effects of metal surfaces. Among numerous awards, Professor Somorjai received the Wolf Prize in Chemistry in 1998, the Priestly Medal in 2008 and the William Nichols Medal Award from the American Chemical Society in 2005.

Professor Wüthrich

Professor Wüthrich was awarded the Nobel Prize in Chemistry in 2002 for the nuclear magnetic resonance techniques which he developed for the study of biological macromolecules. Professor Wüthrich has two laboratories: one at the ETH Zurich and the other at the Scripps Research Institute in La Jolla, California. He is the Chairman of the International Solvay Committee for Chemistry. As a member of the Advisory Board of the USA Science and Engineering Festival, he has always shown great interest in stirring the enthusiasm of young people for exact science.

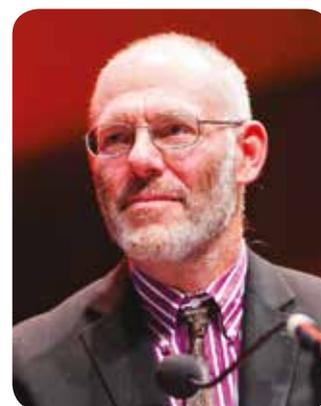


Professor Goldberg

Professor Goldberg is the Nicole Board endowed Professor of Chemistry at the University of Washington. Her research aims at the understanding of fundamental reactions in organometallic chemistry and the creation of catalysts. Professor Goldberg obtained the 2015 Award for Organometallic Chemistry from the American Chemical Society and she has been distinguished in 2006 as an Outstanding Women Scientist by the New York Metropolitan Chapter of the Association for Women in Science.

Professor Herschlag

Professor Herschlag is Professor of Biochemistry at the Stanford University School of Medicine. His research aims at improving our understanding of the fundamental behaviour of RNA and proteins, by means of rigorous kinetic and mechanistic approaches. Among other distinctions and awards, Professor Herschlag obtained the Pfizer Award in Enzyme Chemistry in 1997 and the William Rose Award from the American Society for Biochemistry and Molecular Biology in 2010.



Program

15:00 - 15:05	Opening by Professor Marc Henneaux ULB & International Solvay Institutes
15:05 - 15:30	Solvay Awards Ceremony introduced by Jean-Pierre Clamadieu CEO, Solvay Group and Nicolas Cudré-Mauroux Solvay Research & Innovation Group General Manager
15:30 - 16:15	<i>Translation of Academic Science into the Commercial</i> Professor Robert Grubbs California Institute of Technology, USA
16:20 - 17:05	<i>The Art of Building Small</i> Professor Ben Feringa University of Groningen The Netherlands
17:10 - 17:55	Debate chaired by Prof. Kurt Wüthrich 2002 Chemistry Nobel Laureate Scripps Institute, USA and ETH-Zurich, Switzerland and with the participation of Profs. Ben Feringa University of Groningen, The Netherlands Karen Goldberg University of Washington, USA Robert Grubbs Caltech, USA Daniel Herschlag Stanford, USA Gabor Somorjai UC Berkeley, USA
Moderator	Professor Franklin Lambert VUB & International Solvay Institutes
17:55 - 18:00	Closing
18:00 - 18:30	Drink



Solvay Awards Ceremony



Every year, Solvay presents the Solvay Awards in recognition of high-quality research work carried out by the students of the Science Faculty or Applied Science Faculty/Polytechnic School of the Université libre de Bruxelles or Vrije Universiteit Brussel.

The Solvay Awards are presented to university graduates studying at the Master's degree level (MSc or Master's in Engineering Science) or at the PhD level.

Solvay awards these prizes in order to stimulate the inventiveness and reflection of highly promising young graduates and research scientists regarding the application of their work and research in society at large.

The ceremony was introduced by Jean-Pierre Clamadieu, CEO Solvay Group. Nicolas Cudré-Mauroux, Solvay Research & Innovation Group General Manager, gave the awards to the laureates.



Laureates

Audrey Cuvelier | VUB

Saskia Demulder | VUB

Jean-François Derivaux | ULB

Kevin Garnir | ULB

Mélanie Hercor | ULB

Christophe Labar | ULB

Margaux Leemans | VUB

Alexandre Lutz | VUB

Chloé Martens | ULB

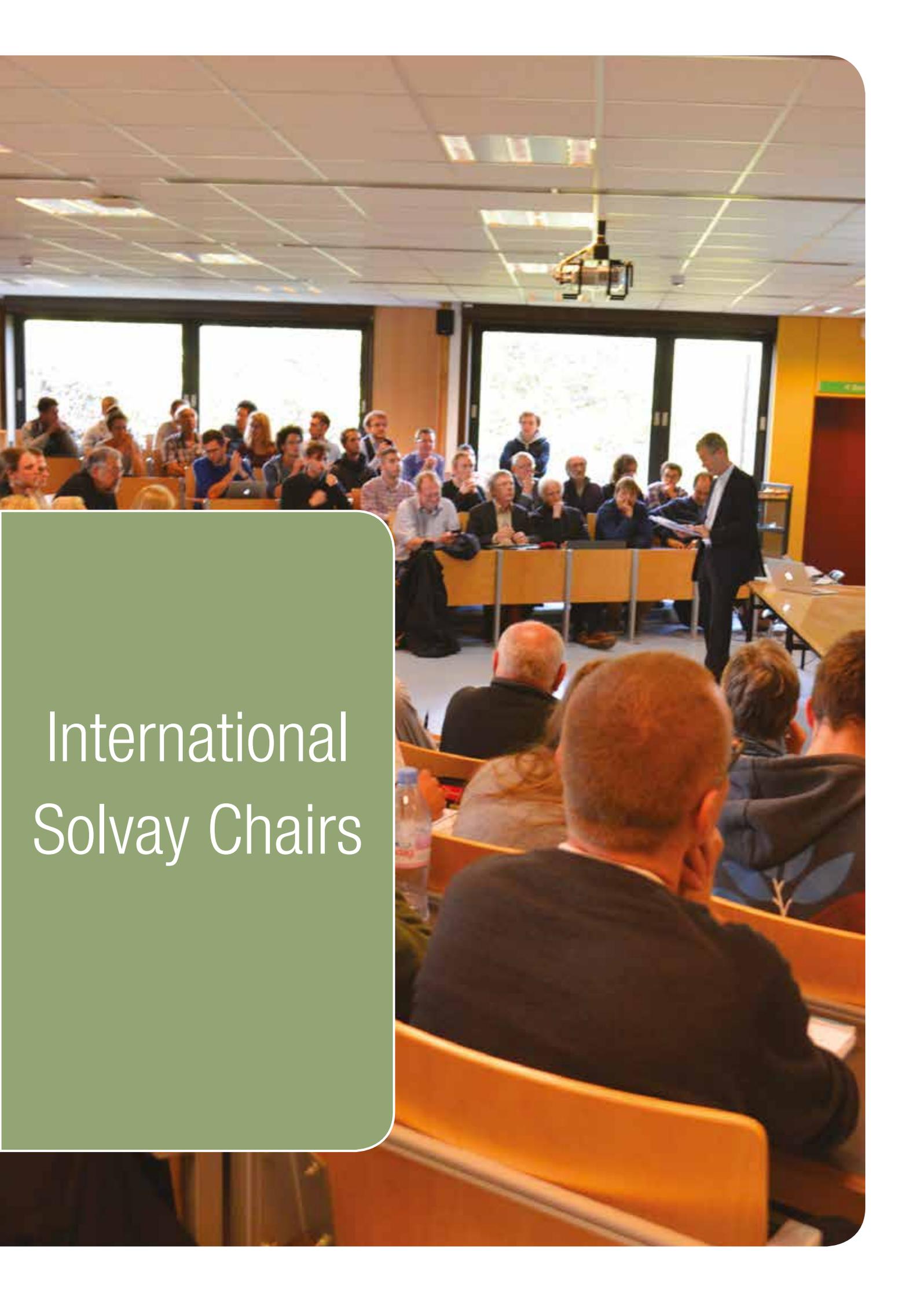
Minh Duc Nguyen | VUB

Edith Oyen | VUB

Nandi Vrancken | VUB

Bert Wouters | VUB





International Solvay Chairs

International Solvay Chairs

The International Solvay Chair programme enables the Institutes to invite in Brussels eminent scientists for a period of one to two months in order to give lectures on their work to researchers in the corresponding fields, not only from the ULB and the VUB, but also from other Belgian universities and abroad.

The programme started in 2006 for physics. In 2011 the physics chair was renamed the International “Jacques Solvay Chair in Physics” in memory of Jacques Solvay, who was president of the Institutes for more than 50 years.

The chair programme in chemistry was launched in 2008 thanks to a generous grant from the Solvay Company, which the Institutes gratefully acknowledge.

2016 International Jacques Solvay Chair in Physics

Professor Dam Thanh Son | University of Chicago, USA

The 2016 International Jacques Solvay Chair in Physics was held by Professor Dam Thanh Son from the Enrico Fermi Institute (University of Chicago, USA).



Professor Dam Thanh Son gave his inaugural lecture on October 4, 2016. He will come back in the Fall of 2017 to deliver his other lectures in the context of the International Doctoral School on theoretical physics organized by the University of Amsterdam, the ULB, the VUB, a consortium of French theoretical groups led by ENS Paris, and a consortium of Swiss theoretical groups led by ETH Zurich.



Professor Dam Thanh Son is a leading figure in theoretical physics, with broad interests covering string theory, nuclear physics, condensed matter physics and atomic physics, areas to which he made central contributions.

In particular, he discovered remarkable connections between fluid viscosity and black hole physics through techniques originating from string theory. These techniques, applicable to strongly interacting systems, enabled him to make breakthroughs in the understanding of the quark-gluon plasma in nuclear physics, where standard perturbation theory breaks down.

His ideas have a wide range of applicability and open many promising lines of developments reaching also to atomic physics and condensed matter physics.

The subject of the inaugural lecture delivered by Professor Dam Thanh Son was devoted to the exciting field of black holes and fluid viscosity.

During his stays in Brussels, Professor Dam Thanh Son was hosted in the group of Professors Jean-Marie Frère and Peter Tinyakov (ULB), to which the International Solvay Institutes are most grateful.

Professor Dam Thanh Son studied physics at Moscow State University, where he got his Master Degree in 1991. He received his PhD in physics in 1995 from INR - the Institute for Nuclear Research - in Moscow.

He subsequently held postdoctoral positions at the University of Washington and at MIT, before getting a faculty appointment at Columbia University. He was also at the same time a fellow at the Brookhaven National Laboratory in Long Island.

In 2002, he became a Senior Fellow at the Institute for Nuclear Theory and a professor in the Physics Department at the University of Washington.

Then, in 2012, he moved to Chicago and became the 19th person to hold a University Professorship at the University of Chicago.

For his remarkable achievements, Professor Dam Thanh Son received many awards. He was an Alfred P. Sloan Research Fellow and received an Outstanding Junior Investigator Award from the US Department of Energy.

In 2013, he received a Simons Investigator Award. He was elected to the American Academy of Arts and Sciences in 2014, and to the National Academy of Sciences the same year.

The research areas covered by Professor Dam Thanh Son are broad. His ideas have played a seminal role in many fields of theoretical physics.



Inaugural Lecture I 4 October 2016

Fluid viscosity: from Maxwell to black holes

There has been tremendous progress in recent years in our understanding of the behavior of matter in extreme conditions - at very high and very low temperatures. Unexpectedly, physicists have found that some techniques originating from string theory are very useful and gives information about the viscosity of strongly interacting liquids that cannot be obtained by other methods. We trace the history of the notion of viscosity from Maxwell to modern days, and elucidate the relationship between the viscosity and the behavior of black hole horizons.

2015 International Jacques Solvay Chair in Physics

Professor Peter Zoller | University of Innsbruck, Austria

The last lecture of the 2015 Solvay Chair in Physics, held by Professor Peter Zoller (University of Innsbruck, Austria) took place on 18 February 2016.

Driven-dissipative quantum many-body systems: a quantum optical perspective

We will start with a brief introduction to quantum noise from the perspective of quantum optics. We then present examples from quantum optics, and cold atomic gases on engineered driven-dissipative manybody quantum systems, where the goal is to produce interesting and novel quantum phases and entangled states in this non-equilibrium setting. We will outline both the underlying theoretical aspects, as well as show recent experimental results with cold atoms and ions.

On the occasion of the second stay of Professor Zoller in Brussels, a workshop was organized on “Quantum Simulation with Cold Matter and Photons” (see corresponding section).

2016 Solvay International Chair in Chemistry

Professor Raymond Kapral | University of Toronto, Canada

The ninth International Chair in Chemistry was held by Professor Raymond Kapral from the University of Toronto (Canada), one of the world leaders working on the theoretical aspects of self-organization, pattern formation, and nonequilibrium systems.

Raymond Kapral has also pioneered research on self-propelled nanoparticles, establishing their theory, and inspiring many recent experiments in the nanosciences, with remarkable potential applications to molecular machines and synthetic motors.

His inaugural lecture, given on the 19th of April 2016, was precisely devoted to this fascinating field.

During his stay in Brussels, Professor Kapral was hosted in the group of “Physics of Complex Systems and Statistical Mechanics” at the ULB. The Institutes thank both Professor Pierre Gaspard and Professor Jean-Pierre Boon for their efficient help in organizing the chair.

In the context of the Solvay Chair of Professor Kapral, a workshop was organized at the Institutes on “Bridging the gaps at the PCB interface - Multiscale modelling in physics chemistry and biology” (see corresponding section).

After a PhD degree in 1967 at the University of Princeton and a postdoctoral stay at MIT, Professor Kapral joined the University of Toronto, where he is Professor at the department of chemistry and one of the group leaders of the Chemical Physics Theory Group.

The research interests of Raymond Kapral cover a wide range of topics at the interface of Chemistry, Physics, Biology, Applied Mathematics and Computer Science. He made exceptional contributions to theoretical chemistry and nonlinear dynamical systems.

For his work, Professor Kapral received many prestigious awards, such as the John Polanyi Award from the Canadian Society for Chemistry in 1996, a Humboldt Award in 2004, the Steacie Award from the Canadian Society for Chemistry in 2011, and many more.

Professor Raymond Kapral is also a good friend of the Belgian scientific community since he came to Brussels in the eighties as a visiting professor. The Institutes were extremely pleased that he came back in the context of the Solvay Chair.



Inaugural Lecture I 19 April 2016

Molecular Machines and Synthetic Motors: Active Motion on the Nanoscale

Molecular machines operate far from equilibrium and are subject to strong thermal fluctuations. They use chemical energy to perform a variety of tasks, acting as motors, enzymes or pumps, and in doing so play important roles in the operation of the cell. Synthetic chemically-powered nanomotors, with and without moving parts, operate under similar conditions and are being studied because of their potential applications involving active transport on small scales and the challenges they pose for theory and simulation. Two examples will be used to illustrate the phenomena that such systems display: synthetic chemically-powered nanomotors and hydrodynamic collective effects arising from active protein machines.

The kinds of synthetic nanomotors that have been constructed and their potential applications will be described, and the mechanisms they use for propulsion and how their dynamics may be simulated will be discussed. Experimental observations have shown that transport in the cell is influenced by protein activity. It will be shown that one mechanism that may contribute to the enhanced transport of passive particles and other enzymes in the cell and in solution is due to the hydrodynamic flows that are generated by the nonequilibrium conformational changes of active enzymes.



Lecture 1 I 11 April 2016

Quantum Dynamics in Complex Systems

Quantum processes, such as electron, proton and coherent energy transfer, often take place in large complex many-body environments. While the dynamics of a subsystem of the entire system is often of primary interest, its interaction with the remainder of the system is responsible for decoherence and other environmental effects. Coupling between the subsystem and environment can lead to the breakdown of the Born-Oppenheimer approximation.

The resulting nonadiabatic dynamics plays an important role in many physical phenomena, such as population relaxation following initial preparation of the system in an excited electronic state. The talk will focus on a mixed quantumclassical description of nonadiabatic dynamics and discuss how coherence and decoherence are accounted for in this framework, and how it can be used to simulate the quantum dynamics of chemical rate processes.

Lecture 2 | 25 April 2016

Chemically-Powered Nanomotors

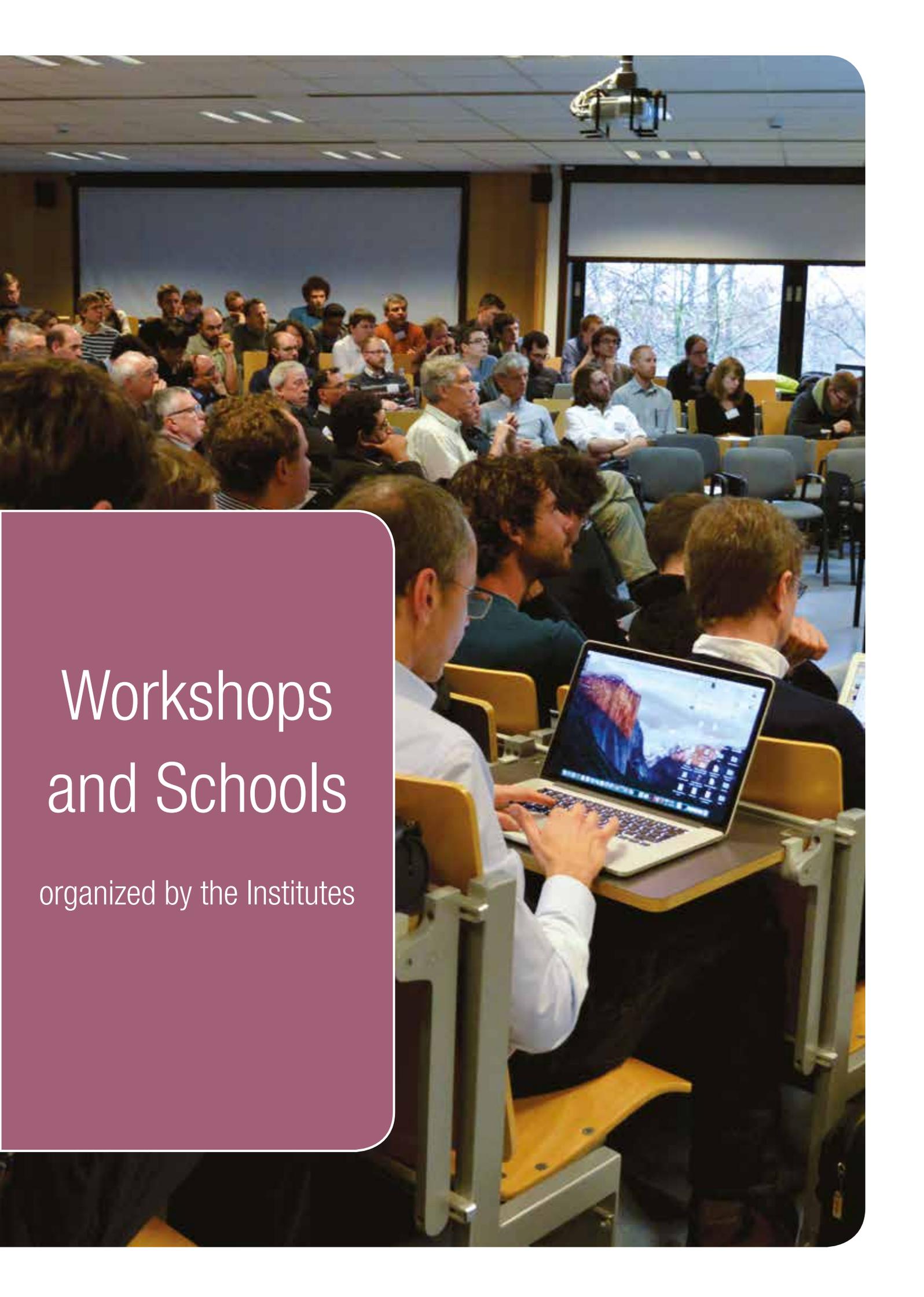
Synthetic chemically-powered motors that do not make use of conformational changes for their propulsion will be described. They operate under far-from-equilibrium conditions and are subject to strong fluctuations from the environment in which they move. In particular, motors that operate by diffusiophoresis, where a self-induced chemical gradient is responsible for motion, will form the focus of the discussion. The propulsion mechanism based on the continuum reaction-diffusion and hydrodynamic equations will be given, as well as a mesoscopic model for motor motion. The properties of these motors will be described. The manner in which different chemical reactions on the catalytic sites of the motor and in its environment influence motor propulsion properties will be considered. In collections of such motors, the individual motors interact through forces that arise from concentration gradients, hydrodynamic coupling and direct intermolecular forces. Motors self-assemble into transient aggregates with distinctive structural correlations and exhibit swarming where the aggregates propagate through the system. These phenomena will be illustrated by simulations of the dynamics of many-motor systems.



Lecture 3 | 27 April 2016

Protein Dynamics and Hydrodynamics

The dynamics of proteins in solution and in crowded molecular environments, which mimic some features of the interior of a biochemical cell, will be discussed. The translational and internal dynamics and catalytic activity of enzymes that utilize chemical energy to effect cyclic conformational changes to carry out their catalytic functions will be described. Proteins often function when bound to lipid membranes and the nature of the mutual interactions between the lipid membrane and active protein will be discussed. The emphasis in these studies is on the role that hydrodynamics plays in determining the protein dynamics. The investigation of the dynamics of such complex systems requires knowledge of the time evolution on physically relevant long distance and time scales, necessitating a coarse grained or mesoscopic treatment of the dynamics.



Workshops and Schools

organized by the Institutes

Workshop on “Quantum Simulation with Cold Matter and Photons”

8 - 11 February 2016



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INSTITUTES
BRUSSELS

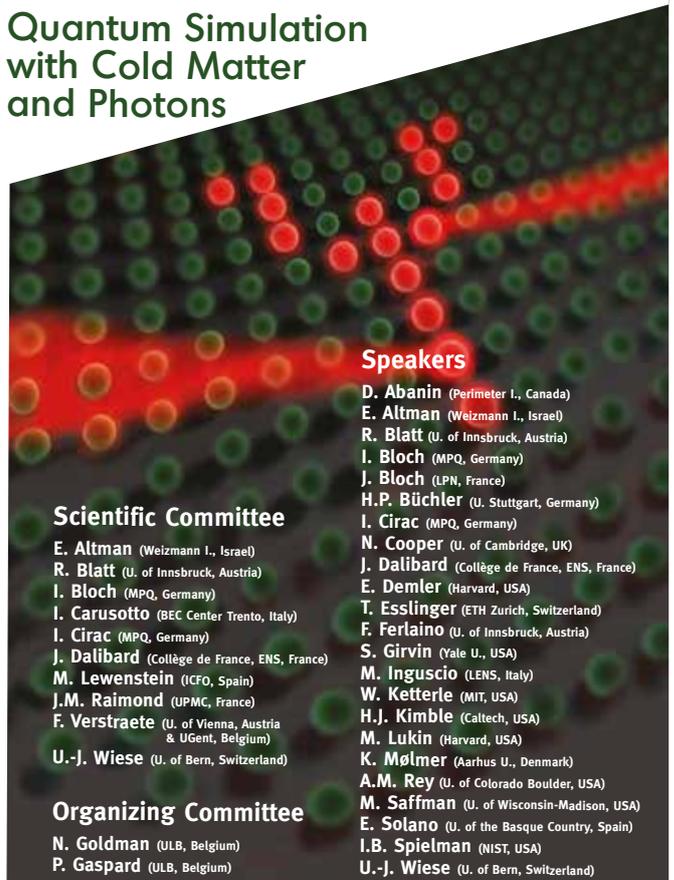
Brussels, 8 - 11 February 2016

ULB - Campus Plaine - Solvay Room

www.solvayinstitutes.be

Workshop on

Quantum Simulation with Cold Matter and Photons



Speakers

D. Abanin (Perimeter I., Canada)
E. Altman (Weizmann I., Israel)
R. Blatt (U. of Innsbruck, Austria)
I. Bloch (MPQ, Germany)
J. Bloch (LPN, France)
H.P. Büchler (U. Stuttgart, Germany)
I. Cirac (MPQ, Germany)
N. Cooper (U. of Cambridge, UK)
J. Dalibard (Collège de France, ENS, France)
E. Demler (Harvard, USA)
T. Esslinger (ETH Zurich, Switzerland)
F. Feriaino (U. of Innsbruck, Austria)
S. Girvin (Yale U., USA)
M. Inguscio (LENS, Italy)
W. Ketterle (MIT, USA)
H.J. Kimble (Caltech, USA)
M. Lukin (Harvard, USA)
K. Mølmer (Aarhus U., Denmark)
A.M. Rey (U. of Colorado Boulder, USA)
M. Saffman (U. of Wisconsin-Madison, USA)
E. Solano (U. of the Basque Country, Spain)
I.B. Spielman (NIST, USA)
U.-J. Wiese (U. of Bern, Switzerland)

Scientific Committee

E. Altman (Weizmann I., Israel)
R. Blatt (U. of Innsbruck, Austria)
I. Bloch (MPQ, Germany)
I. Carusotto (BEC Center Trento, Italy)
I. Cirac (MPQ, Germany)
J. Dalibard (Collège de France, ENS, France)
M. Lewenstein (ICFO, Spain)
J.M. Raimond (UPMC, France)
F. Verstraete (U. of Vienna, Austria & UGent, Belgium)
U.-J. Wiese (U. of Bern, Switzerland)

Organizing Committee

N. Goldman (ULB, Belgium)
P. Gaspard (ULB, Belgium)

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“Quantum Simulation with Cold Matter and Photons”

8 - 11 February 2016

The Workshop on “Quantum Simulation with Cold Matter and Photons” was organized in the context of the 2015 International Jacques Solvay Chair in Physics attributed to Professor Peter Zoller.



Quantum simulation denotes the approach by which controllable many-body quantum systems are designed and analysed in view of revealing complex and intriguing quantum phenomena. This fast growing field of research gathers a huge community of scientists specialized in various branches of quantum physics, including condensed-matter physics, atomic and molecular physics, quantum optics, quantum information and high-energy physics.

The Workshop has assembled a unique group of leading experts, who significantly contributed to the development of quantum simulation in the recent years.

The subjects discussed at the Workshop included:

- Cold atoms in optical lattices, Rydberg atoms and cold molecules
- Physics of trapped ions
- Hybrid quantum systems
- Quantum fluids of light: Photonic crystals, polaritons, and cavity quantum electrodynamics
- Superconducting circuits
- Quantum Hall physics, topological states of matter and strongly-correlated systems
- Quantum many-body dynamics, non-equilibrium dynamics, many-body localization
- Quantum simulation of lattice gauge theories

Organizing Committee

Nathan Goldman | ULB, Belgium
Pierre Gaspard | ULB, Belgium

Scientific Committee

Ehud Altman | Weizmann I., Israel
Rainer Blatt | U. of Innsbruck, Austria
Immanuel Bloch | MPQ, Garching, Germany
Iacopo Carusotto | U. of Trento, Italy
Ignacio Cirac | MPQ, Garching, Germany
Jean Dalibard | Collège de France, ENS, France
Maciej Lewenstein | ICFO, Spain
Jean-Michel Raimond | UPMC, France
Frank Verstraete | U. of Vienna, Austria
Uwe-Jens Wiese | U. of Bern, Switzerland

Speakers

Dmitry Abanin Perimeter Institute, Canada	Wolfgang Ketterle MIT, USA
Ehud Altman Weizmann I., Israel	H. Jeff Kimble Caltech, USA
Rainer Blatt U. of Innsbruck, Austria	Mikhail Lukin Harvard, USA
Jérôme Beugnon Collège de France, France	Klaus Molmer Aarhus U., Denmark
Immanuel Bloch MPQ Garching, Germany	Mikael Rechtsman Pennsylvania State U., USA
Jacqueline Bloch LPN, CNRS, France	Ana Maria Rey U. of Colorado Boulder, USA
Hans Peter Büchler U. Stuttgart, Germany	Mark Saffman U. of Wisconsin-Madison, USA
Ignacio Cirac MPQ Garching, Germany	Moti Segev Technion, Israel
Nigel Cooper U. of Cambridge, UK	Enrique Solano U. of the Basque Country, Spain
Jean Dalibard Collège de France, France	Ian B. Spielman NIST, USA
Eugene Demler Harvard, USA	Uwe-Jens Wiese U. of Bern, Switzerland
Tilman Esslinger ETH Zurich, Switzerland	
Francesca Ferlino U. of Innsbruck, Austria	
Steven Girvin Yale U., USA	
Mohammad Hafezi U. of Maryland, USA	
Massimo Inguscio LENS, Firenze, Italy	



Program

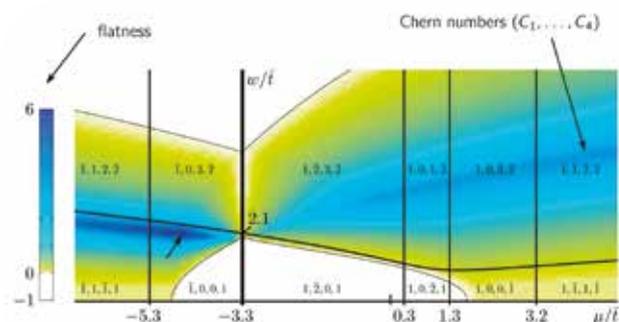
Monday 8 February 2016

Opening by Marc Henneaux and Peter Zoller

- | | |
|--------------------|--|
| Rainer Blatt | <i>Quantum simulations with cold trapped ions</i> |
| Ignacio Cirac | <i>Quantum simulation and quantum optics in photonic crystals</i> |
| Hans Peter Büchler | <i>Topological states of matter with cold atomic gases and Rydberg atoms</i> |
| Mikhail Lukin | <i>Quantum dynamics of strongly interacting photons and atoms</i> |
| Klaus Mølmer | <i>The good, the better, and the theoretically best precision measurements with matter and light</i> |
| H. Jeff Kimble | <i>Quantum matter built from strong atom-photon interactions in nanoscopic lattices</i> |

Tuesday 9 February 2016

- | | |
|--------------------|---|
| Ehud Altman | <i>Many-body localization: new insights from theory and experiments with cold atoms</i> |
| Dmitry Abanin | <i>Many-body localization and prethermalization in periodically driven systems</i> |
| Enrique Solano | <i>Digital quantum computers versus analog quantum simulators</i> |
| Steven Girvin | <i>Quantum bath engineering for circuit QED systems</i> |
| Francesca Ferlaino | <i>The fascination of Lanthanides for ultracold quantum physics</i> |
| Tilman Esslinger | <i>Quantum problem generators</i> |
| Nigel Cooper | <i>Quantum quenches in Chern insulators</i> |



Wednesday 10 February 2016

- Massimo Inguscio *Observing ultracold symmetries*
- Ana Maria Rey *New perspectives on quantum simulation with alkaline earth atoms*
- Immanuel Bloch *From many-body localization to Rydberg gases - new frontiers for ultracold atoms*
- Ian B. Spielman *Gauge fields in multi-level atoms: a tutorial*
- Mohammad Hafezi *New prospects in topological photonics*
- Jérôme Beugnon *Direct measurement of Chern numbers in the diffraction pattern of a Fibonacci chain*
- Jacqueline Bloch *Toward quantum simulation with cavity polaritons*
- Moti Segev / Mikael Rechtsman *Aspects of photonic topological insulators*



Thursday 11 February 2016

- Mark Saffman *Quantum bits with Rydberg atoms: results, challenges, and new ideas*
- Wolfgang Ketterle *Quantum simulations with laser-assisted tunneling*
- Eugene Demler *Interferometric probes of many-body systems: from ultracold atoms to quantum materials*
- Uwe-Jens Wiese *Atomic quantum simulation of Abelian and non-Abelian gauge theories*

Concluding remarks by Peter Zoller and colleagues

Workshop on “Conceptual Quantum Chemistry: Present Aspects and Challenges for the Future”

4 - 8 April 2016



INTERNATIONAL
SOLVAY
INSTITUTES
BRUSSELS

Solvay Workshop on

Conceptual Quantum Chemistry Present Aspects and Challenges for the Future

with a special session celebrating the contributions of Paul Geerlings

www.solvayinstitutes.be

ULB, Campus Plaine, Solvay Room
Brussels, Belgium, April 4-8, 2016

Invited Speakers

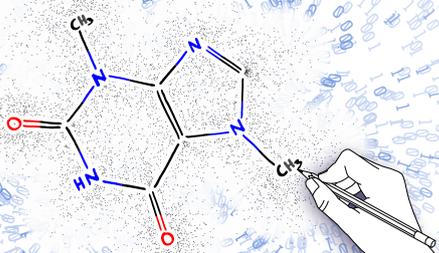
Paul W. Ayers
McMaster U., Hamilton, Canada
F. Matthias Bickelhaupt
VU, Amsterdam, The Netherlands
Alexander I. Boldyrev
Utah State U., Logan, USA
Pratim K. Chattaraj
IIT, Kharagpur, India
Carlos Cárdenas
U. de Chile, Santiago, Chile
Julia Contreras-García
UPMC/CNRS, Paris, France
Clémence Corminboeuf
EPFL, Lausanne, Switzerland
Gernot Frenking
Philipps-U. Marburg, Germany
Patricio Fuentealba
U. de Chile, Santiago, Chile
José Luis Gázquez
UAM-Iztapalapa, Mexico City, Mexico
Martin Head-Gordon
UC Berkeley, Berkeley CA, USA
Erin R. Johnson
Dalhousie U., Halifax, Canada
Eduard Matito
UPV/EHU, Donostia, Spain
Ángel Martín Pendás
U. de Oviedo, Oviedo, Spain
Paul Popelier
U. of Manchester, Manchester, UK
Andreas Savin
UPMC/CNRS, Paris, France
W.H. Eugen Schwarz
NTHU, Beijing, China and
U. Siegen, Siegen, Germany
Miquel Solà
UdG, Girona, Spain
Alejandro Toro-Labbé
PDC, Santiago, Chile
Israel Fernández
UCM, Madrid, Spain
Judy I. Wu
U. of Houston, Houston, USA

Scientific Committee

Paul W. Ayers
McMaster U., Hamilton, Canada
F. Matthias Bickelhaupt
VU, Amsterdam, The Netherlands
Pratim K. Chattaraj
IIT, Kharagpur, India
Clémence Corminboeuf
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Patricio Fuentealba
U. de Chile, Santiago, Chile
Andreas Savin
UPMC/CNRS, Paris, France
Miquel Solà
UdG, Girona, Spain

Organizing Committee

Frank De Proft VUB
Mercedes Alonso VUB
Patrick Bultinck UGent
Freija De Vleeschouwer VUB
Stijn Fias VUB
Michel Godefroid ULB
Jacky Liévin ULB
Balazs Pinter VUB
Nathalie Vaeck ULB
Sofie Van Damme UGent
Toon Verstraelen UGent



“Conceptual Quantum Chemistry: Present Aspects and Challenges for the Future”

4 - 8 April 2016

Quantum chemistry applies quantum mechanics to problems in chemistry. In the last 30 years, various accurate and powerful electronic structure methods have been developed and implemented allowing quantum chemists to compute various molecular properties to very high accuracy. Also, potential energy surfaces can now be studied highly accurately, including the critical points on these surfaces (minima and transition states). Electronic structure and potential energy surfaces lie at the very heart of chemistry and so it would seem that all of chemistry can be computed. However, chemistry as the science of rationalization and classification has always employed a set of very powerful “concepts”. These have shaped much of chemistry and have found wide use not only to rationalize a posteriori but also to predict, e.g. in synthesis. From the early days of quantum chemistry, much attention has been devoted to the computation of these (often non-observable) chemical concepts. Although many of these concepts are still widely used, with the above-mentioned increasing accuracy of methods available and their ever-increasing possibility to treat larger molecular systems, it is important to raise the question whether a conceptual approach is still desirable.

It remains important to keep on reflecting on the question of the usefulness of a conceptual approach, especially since “old” concepts get more and more often also applied to new classes of molecules and compounds. In this context, concepts are not fading away with the increased sophistication of our calculations but rather get extended to new areas.

The Solvay workshop “Conceptual Quantum Chemistry: Present Aspects and Challenges for the Future” aimed at celebrating the achievements made in the field of conceptual quantum chemistry field and at critically and thoroughly discussing the challenges ahead, among others the discussion whether chemical concepts from quantum mechanics still need to have an important place in contemporary quantum chemistry.

During the workshop, a special half-day session on the topic of “conceptual DFT” in honor of Paul Geerlings, on the occasion of his retirement in October 2015, was organized.

Organizing Committee

Paul Ayers | McMaster U., Canada
Matthias Bickelhaupt | VU Amsterdam, The Netherlands
Pratim Kumar Chattaraj | IIT Kharagpur, India
Clémence Corminboeuf | EPFL, Switzerland
Gernot Frenking | Philipps-U. Marburg, Germany
Patricio Fuentealba | U. de Chile, Chile
Andreas Savin | CNRS & Sorbonne, France
Miquel Solà | U. de Girona, Spain

Scientific Committee

Mercedes Alonso VUB, Belgium	Jacques Lievin ULB, Belgium
Patrick Bultinck UGent, Belgium	Balazs Pinter VUB, Belgium
Frank De Proft VUB, Belgium	Nathalie Vaeck ULB, Belgium
Freija De Vleeschouwer VUB, Belgium	Sofie Van Damme UGent, Belgium
Stijn Fias VUB, Belgium	Toon Verstraelen UGent, Belgium
Michel Godefroid ULB, Belgium	

Speakers

Paul Ayers McMaster U., Canada	Patricio Fuentealba U. de Chile, Chile
Matthias Bickelhaupt VU Amsterdam, The Netherlands	José Luis Gázquez UAM, Iztapalapa, Mexico
Alexander Boldyrev Utah State U., USA	Martin Head-Gordon U. of California, USA
Carlos Cardenas U. de Chile, Chile	Eduard Matito UPV - EHU, Spain
David Cooper Liverpool U., UK	Ángel Martin Pendás U. de Oviedo, Spain
Pratim Kumar Chattaraj IIT Kharagpur, India	Andreas Savin CNRS and Sorbonne, France
Julia Contreras-García UPMC, France	Eugen Schwarz U. Siegen, Germany
Clémence Corminboeuf EPFL, Switzerland	Miquel Solà U. de Girona, Spain
Israel Fernández U. Complutense de Madrid, Spain	Alejandro Toro-Labbé Pontificia U. Católica de Chile, Chile
Gernot Frenking Philipps-U. Marburg, Germany	Judy Wu U. of Houston, USA

Program

The program consisted of a series of invited lectures (35 mins of lecture plus 10 mins of discussion). Also, a total of 10 contributed talks (20 mins of lectures and 5 mins of discussion) were scheduled.

Monday 4 April 2016

Welcome reception

Tuesday 5 April 2016

Opening session - Frank De Proft and Lode Wyns

Chair: Paul Geerlings

Gernot Frenking *Molecules With Unusual Bonding Situations –
A Challenge for Chemical Bonding Models*

Alexander Boldyrev *Multicenter Bonding in Chemistry*

Chair: Toon Verstraelen

Matthias Bickelhaupt *Theory of chemical bonding and reactivity
Quantitative orbital and activation strain
models*

Israel Fernández *A different approach to understand
and control reactivity*

Ángel Martín Pendás *Some insights into the nature of ground
and excited states from real space
descriptors*

Contributed talk

R. Ramakrishnan *Towards reliable electron dynamics
across molecular wires and
nanostructures*

Chair: Jeremy Harvey

Andreas Savin *Is conceptual chemistry ready to work
on open systems?*

David Cooper *Visual Descriptions of Electronic Structure
from Modern Valence Bond Theory:
O₃ and SO₂*

Wednesday 6 April 2016

Developments in Conceptual Density Functional Theory:
Session in honour of Paul Geerlings

Chair: Kris Van Alsenoy

- Carlos Cardenas *Chemical response functions in degenerate states and extended systems*
- Alejandro Toro-Labbé *Four concepts to characterize the mechanisms of chemical reactions*
- Patricio Fuentealba *On the concepts of electron donor and electron acceptor systems*

Chair: Anatole von Lilienfeld

- Paul Ayers *Learning new, and old, chemical concepts from data*
- José Luis Gázquez *Temperature in density functional theory of chemical reactivity*

Chair: Henri Chermette

Contributed talk

- Thijs Stuyver *Qualitative insights into molecular transmission: a curly arrow approach*

Contributed talk

- Christophe Morell *Towards the first theoretical scale of the trans effect in octahedral complexes*

Contributed talk

- Andrés Cedillo *Group and fragment electronegativities from constrained SCF methods*

Poster session



Thursday 7 April 2016

Chair: Minh Tho Nguyen

Miquel Solà *Connecting hydrocarbon and boronhydride chemistries and bidimensional and three-dimensional aromaticities*

Martin Head-Gordon *Some advances in energy decomposition analysis of electronic structure calculations*

Chair: Christophe Morell

Clémence Corminboeuf *On the many facets of analyzing (non)-covalent interactions*

Julia Contreras-García *Non covalent interactions: achievements and unsolved challenges of topology*

Chair: Laurent Joubert

Contributed talk

Roberto Boto *On the topology of the reduced density gradient*

Contributed talk

Vincent Tognetti *Electron density and reactivity: A synergetic DFT-CDFT-QTAIM approach*

Contributed talk

Marco Antonio Franco *Beyond the three state ensemble model, Chemical Reactivity Theory for the general case*

Contributed talk

Steven Vandenbrande *Constructing complete non-covalent force fields based on *ab initio* monomer densities*

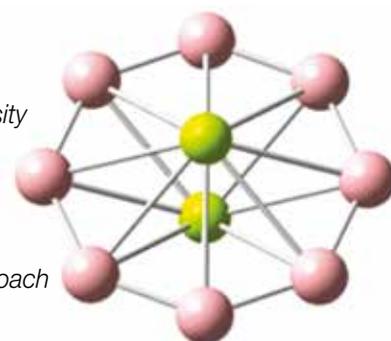
Contributed talk

Jacek Korchowiec *Application of charge sensitivity analysis to improve the accuracy of the fragmentation based methods of electronic structure calculations*

Chair: Brian Sutcliffe

Arnout Ceulemans *The Symmetry of the Periodic System*

Eugen Schwarz *The Hidden Physics behind the Periodic Table of Chemical Elements and New Aspects of Valence, Oxidation, Charge and Correlation Numbers*



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Friday 8 April 2016

Chair: Nathalie Vaeck

Judy Wu *Hydrogen Bond – π -Conjugation Coupling in Enzyme Catalysis: Turning Weak Acids into Strong Proton Donors*

Contributed talk

Mario Van Raemdonck *Constrained CI calculations to investigate charge transfer and the effects of the integer nature of the electron*

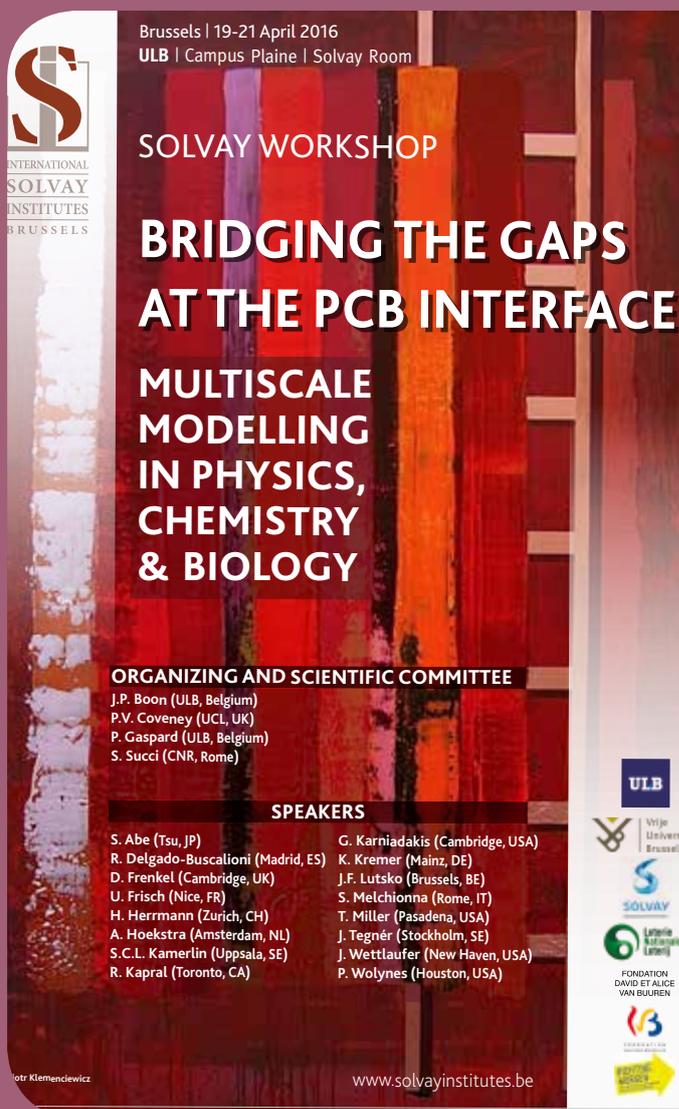
Eduard Matito *Characterization and identification of molecular electrides*

Closing remarks by Patrick Bultinck



Workshop on “Bridging the gaps at the PCB interface”

19 - 21 April 2016



Brussels | 19-21 April 2016
ULB | Campus Plaine | Solvay Room

SOLVAY WORKSHOP

BRIDGING THE GAPS AT THE PCB INTERFACE

MULTISCALE MODELLING IN PHYSICS, CHEMISTRY & BIOLOGY

ORGANIZING AND SCIENTIFIC COMMITTEE

J.P. Boon (ULB, Belgium)
P.V. Coveney (UCL, UK)
P. Gaspard (ULB, Belgium)
S. Succi (CNR, Rome)

SPEAKERS

S. Abe (Tsu, JP)	G. Karniadakis (Cambridge, USA)
R. Delgado-Buscalioni (Madrid, ES)	K. Kremer (Mainz, DE)
D. Frenkel (Cambridge, UK)	J.F. Lutsko (Brussels, BE)
U. Frisch (Nice, FR)	S. Melchionna (Rome, IT)
H. Herrmann (Zurich, CH)	T. Miller (Pasadena, USA)
A. Hoekstra (Amsterdam, NL)	J. Tegnér (Stockholm, SE)
S.C.L. Kamerlin (Uppsala, SE)	J. Wettlaufer (New Haven, USA)
R. Kapral (Toronto, CA)	P. Wolynes (Houston, USA)

photo: Klemenciewicz

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3
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SCIENTIFIQUES

“Bridging the gaps at the PCB interface”

Multiscale Modelling in Physics, Chemistry and Biology

19 - 21 April 2016

It is commonly agreed that the most challenging problems in modern science and engineering involve the concurrent and non-linear interaction of multiple phenomena, acting on a broad and disparate spectrum of scales in space and time. It is also understood that such phenomena lie at the interface between different disciplines, such as physics, chemistry, material science and biology. The multiscale and multi-level nature of these problems commands a paradigm shift in the way they need to be handled, both conceptually and in terms of the corresponding problem-solving computational tools.

The triple interface between biology, chemistry and physics provides a most fertile ground for these kind of phenomena; the design of environmental friendly catalytic devices or smart-drug delivery devices for nanomedicine purposes, being just two examples in point, where atomic-scale details organize coherently across the hierarchy of scales, all the way up to the macroscopic level which dictates the functional operation of the actual device.

The above phenomena take place far from equilibrium, where the organizing power of non-linearity is fully exposed and universality must be (partially) compromised with the necessary degree of microscopic (molecular) individualism. Indeed, the ability to sensibly integrate universality and molecular individualism is possibly the most challenging frontier of modern multi-modelling science. Computer technology, a key enabling technology for the quantitative modeling of such complex phenomena

across scales, has experienced an extraordinary and relentless growth in both computational speed and memory, along with dramatic cost reductions. At the same time, the last decades have also witnessed tremendous progress in modelling methodologies at all levels of scales, e.g. ab initio MD and QM/MM techniques for atomic and nano-scales, Lattice Boltzmann and Dissipative Particle Dynamics for mesoscales and various gridbased methods for macroscales, culminating with the 2013 Chemistry Nobel Prize for “multiscale modelling of complex chemical system”.

The Solvay Symposium centered about the rising multi-modelling paradigm, with special focus on emergent phenomena flourishing at the PCB interface, and should not only help to gain focus on the present state of the art in the field, but, most importantly, also to foster and shape up new cooperative research efforts to advance this exciting forefront of modern science.

There will be an accompanying publication under the same title as a Theme Issue of Proceedings of the Royal Society of London (Series A).



Organizing and Scientific Committee

J.P. Boon | ULB, Belgium
P.V. Coveney | UCL, UK
P. Gaspard | ULB, Belgium
S. Succi | CNR, Rome

Speakers

S. Abe | Tsu, JP
R. Benzi | Rome, IT
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D. Frenkel | Cambridge, UK
H. Herrmann | Zurich, CH
A. Hoekstra | Amsterdam, NL
S.C.L. Kamerlin | Uppsala, SE
R. Kapral | Toronto, CA
K. Kremer | Mainz, DE
J.F. Lutsko | Brussels, BE
S. Melchionna | Rome, IT
T. Miller | Pasadena, USA
J. Tegnér | Stockholm, SE
P. Wolynes | Houston, USA



Program

Tuesday 19 April 2016

Welcome by Marc Henneaux (Director of the Solvay Institutes)
and introduction by Jean-Pierre Boon (Université Libre de Bruxelles).

Chair: Jean-Pierre Boon

Sauro Succi *Mesoscale modeling of complex moving matter across scales*

Sumiyoshi Abe *Anomalous diffusion in volcanic seismicity*

Contributed talk

Ilya Karlin *Mechanisms of droplet bouncing from micro-textured surfaces*
ETH Zurich

Rafael Delgado-Buscalioni *Combined strategies to climb up the scales in complex liquids simulations*

Daan Frenkel *Multi-scale modelling of self assembly*

Chair: Pierre Gaspard

Hans Herrmann *Packing of wires in cavities and growing surfaces*

Alfons Hoekstra *Multiscale Modelling in Vascular Disease*

Contributed talk

Riccardo Rao *Nonequilibrium Thermodynamics of
U. of Luxembourg Chemical Reaction Networks*

Inaugural Lecture Solvay Chair in Chemistry

Raymond Kapral *Molecular Machines and Synthetic
Motors: Active Motion on the Nanoscale*

Wednesday 20 April 2016

Chair: Raymond Kapral

Roberto Benzi *Statistical properties of Soft Glasses
at the yield stress transition*

Kurt Kremer *Multiscale Simulations for Soft Matter:
Applications and New Developments*

Contributed talk

S. Kashif Sadiq *Towards multiscale spatiotemporal
Heidelberg Institute modeling of retroviral self-assembly*

Discussion

Peter Coveney *Big Data Need Big Theory Too*

Chair: Peter Coveney

James Lutsko *Bridging length scales in the theory of nucleation*

Simone Melchionna *Macromolecules and hydrodynamics: a simulation approach*

Contributed talk

Marco Lauricella *A Computational Study of Hydrate Methane Nucleation by Metadynamics*
CNR

Contributed talk

Josip Lovric *Molecular level study of Palmitic acid substrate on NaCl(100): physical phenomena of atmospheric interest*
University Lille

Contributed talk

Pierre de Buyl *Self-propulsion through symmetry breaking*
KU Leuven

Contributed talk

Agastya Prakash Bhati *Computing ligand-protein free energies using multiscale methods*
U. College London

Poster Session and Conference Dinner



Thursday 21 April 2016

Chair: James Lutsko

Thomas Miller *Computationally guided design of next-generation polymer electrolytes*

Jesper Tegnér *On Bridging the Gap between Data and System Dynamics: Multi-omics Integrative Analysis of State-transitions in Cells and Data-driven formulation of System Equations*

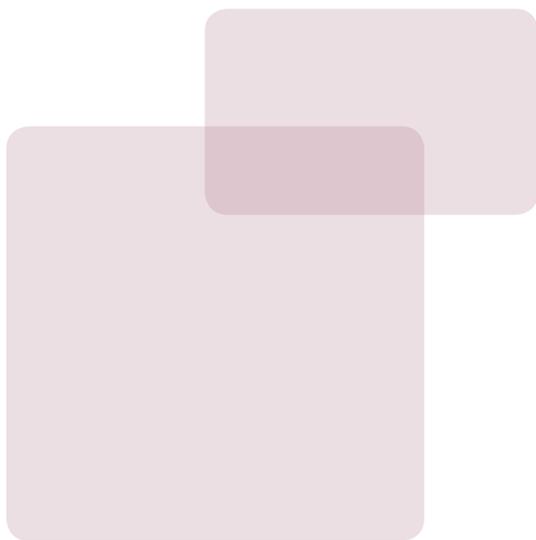
Contributed talk

Alya Arabi *Electric-Field Effects on the Double-Proton Transfer. Reaction in Formic Acid Dimer*
Zayed University

Contributed talk

Nikolay Brilliantov *Generation of mechanical force by grafted polyelectrolytes in an electric field: Application to polyelectrolyte-based nano-devices.*
University of Leicester

Peter Wolynes *From Folding Proteins to Folding Chromosomes*



Chair: Sauro Succi

Contributed talk

Fabrizio Pucci
Université Libre
de Bruxelles

*More insight into protein thermal stability:
from the molecular level to the analysis at
the structuromic scale*

Contributed talk

Gianluca Di Staso
University of
Eindhoven

*Hybrid MonteCarlo and lattice Boltzmann
equation model for rarefied and non-
rarefied gas flows*

Contributed talk

Robin Richardson
University College
London

*Multiscale Modelling of Cerebral Blood
Flow with lattice-Boltzmann for Clinical
Decision-making*

Pierre Gaspard

*Kinetics and thermodynamics of living
copolymerization processes*

Closing Remarks by Sauro Succi



Workshop on “Nonequilibrium and Nonlinear Phenomena in Statistical Mechanics”

11 - 13 July 2016

11-13 July 2016 | ULB - Campus Plaine - Solvay Room

Solvay Workshop on

“Nonequilibrium & nonlinear phenomena in statistical mechanics”

SPEAKERS

- Vijay Balasubramanian (U. of Pennsylvania, USA)
- Felipe Barra (U. de Chile, Santiago, Chile)
- Bernard Derrida (ENS, Paris, France)
- Jean-Pierre Eckmann (Geneva U., Switzerland)
- Massimiliano Esposito (U. du Luxembourg, Luxembourg)
- Giovanni Gallavotti (Sapienza U., Rome, Italy)
- Theo Geisel (MPI for Dynamics and Self-Organization, Göttingen, Germany)
- Rosemary Harris (Queen Mary University of London, UK)
- Mehran Kardar (Massachusetts Inst. of Technology, USA)
- Jürgen Kurths (Potsdam U., Germany)
- David Lacoste (ESPCI, Paris, France)
- Valerio Lucarini (U. of Hamburg, Hamburg, Germany)
- Eric Lutzu (U. of Erlangen-Nürnberg, Germany)
- Anna Maciolek (Max Planck Institute, Stuttgart, Germany)
- Antonio Politi (U. of Aberdeen, UK)
- Itamar Procaccia (Weizmann Inst. of Science, Rehovot, Israel)
- Linda Reichl (U. of Texas, Austin, USA)
- Peter Reimann (U. Bielefeld, Bielefeld, Germany)
- Miguel Rubi (U. de Barcelona, Barcelona, Spain)
- Maxi San Miguel (U. de les Illes Balears, Spain)
- Tanja Schilling (U. du Luxembourg, Luxembourg)
- Lutz Schimansky-Geier (Humboldt-U. zu Berlin, Germany)
- Friederike Schmid (JGU, Mainz, Germany)
- Udo Seifert (U. Stuttgart, Germany)
- Herbert Spohn (Technische U. München, Germany)
- Tyvi Tlusty (IAS, Princeton, USA)
- Raul Toral (U. de les Illes Balears, Spain)
- Carolynne M. Van Vliet (U. of Miami, USA)
- David H. Wolpert (Santa Fe Institute, USA)
- Annette Zippelius (Georg-August-U. Göttingen, Germany)

Scientific & Organising Committee

- Jan Danckaert (VUB, Belgium)
- Pierre Gaspard (ULB, Belgium)
- Josephindekeu (KU Leuven, Belgium)
- Christian Van den Broeck (UHasselt, Belgium)

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ULB Vrije Universiteit Brussel

6 Letelier Laboratory

FONDATION DAVID ET ALICE VAN BUUREN

INSTITUT SOLVAY

SOLVAY

“Nonequilibrium and Nonlinear Phenomena in Statistical Mechanics”

11 - 13 July 2016

Scientific & Organizing Committee

Jan Danckaert | VUB, Belgium

Pierre Gaspard | ULB, Belgium

Joseph Indekeu | KU Leuven, Belgium

Christian Van den Broeck | UHasselt, Belgium

This workshop has been devoted to the statistical physics of nonequilibrium and nonlinear phenomena, including stochastic thermodynamics, fluctuation theorems, as well as applications of statistical mechanics to interfaces, nonlinear dynamics, and complex systems. Statistical mechanics is the theory providing the scientific concepts and mathematical methods to bridge the scales separating the microscopic and macroscopic worlds. At the forefront of this field, nonequilibrium and nonlinear phenomena are the focus of an intense research activity that the Solvay workshop has highlighted. During the three days of the workshop, the thirty talks have brought out the unifying role of fluctuations and heterogeneity in systems as diverse as the nuclear spin of a carbon-13 atom in the chloroform molecule to detect the arrow of time, isolated quantum gases, open quantum spin chains, heat conducting chains, driven optical lattices, out-of-equilibrium radiation, waves in random media, arrays of superfluid cells, nonequilibrium diffusive media, active ion channels, amorphous materials, matter with broken symmetry, growing interfaces, stochastic systems with memory, self-assembling polymers and nanoparticles, granular matter, chemotactic walkers, self-propelled particles, computing machines, chemical reaction networks, the evolving protein universe, the immune system, the climate, or socio-economic networks.

The workshop has gathered about seventy participants from seventeen different countries. The International Union of Pure and Applied Physics has approved, under the C3 Commission on statistical physics, the support of the workshop as a topical IUPAP satellite meeting of the triannual conference STATPHYS26, July 18-22, 2016 in Lyon.



Speakers

- | | |
|--|---|
| Vijay Balasubramanian U. of Pennsylvania, USA | Linda Reichl U. of Texas, Austin, USA |
| Felipe Barra U. de Chile, Santiago, Chile | Peter Reimann U. Bielefeld, Germany |
| Bernard Derrida ENS, Paris, France | Miguel Rubi U. de Barcelona, Spain |
| Jean-Pierre Eckmann Geneva U., Switzerland | Maxi San Miguel U. de les Illes Balears, Spain |
| Massimiliano Esposito U. du Luxembourg, Luxembourg | Grégoire Nicolis ULB, Belgium |
| Giovanni Gallavotti Sapienza U., Rome, Italy | Tanja Schilling U. du Luxembourg, Luxembourg |
| Theo Geisel MPI for Dynamics and Self-Organization, Göttingen, Germany | Lutz Schimansky-Geier Humboldt-U. zu Berlin, Germany |
| Rosemary Harris Queen Mary University of London, UK | Friederike Schmid JGU, Mainz, Germany |
| Mehran Kardar Massachusetts Inst. of Technology, USA | Udo Seifert U. Stuttgart, Germany |
| Jürgen Kurths Potsdam U., Germany | Herbert Spohn Technische U. München, Germany |
| David Lacoste ESPCI, Paris, France | Tsvi Tlusty IAS, Princeton, USA |
| Valerio Lucarini U. of Hamburg, Germany | Raul Toral U. de les Illes Balears, Spain |
| Eric Lutz U. of Erlangen-Nürnberg, Germany | Carolyn M. Van Vliet U. of Miami, USA |
| Anna Maciolek Max Planck Institute, Stuttgart, Germany | David H. Wolpert Santa Fe Institute, USA |
| Antonio Politi U. of Aberdeen, UK | Annette Zippelius Georg-August-U., Göttingen, Germany |
| Itamar Procaccia Weizmann Inst. of Science, Rehovot, Israel | |

Program

Monday 11 July 2016

Chair: Pierre Gaspard

Welcome and introductory speech by Grégoire Nicolis

- | | |
|-------------------|---|
| Mehran Kardar | <i>Non-equilibrium fluctuation-induced forces</i> |
| Anna Maciolek | <i>Emergent long-range couplings in arrays of fluid cells</i> |
| Friederike Schmid | <i>Non-equilibrium self-assembly of polymeric nanoparticles in flow</i> |
| Herbert Spohn | <i>Universal distributions for growing interfaces in one dimension</i> |
| Annette Zippelius | <i>Dense Granular flow of frictional particles</i> |

Chair: Herbert Spohn

- | | |
|-----------------------|---|
| Bernard Derrida | <i>Current fluctuations in non-equilibrium diffusive systems</i> |
| Udo Seifert | <i>Universal features of NESS-fluctuations of single molecules and small networks</i> |
| Massimiliano Esposito | <i>Dynamics and thermodynamics of open chemical reaction networks</i> |
| Miguel Rubi | <i>Far-from-equilibrium activated processes</i> |
| Itamar Procaccia | <i>Mechanical yield to plastic flow in amorphous materials</i> |

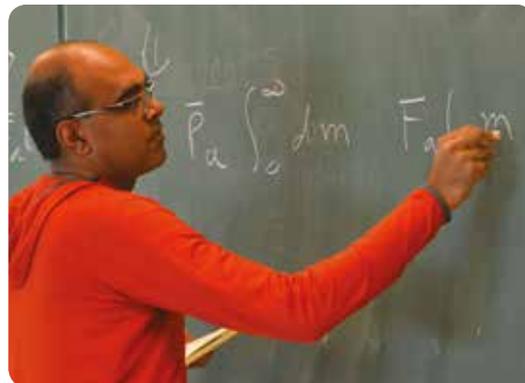
Tuesday 12 July 2016

Chair: Jan Danckaert

- | | |
|-----------------------|--|
| Jürgen Kurths | <i>Quantifying stability in complex networks : From linear to basin stability</i> |
| Maxi San Miguel | <i>Transitions in networks co-evolution dynamics</i> |
| Raul Toral | <i>Macroscopic effects in heterogeneous stochastic systems</i> |
| Tsvi Tlusty | <i>Proteins as learning amorphous matter: dimension and spectrum of the genotype-to-phenotype maps</i> |
| Vijay Balasubramanian | <i>Adaptive Molecular Sensing</i> |

Chair: Massimiliano Esposito

- Theo Geisel *Caustics in random media:
Universal properties on many scales*
- Rosemary Harris *Fluctuations in stochastic systems
with memory*
- David Lacoste *Thermodynamic constraints
on the equilibrium fluctuations of an order
parameter*
- Giovanni Gallavotti *SRB: Interpretation, simulations*
- Valerio Lucarini *Response and Fluctuations in Climate
Science*
- Hans Herrmann *Packing of wires in cavities and growing
surfaces*



Wednesday 13 July 2016

Chair: Mahendra Verma

- Jean-Pierre Eckmann *Hamiltonian chains with dissipation*
- Linda Reichl *Arnold diffusion in a driven optical lattice*
- David H. Wolpert *Extending Landauer's bound from bit erasure
to arbitrary computation*
- Antonio Politi *Transport phenomena in one-dimensional
systems*
- Eric Lutz *Irreversibility and the arrow of time
in a quenched quantum system*

Chair: Daniel Alonso

- Peter Reimann *Typical fast thermalization processes
in closed many-body systems*
- Felipe Barra *Thermodynamics of boundary driven open
quantum systems*
- Tanja Schilling *Pacman has a new exponent*
- Lutz Schimansky-Geier *Stochastic models of self-propelled
particles*

Closing

Modave Summer School in Mathematical Physics

11 - 17 September 2016



Modave Summer School in Mathematical Physics

11 - 17 September 2016



The twelfth edition of the Modave Summer School in Mathematical Physics took place from the 11th to the 17th of September 2016 in Modave (Belgium). The Modave Summer School is organized by PhD students from Belgian universities (ULB, VUB, KUL and UMons) for other young PhD students from all over the world. The lecturers are late

PhD students or young Post-Docs, so that an informal and non-hierarchical environment is assured, facilitating fruitful interactions among young researchers of close fields. The courses consist of pedagogical blackboard lectures on different topics in theoretical physics, ranging from introductory to advanced subjects. The lectures of the twelfth edition have touched the following topics: higher spins and holography, information loss paradox, integrability, on-shell scattering amplitudes, and resurgence.

Modave 2016 organizing committee

Thomas Basile | UMons
Juan Diaz | KUL
Tim De Jonckheere | VUB
Saskia Demulder | VUB
Sybille Driezer | VUB
Marco Fazzi | ULB
Edoardo Lauria | KUL
Victor Lekeu | ULB
Amaury Leonard | ULB

Jonathan Lindgren | VUB
Andrea Marzolla | ULB
Daniel Naegels | ULB
Blagoje Oblak | ULB
Roberto Oliveri | ULB
Arash Ranjbar | ULB
Ellen van der Woerd | KUL
Yannick Vreys | KUL
Céline Zwikel | ULB

Lectures

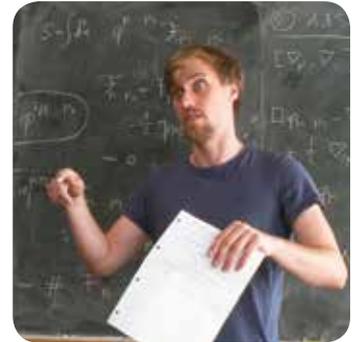
Higher Spins (6h)



Charlotte Sleight & Pan Kessel

We aim to give a pedagogical introduction to theories of higher-spin gauge fields, and review aspects of higher-spin holography. The lecture will revolve around the following topics:

- No-go results
- Higher-spins on AdS
- CFT in $d > 2$
- Higher-spin holographic dualities



Information loss paradox (5h)



David Turton

The black hole information paradox represents a strong consistency test for any theory of quantum gravity. I will review Hawking's original derivation of the paradox, as well as some more recent formulations using results from quantum information theory. I will also introduce some proposed possible resolutions to the paradox, discuss the status of these proposals, and their implications for the physics of an observer falling into a black hole.

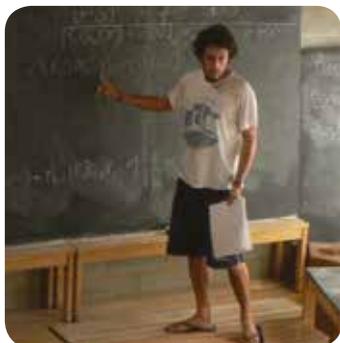
Integrability (5h)



Stijn Van Tongeren

I will provide a conceptual overview of integrable models, linked to their relevance in AdS/CFT. I will address the basics of integrability in classical two dimensional field theory in terms of Lax connections, and then move to quantum spin chains and quantum field theory, leading to topics such as factorized scattering and the Bethe ansatz.

On-Shell Amplitudes with spinor/helicity formalism (5h)



Andrea Marzolla

I will review the spinor/helicity formalism as an efficient tool to test the power of Poincaré invariance in constraining scattering amplitudes, independently of the specific theory and of the existence of a Lagrangian. I will show the advantages of working with complex momenta and the potentiality of BCFW recursion relations.

Resurgence (6h)



Daniele Dorigoni

I will introduce some basic concepts in asymptotic expansions and resurgent theory and explain why these are relevant when computing physical observables in perturbation theory. I will then apply these methods in some simple quantum mechanics and quantum field theory models to extract non-perturbative information from the perturbative expansion of specific physical quantities.

The proceedings of the lectures of the summer school will be published in Proceedings of Science, the open access online journal organized by SISSA, the International School for Advanced Studies based in Trieste.

Participants

Thomas Basile | Université de Mons, Belgium

Charles Cosnier-Horeau | Ecole Polytechnique / UPMC, Paris, France

David De Filippi | Université de Mons, Belgium

Saskia Demulder | VUB, Brussels, Belgium

Daniele Dorigoni | Durham University, UK

Sibylle Driezen | VUB, Brussels, Belgium

Joseph Farrow | Durham University, UK

Paolo Gregori | ULB & Università di Torino, Italy

Renjan Rajan John | Institute of Mathematical Sciences, Chennai, India

Tim De Jonckheere | VUB, Brussels, Belgium

Pan Kessel | Max Planck Institute, Potsdam, Germany

Rob Klabbers | Hamburg University, Germany

Marcela Lagos | Universidad de Concepción, Chile

Victor Lekeu | ULB, Brussels, Belgium

Tom Lemmens | KU Leuven, Belgium

Amaury Leonard | ULB, Brussels, Belgium

Jonathan Lindgren | VUB, Brussels, Belgium

Vincent Luyten | VUB, Brussels, Belgium

Andrea Marzolla | ULB, Brussels, Belgium

Vincent Min | KU Leuven, Belgium

Jesse van Muiden | KU Leuven, Belgium

Daniel Naegels | ULB, Brussels, Belgium

Zainab Nazari | Bogaziçi University, Istanbul, Turkey

Kevin Nguyen | VUB, Brussels, Belgium

Pablo Pais | ULB & CECs, Valdivia, Chile

Cihan Pazarbasi | Bogaziçi University, Istanbul, Turkey

Madhusudhan Raman | Institute of Mathematical Sciences, Chennai, India

Arash Ranjbar | ULB, Brussels, Belgium

Romain Ruzziconi | ULB, Brussels, Belgium

Sergei Savin | Hamburg University, Germany

Charlotte Sleight | Max Planck Institute, Munich, Germany

Lucas Traina | Université de Mons, Belgium

David Turton | Saclay, Paris, France

Guillaume Valette | ULB, Brussels, Belgium

Stijn Van Tongeren | Humboldt University, Berlin, Germany

Aldo Vera Serón | Universidad de Concepción, Chile

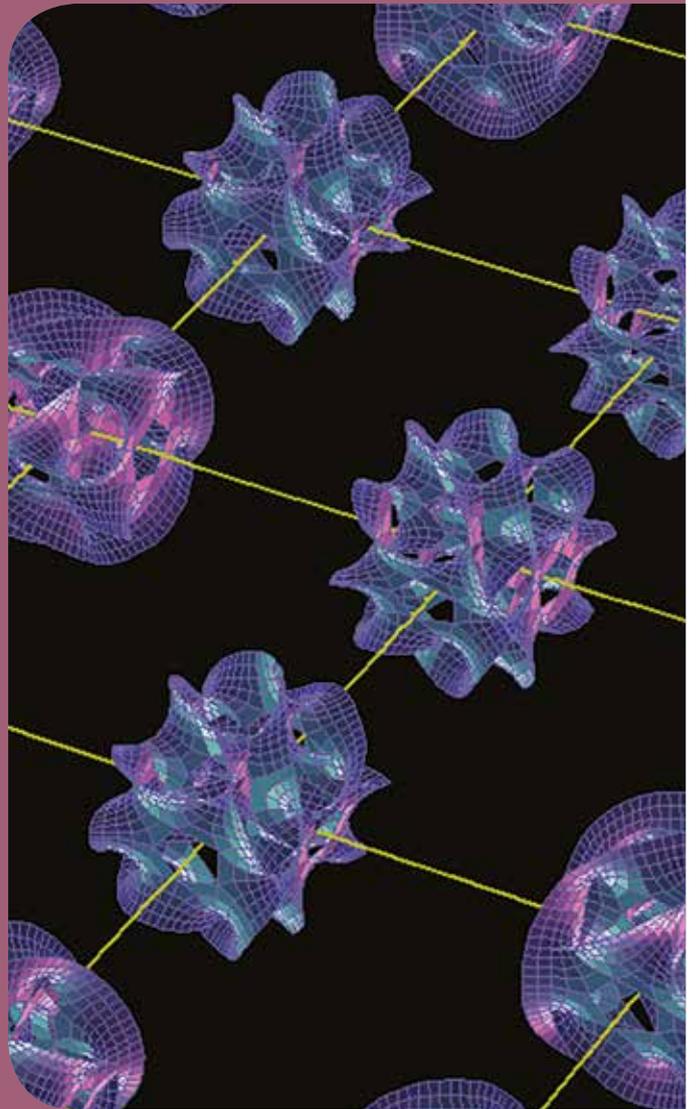
Yannick Vreys | KU Leuven, Belgium

Céline Zwickel | ULB, Brussels, Belgium



The International Doctoral School
“Quantum Field Theory,
Strings and Gravity”

3 - 21 October 2016



The International Doctoral School “Quantum Field Theory, Strings and Gravity”



The aim of the Amsterdam-Brussels-Geneva-Paris Doctoral School on “Quantum Field Theory, Strings and Gravity” is to provide first-year PhD students with advanced courses in theoretical physics that help bridge the gap between Master-level

courses and the most recent advances in the field. Responsible for the organization as well as for teaching the courses are the ULB, the VUB, the University of Amsterdam, various institutions in Paris led by the École Normale Supérieure, and various institutions in Switzerland led by ETH Zurich.

The program typically starts at the end of September/beginning of October and consists of three times three weeks of lectures in three cities among Amsterdam, Brussels, Geneva (CERN) and Paris (depending on the year), with a one-week break between the segments. This way, the students are exposed to several institutes, each with their own research and teaching culture, and to professors from the various institutes.

Last but not least, they get to meet fellow students from neighboring institutes and countries, who will be their peers and colleagues throughout (and possibly beyond) their PhD studies.



Organizing Committee Brussels

Riccardo Argurio | ULB
Ben Craps | VUB
Frank Ferrari | ULB

Organizing Institutions

Institute for theoretical physics | University of Amsterdam
Laboratoire de physique théorique | École Normale Supérieure | Paris
Physique théorique et mathématique | ULB | Brussels
Theoretical particle physics | VUB | Brussels
SwissMap | ETH, U. Bern, U. Geneva, CERN

Program

Brussels | 3 - 21 October 2016

String Theory I - Alberto Lerda | Università del Piemonte Orientale, Alessandria, Italy
String Theory II - Marco Billò | Università di Torino, Italy
Advanced Quantum Field Theory - Adel Bilal | ENS, Paris, France
General Relativity and Black Holes - Glenn Barnich | ULB, Belgium
Quantum Hall physics and field-theoretic dualities
Dam Thanh Son | Chigago, USA (2016 Solvay Chair in Physics)

Amsterdam | 31 October - 18 November 2016

String Theory II - Elias Kiritsis
Supergravity - Antoine van Proeyen
Susy QFT / CFT - Nikolay Bobev
Quantum Fields in Curved Space-Time - Guilherme Pimentel
Introduction to AdS/CFT - Kyriakos Papadodimas

Geneva | 28 November - 16 December 2016

4d N=2 susy QFT - Wolfgang Lerche
Lie algebras - Matthias Gaberdiel
Large N - Marcos Marino
Foundations of AdS/CFT - Ben Hoare
Applied AdS/CFT - Julian Sonner



Participants

Alves da Silva João Pedro EPFL, Lausanne, Switzerland	Manenti Andrea EPFL, Lausanne, Switzerland
Anagiannis Vasileios UvA, The Netherlands	Mazuet Charles University of Tours, France
Berthiere Clément University of Tours, France	Nguyen Kevin VUB, Brussels, Belgium
Biasi Anxo Universidad de Santiago de Compostela, Spain	Novak Igor University of Geneva, Switzerland
Bomans Pieter KU Leuven, Belgium	Reehorst Martin EPFL, Lausanne, Switzerland
Bonnefoy Quentin Ecole Polytechnique, Palaiseau, France	Ruzziconi Romain ULB, Brussels, Belgium
Ciambelli Luca Ecole Polytechnique, Paris, France	Schotte Alexis UGent, Belgium
De Clerck Marine VUB, Brussels, Belgium	Sekiguchi Yuta University of Bern, Switzerland
De Filippi David UMONS, Belgium	Tournoy Magnus KU Leuven, Belgium
Dei Andrea ETH Zurich, Switzerland	Traina Lucas UMONS, Belgium
Ge Dongsheng École Normale Supérieure, Paris, France	Valette Guillaume ULB, Brussels, Belgium
Gemunden Thomas ETH Zurich, Switzerland	van Breukelen Rik University of Geneva, Switzerland
Godet Victor UvA, The Netherlands	van Muiden Jesse KU Leuven, Belgium
Goelen Frederik KU Leuven, Belgium	Vanhecke Bram UGent, Belgium
Hansen Dennis ETH Zurich, Switzerland	Venken Gerben KU Leuven, Belgium
Heidman Pierre Université Paris-Saclay, France	Verhellen Jonas VUB, Brussels, Belgium
Het Lam Huibert Utrecht University, The Netherlands	Vielma Manuel University of Geneva, Switzerland
Iarygina Oksana Leiden University, The Netherlands	Zhihao Duan ENS Paris, France
Kelley Katharine University of Western, Australia	Zhong Deliang UPMC, France
Kumar Jewel University of Paris 7, France	
Laletin Maxim Université de Liège, Belgium	
Lavdas Ionnis École Normale Supérieure, France	

Student's opinion

This doctoral school was my first contact with an international research environment. One of the aims was to bridge the gap between Master-level courses and the most recent advances in theoretical and mathematical physics. The lectures were given by professors, experts from the various organizing institutes. All participants were PhD students specialized in the field. All were strongly motivated and there was an atmosphere of emulation which permitted the learning of many subjects in a short period of time. It was a wonderful experience from a professional and a personal point of view.

The school consisted of three sessions of three intense weeks of lectures, with one week of break between each session. The first session was held in Brussels. We attended lectures about General Relativity, Quantum Field Theory and String Theory. It was a wonderful opportunity to complete the teaching received during the Master and constitutes for me an essential background that all theoretical physicists should know. The second session of lectures, held in Amsterdam, consisted essentially of going deeper into the previously introduced theories. We received courses about Supersymmetry, Supergravity, Conformal Field Theory, Superstring Theory, Quantum Field Theory in Curved Space-Time and an Introduction to AdS/CFT Correspondence. I learned a lot of material during this period and it procured me knowledge of many concepts appearing repeatedly in high energy physics. This has also permitted me to easily consult many textbooks and specialized reviews about these subjects. The last session of lectures was held in Geneva. The aim was to bring PhD students up to the state of the art level in the modern and mainstream subjects of research in the discipline. It consisted mainly of more specific courses like Large N, 4d N=2 Susy/QFT, Integrability with a special emphasize on AdS/CFT, Applied AdS/CFT and a course about Lie Algebra. After this last session, we are now able to follow talks given by experts in a broad range of subjects, even if we are not working on them directly.

Romain Ruzziconi

In addition to these lectures, the school was a wonderful opportunity to meet some PhD students working on similar subjects in other European universities. I had many exchanges with the other participants about our particular research interests. I learned as many things during these conversations as during the lectures. I have kept in touch with some of them that I still encounter in some conferences, which will probably lead to future collaborations. Both from a social and a professional point of view, this

doctoral school is a huge advantage that we have compared to other institutions and constitutes a very valuable experience for the future.



Workshop on “Charge, spin, and heat transport in organic semiconductors”

15 - 17 November 2016



15 - 17 November 2016
ULB - Campus Plaine - Solvay Room

Solvay Workshop on
Charge, spin, & heat transport
in organic semiconductors

SPEAKERS

Chihaya Adachi (Kyushu, Japan)
John Anthony (Lexington, USA)
Narcis Avarvari (Angers, France)
Fabio Biscarini (Modena, Italy)
Jean-Luc Brédas (KAUST, Saudi Arabia)
Xavier Crispin (Linköping, Sweden)
Daniel Frisbie (Minneapolis, USA)
Ferdinand Grozema (Delft, The Netherlands)
Bert Koopmans (Eindhoven, The Netherlands)
Karl Leo (Dresden, Germany)
Yueh Lin Loo (Princeton, USA)
Christian Maes (Leuven, Belgium)
Ron Naaman (Rehovot, Israel)
Yoann Olivier (Mons, Belgium)
Vitaly Podzorov (Rutgers, USA)
Alberto Salao (Stanford, USA)
Guillaume Schweicher (Cambridge, UK)
Shu Seki (Kyoto, Japan)
Erik McNellis (Mainz, Germany)
Henning Sirringhaus (Cambridge, UK)
Zhigang Shuai (Beijing, China)
Jun Takeya (Tokyo, Japan)
Kazuo Takimiya (Riken, Japan)

SCIENTIFIC & ORGANISING COMMITTEE

Basab Chattopadhyay (ULB, Belgium)
Yves Geerts (ULB, Belgium)

www.solvayinstitutes.be

 INTERNATIONAL SOLVAY INSTITUTES BRUSSELS

“Charge, spin, and heat transport in organic semiconductors”

15 - 17 November 2016

This workshop intended to be a brainstorming session in which the latest results on charge, spin, and heat transport were presented and discussed. The aim was to get a comprehensive view of transport properties in organic semiconductors that differ from inorganic ones by many aspects. Current understanding of these phenomena based on both experimental and theoretical evidences is not absolute. Charge transport mechanism cannot be uniquely described by hopping or band-like models. Spin diffusion length are larger because of weak spin-orbit coupling. Heat transport is limited by low and anisotropic thermal conductivity coefficients. Internationally-recognized researchers, with very different backgrounds have been invited. Chemists, physicists, experimentalists, and theoreticians will confront their viewpoints to get a deep and comprehensive fundamental understanding of transport phenomena in organic semiconductors.

Scientific & Organizing Committee

Basab Chattopadhyay | ULB, Belgium
Yves Geerts | ULB, Belgium

Speakers

Chihaya Adachi | Kyushu, Japan
John Anthony | Lexington, USA
Narcis Avarvari | Angers, France
Fabio Biscarini | Modena, Italy
Jean-Luc Brédas | KAUST, Saudi Arabia
Xavier Crispin | Linköping, Sweden
Daniel Frisbie | Minneapolis, USA
Ferdinand Grozema | Delft, The Netherlands
Georges Hadziioannou | U. Bordeaux, France
Bert Koopmans | Eindhoven, The Netherlands
Karl Leo | Dresden, Germany
Yueh Lin Loo | Princeton, USA
Christian Maes | Leuven, Belgium
Erik McNellis | Mainz, Germany
Ron Naaman | Rehovot, Israel
Yoann Olivier | Mons, Belgium
Alberto Saleo | Stanford, USA
Guillaume Schweicher | Cambridge, UK
Shu Seki | Kyoto, Japan
Henning Sirringhaus | Cambridge, UK
Zhigang Shuai | Beijing, China
Jun Takeya | Tokyo, Japan
Kazuo Takimiya | Riken, Japan

Program

Tuesday 15 November 2016

Welcome and introductory speech by Yves Geerts

- Georges Hadziioannou *Structure - Properties correlations for thermoelectric polymers: Towards efficient material design*
- Zhigang Shuai *Modeling charge and heat transports in organic/polymeric materials*
- Shu Seki *Electron mass and conductivity on pi-conjugated molecules in their condensed phases and at interfaces*
- Daniel Frisbie *Structure-Transport Relationships in Single Crystal Organic FETs*
- Alberto Saleo *A new plastic artificial synapse*
- Kazuo Takimiya *Thienoacenes; molecules for organic semiconductors and beyond*
- Karl Leo *Novel organic transistors*
- Jean-Luc Brédas *The Impact of Coherence Effects in Organic Electronics*
- Fabio Biscarini *Electrolyte-gated organic field effect transistors: doping effects in organic semiconductors in water*

Poster session



Wednesday 16 November 2016

Erik McNellis	<i>Modeling spin transport and spin-phenomena in organics</i>
Yueh Lin Loo	<i>Polymorphic transformations in Thin Films of Core-Chlorinated Naphthalene Diimide Derivatives</i>
Narcis Avarvari	<i>Chiral conducting molecular materials</i>
Bert Koopmans	<i>Magnetic field effects in organic semiconductors</i>
Chihaya Adachi	<i>Triplet exciton management in organic light emitting devices</i>



Henning Sirringhaus	<i>Charge and spin transport physics of high mobility organic semiconductors</i>
Jun Takeya	<i>Materials and integrated circuits of organic semiconductors</i>
Christian Maes	<i>Non-dissipative aspects in structure and transport out-of-equilibrium</i>

Solvay Colloquium

Ron Naaman	<i>The chiral induced spin selectivity effect- from spintronics to Biology</i>
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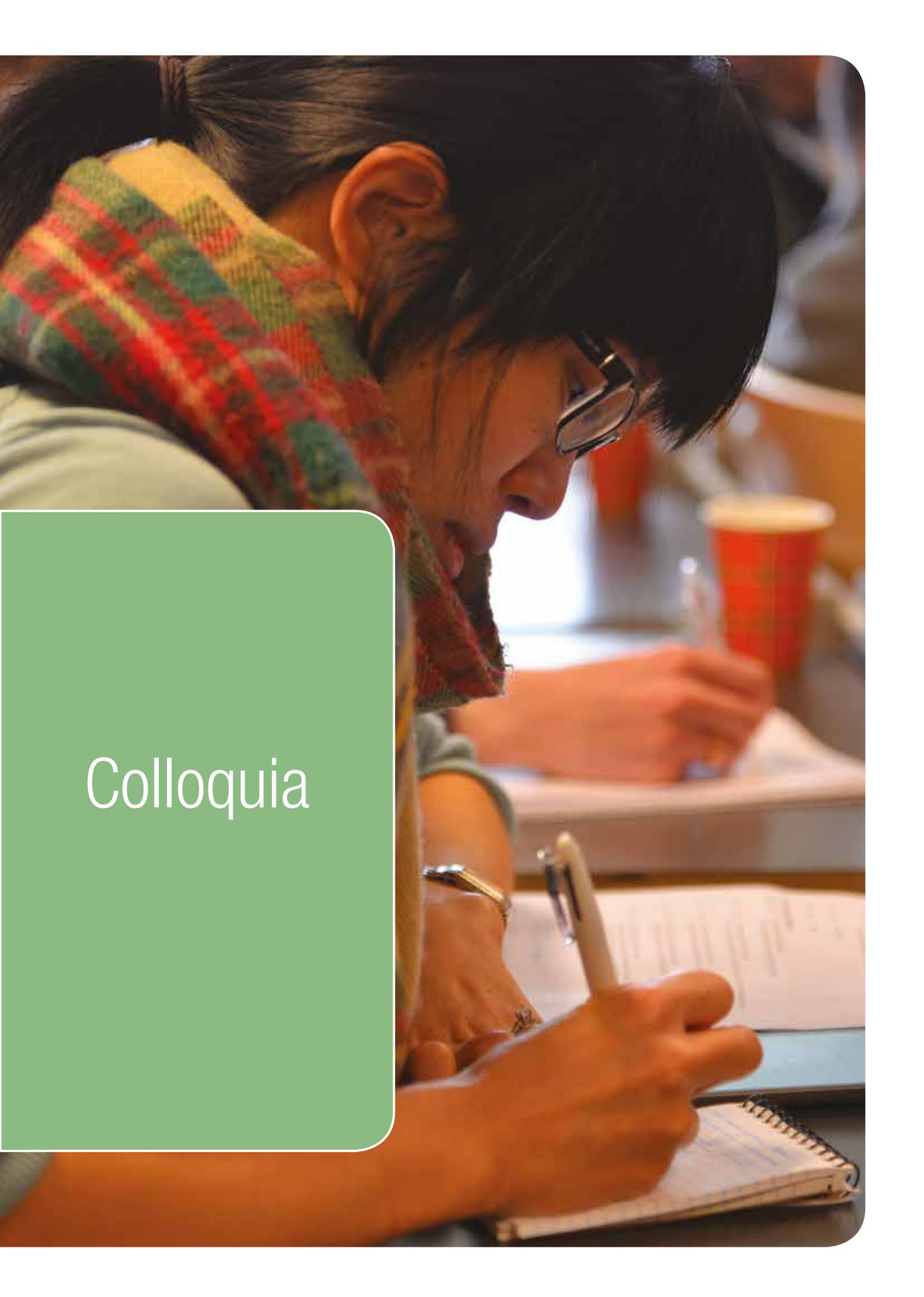
Conference Banquet



Thursday 17 November 2016

- | | |
|----------------------|--|
| Xavier Crispin | <i>Thermoelectric properties of Poly (3,4-ethylenedioxythiophene) derivatives</i> |
| Guillaume Schweicher | <i>Structure-property relationship of thienoacenes</i> |
| John Anthony | <i>Structure / transport relationships in crystalline organic semiconductors</i> |
| Ferdinand Grozema | <i>Effect of molecular packing and structural dynamics on charge transport in organic semiconductors</i> |
| Yoann Olivier | <i>How microstructure defines function in organic conjugated materials: insight from modeling</i> |
| Yves Geerts | Conclusions |



A close-up, side-profile photograph of a young woman with dark hair and glasses, wearing a colorful, patterned scarf. She is focused on writing in a spiral notebook with a white pen. The background is softly blurred, showing another student at a desk with a red cup. The overall atmosphere is one of quiet concentration in a classroom or lecture hall.

Colloquia

Oscillations, no-oscillations and neutrino mass

Professor Alexei Smirnov | *MPIK Heidelberg, Germany* | 26 January 2016

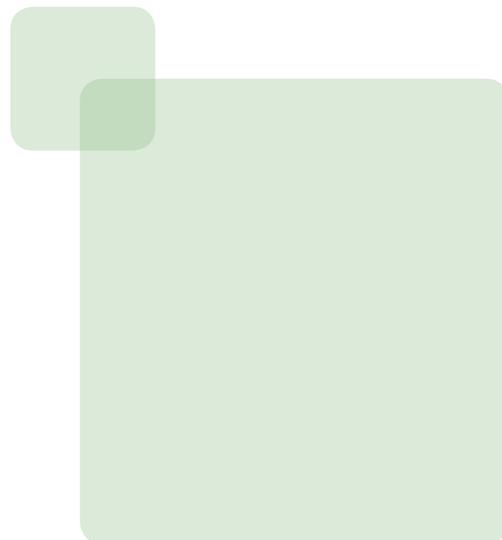


The Nobel prize in physics 2015 has been awarded “for the discovery of neutrino oscillations”. In this connection I will describe the SuperKamiokande (SK) and SNO experiments and give the present day interpretation of their results. While SK has discovered vacuum oscillations, the SNO observed mainly effect of the adiabatic flavor conversion in matter of the Sun with

only small corrections due to the averaged oscillations. In general, oscillations imply existence of mixing but not a mass. Further studies required to show that the neutrino masses are behind the SK and SNO observations.

In continuation I will discuss the present status of exploration of the solar neutrinos as well as oscillations of neutrinos of various origins.

Some recent developments of the theory of neutrino oscillations in vacuum and in different media will be outlined. That includes, in particular, effects of spread of the neutrino wave packets, splitting of eigenstates in multilayer media, collective oscillations related to scattering of neutrinos on neutrinos.



Nanostructuring in polymeric materials: macro-performance via nano-scale chemical tailoring

Professor Philippe Dubois | *Université de Mons, Belgium* | 16 February 2016

Recent advances in polymer blends and (nano) filled polymers clearly highlight how much versatile and rich these research domains can be. Particularly polymer nanocomposites, singularly based on polymer blends compatibilized by nanoparticles, appear highly promising paving the way to novel families of materials offering extraordinary property improvement.



This contribution aims at presenting new orientations currently given in the search of such polymeric materials, actually by combining two (or more) nanofillers providing synergistic behaviour, developing new processing technologies (reactive extrusion and layer-by-layer techniques,...) and nanostructuring

the nanocomposite materials by specifically localizing/orienting the nanofillers, e.g., in co-continuous polymer blends using surface-treated nanoparticles as interfacial compatibilizers.

Mostly three types of nanofillers will be studied, i.e., carbon nanotubes, silica nanoparticles and cellulose nanocrystals, each finely dispersed and even oriented in either thermoplastic, thermosetting or elastomeric matrices. The resulting polymeric materials will display remarkable thermo-mechanical performances (good stiffness/toughness balance) but also more specific properties such as electrical conductivity, flame-resistance, and anti-biofouling. Some industrial applications currently developed based on these novel (nano)materials will be presented as well.



New mobile instruments to get in situ chemical analysis of paintings

Professor Philippe Walter | *UPMC, France* | 1 March 2016



The study of Cultural Heritage materials requires advanced techniques to shed new lights on ancient technologies and help in their preservation. The precious character of the most famous works of art and their uniqueness imply particular cautions and require instruments which may give the maximum of information directly on the objects, in-situ in the museums or in the

archaeological sites.

The implementation of new analytical tools, including mobile instruments, allows a deep insight on the archaeological and artistic materials. We will show the performances of different new mobile instruments we built to allow in situ characterization of the nature, the alteration and the mode of preparation of different pigments. Through several examples, we will show how the painters were able to create the perception of depth in their paintings by modulating carefully the relationship between shadows and light, thanks to the realization of dark areas, the work in sub-layers and the choice of pigments. It was then possible to obtain particular shades reproducing light reflection on metallic objects or performing an atmospheric perspective.

Black holes, a century after the birth of General Relativity

Professor Eric Gourgoulhon | *LUTH, France* | 15 March 2016



Black holes are nowadays part of standard astrophysics, on (almost) the same footing as planets, stars or galaxies. I shall review their theoretical properties and their current observational status. Then, I shall discuss the prospects opened by a new generation of instruments, which, for the first time, will allow us to probe the immediate vicinity of the event horizon the black hole at the

center of our galaxy, thereby providing a unique opportunity to test General Relativity in the strong field regime.

Planck mission: the large scale CMB polarisation data

Professor Jean-Loup Puget | *Université Paris Sud, Orsay, France* | 12 April 2016



The Planck mission measured the Cosmic Microwave Background anisotropies with unprecedented sensitivity and deduced the cosmological parameters of the Cold-Dark-Matter with Cosmological constant and of extensions of this model. It will be argued that we now have a first incarnation of a standard cosmological model.

The Thomson Optical depth parameter τ measuring the column density of free electrons since the first stars and galaxies form was the parameter measured with the lowest accuracy. The polarization E-modes of the CMB anisotropies at large scale allows to measure it nearly independently of the other parameters. The implications for the other parameters will be discussed.

New results on τ remove the tensions between earlier CMB measurements and observations of high redshift sources. Furthermore this measurement starts to constrain the ionising radiation from first stars and galaxies at high redshifts.

Future use of the polarisation Planck data on large scale to search for B modes signal associated with primordial gravity waves from the inflation phase will also be presented.

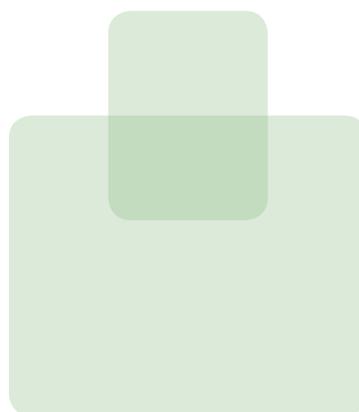
Molecular Machines and Synthetic Motors: Active Motion on the Nanoscale

Professor Raymond Kapral | *University of Toronto, Canada* | 19 April 2016



Molecular machines operate far from equilibrium and are subject to strong thermal fluctuations. They use chemical energy to perform a variety of tasks, acting as motors, enzymes or pumps, and in doing so play important roles in the operation of the cell. Synthetic chemically-powered nanomotors, with and without moving parts, operate under similar conditions and are

being studied because of their potential applications involving active transport on small scales and the challenges they pose for theory and simulation. Two examples will be used to illustrate the phenomena that such systems display: synthetic chemically-powered nanomotors and hydrodynamic collective effects arising from active protein machines. The kinds of synthetic nanomotors that have been constructed and their potential applications will be described, and the mechanisms they use for propulsion and how their dynamics may be simulated will be discussed. Experimental observations have shown that transport in the cell is influenced by protein activity. It will be shown that one mechanism that may contribute to the enhanced transport of passive particles and other enzymes in the cell and in solution is due to the hydrodynamic flows that are generated by the nonequilibrium conformational changes of active enzymes.



Protein structure and dynamics using X-ray free-electron lasers

Professor Ilme Schlichting | *Max Planck Institute, Germany* | 14 June 2016

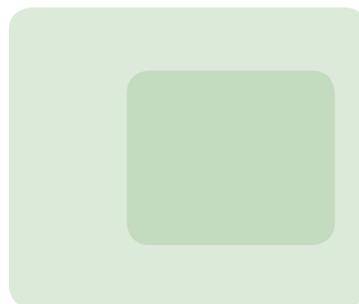


Protein crystallography using synchrotron radiation sources has had tremendous impact on biology, having yielded the structures of thousands of proteins and given detailed insight into their working mechanisms. However, the technique is limited by the requirement for macroscopic crystals, which can be difficult to obtain, as well as by the often severe radiation damage

caused in diffraction experiments, in particular when using tiny crystals. To slow radiation damage, data collection is typically performed at cryogenic temperatures.

The femtosecond X-ray pulses provided by X-ray free-electron lasers (FELs) allow the acquisition of high resolution diffraction data from micron-sized macromolecular crystals at room temperature beyond the limitations of radiation damage imposed by conventional X-ray sources. Moreover, the short duration of the pulses enable time-resolved studies at the chemical time-scale of femtoseconds. The novel sources require new approaches for sample preparation, delivery, data collection and analysis. These approaches [1] as well as recent results obtained will be presented.

[1] Schlichting, I. (2015) *IUCrJ* 2: 246-255. *Serial femtosecond crystallography: the first five years.*



Fluid viscosity: from Maxwell to black holes

Professor Dam Thanh Son | *University of Chicago, USA* | 4 October 2016



There has been tremendous progress in recent years in our understanding of the behavior of matter in extreme conditions - at very high and very low temperatures. Unexpectedly, physicists have found that some techniques originating from string theory are very useful and gives information about the viscosity of strongly interacting liquids that cannot be obtained by other methods. We

trace the history of the notion of viscosity from Maxwell to modern days, and elucidate the relationship between the viscosity and the behavior of black hole horizons.

Chirality and spin- from spintronics to water splitting

Professor Ron Naaman | *Weizmann Institute, Rehovot, Israel* | 16 November 2016



Spin based properties, applications, and devices are commonly related to magnetic effects and to magnetic materials. However, we found that chiral organic molecules act as spin filters for photoelectrons transmission, in electron transfer, and in electron transport.

The new effect, termed Chiral Induced Spin Selectivity (CISS), has interesting implications for the production of new types of spintronics devices and on electron transfer in biological systems. The effect was found in bio-molecules and in bio-systems like the photosystem I. In addition, the CISS effect may play an important role in controlling multiple electrons processes, like water splitting. The basic effect will be explained and various applications and implications will be discussed.

Toy Models

Professor Tadashi Tokieda | *Cambridge University, UK* | 22 November 2016



Would you like to come see some toys?

'Toys' here have a special sense: objects of daily life which we can find or make in minutes, yet which, if played with imaginatively, reveal surprising phenomena that keep physicists puzzling for a while. We will see table-top demos of many such toys and visit some of the science that they open up. A common theme that emerges is *singularity*.

Gravitational Wave Astronomy: Listening to the Dark Side of the Universe!

Professor Karsten Danzmann | *MPI, Germany* | 13 December 2016



For thousands of years we have been looking at the universe with our eyes. But most of the universe is dark and will never be observable with electromagnetic waves.

After September 14th, 2015, everything is different: we can now detect gravitational waves and finally listen to the universe and nobody knows what dark secrets are waiting for us out there.



Workshops

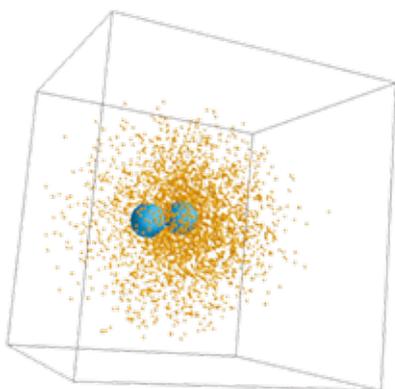
sponsored
by the Institutes

Workshop on “Modeling of chemically powered nanomotors” Organized by KU Leuven

12 - 13 April 2016

Organizing Committee

P. de Buyl, KU Leuven
R. Lambiotte, Université de Namur
C. Maes, KU Leuven
B. Mognetti, Université libre de Bruxelles
C. Van den Broeck, Universiteit Hasselt



Chemically powered nanomotors are studied since about a decade in laboratories worldwide and are of both fundamental and applied interest. They are colloidal devices with a catalytic activity that enables them to harness a source of chemical energy to provide rotational or translational motion.

The focus of the present workshop was to discuss and use simulation models for chemically powered nanomotors.

The methods, despite an almost ten years old history dating to the pioneering paper by Rückner and Kapral (2007), are not widely used. During the workshop, an open-source simulation program was used to demonstrate the methods and show how to conduct simulation of two common types of motors: the dimer nanomotor and the Janus nanomotor. It is hoped that the availability and usability of the code will enable further work at the home institutions of the participants.

The workshop took place on two days, the first one dedicated to scientific presentations, by prominent experts in the field, and the second one to the hands-on session of simulation work. There were two simulation speakers and two experimental speakers, as the field has fruitful and regular exchange between these two communities.

Scientific Committee

H. Chaté, CEA-Saclay, Paris, FR
P. de Buyl, KU Leuven, BE
R. Kapral, University of Toronto, CA
B. Mognetti, Université libre de Bruxelles, BE
C. Maes, KU Leuven, BE
A. Mikhailov, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, DE

Invited speakers

Steve Ebbens, University of Sheffield
Raymond Kapral, University of Toronto
Marisol Ripoll, Forschungszentrum Jülich
Ayusman Sen, Penn State University

Tutorial speakers

Mu-Jie Huang, University of Toronto
Pierre de Buyl, KU Leuven

Program

12 April 2016

Raymond Kapral
Chemically-powered nanomotors: What makes them move, their individual and collective behavior, and why particle-based methods are needed to study their dynamics

Steve Ebbens
Catalytic Micro-swimmers: Progress and Future Challenges

Marisol Ripoll
Thermophoretically powered micromachines

Ayusman Se
Designing Chemically-Powered Nanomotors and Pumps

Poster Session

13 April 2016

Pierre de Buyl & MJ Huang
Setting up software for mesoscopic simulations

Simulation of nanodimer motors

Case studies (flows, motor type)

ERC and Solvay Workshop on “Holography for Black Holes and Cosmology”

Organized by the ULB

9 - 13 May 2016

The workshop welcomed anyone interested in the gauge/gravity correspondence and its realizations in AdS but also in new holographic dualities (non-relativistic holography, flat space, extremal black holes, de Sitter), the tools useful for studying them (symmetries, entanglement, fluids, anomalies,...) and their potential observational consequences (precision cosmology, black hole astrophysics).

Organizing and Scientific Committee

Jay Armas, ULB, Brussels, Belgium
Geoffrey Compère, ULB, Brussels, Belgium
Stéphane Detournay, ULB, Brussels, Belgium
Marc Henneaux, ULB, Brussels, Belgium

Invited Participants

Jan de Boer, UvA, The Netherlands
Arjun Bagchi, MIT, USA
Thomas Faulkner, U. of Illinois, USA
Samuel Gralla, U. of Arizona, USA
Daniel Grumiller, ITP, Austria
Diego Hofman, UvA, The Netherlands
Nabil Iqbal, UvA, The Netherlands
Ted Jacobson, U. Maryland, USA
Aitor Lewkowycz, Princeton, USA
Ramalingam Loganayagam, IAS, USA
Paul McFadden, PI, Canada
Monika Moscibrodzka, Radboud U., The Netherlands
Gim Seng Ng, McGill U., Canada
Donal O’Connell, Edinburgh U., UK
Robert Penna, MIT, USA
Guilherme Pimentel, Cambridge U., UK & UvA, The Netherlands
Suvrat Raju, ICTS Tata Institute, India
Mukund Rangamani, UC Davis, USA
Kostas Skenderis, U. Southampton, UK
Wei Song, Tsinghua U., China
Aron Wall, IAS, USA

Program

Thomas Faulkner

Shape dependence of entanglement entropy and modular energy

Samuel Gralla

Holography and Astrophysics

Daniel Grumiller

Rindler holography

Ted Jacobson

Is the vacuum maximally entangled?

Paul McFadden

Conformality lost: broken conformal invariance in holographic cosmology

Monika Moscibrodzka

Imaging the supermassive black hole in the center of the Milky Way

Jim Seng Ng

Anomaly induced Thermodynamics in Higher dimensional AdS/CFT

Donal O'Connell

Classical squaring relations between gauge theory and gravity

Robert Penna

The membrane paradigm, BMS invariance, and astrophysics

Guilherme Pimentel

On backgrounds with vacuum decay

Suvrat Raju

Smooth causal patches for AdS black holes

Mukund Rangamani

Topological Sigma models and dissipative hydrodynamics

Kostas Skenderis

From Planck data to holography

Wei Song

Holographic Entanglement Entropy for WAdS3

Aron Wall

Negative Energy and the Focussing of Light Rays



Workshop on “Cosmological Frontiers in Fundamental Physics 2016”

Series of Workshops co-organised with APC, Paris and the Perimeter Institute
(held at Perimeter Institute, Canada)

14 - 17 June 2016

The purpose of this workshop was to discuss and exchange ideas on the most stimulating recent developments in cosmology and fundamental physics. This year, the workshop focused on four themes: Next Generation Cosmological Probes, Gravitational Wave Astronomy, Fundamental Strong Gravity, and Theoretical Cosmology. This workshop encouraged new ideas and new collaborations among theorists and observers working in cosmology and gravitation. This workshop was the ninth in a series organized jointly by the International Solvay Institutes, APC (Université Paris VII, Paris) and the Perimeter Institute (Waterloo, Canada). The previous edition was held in Brussels in July, 2015.

Scientific Organizers

Matthew Johnson, Perimeter Institute & York University
Kendrick Smith, Perimeter Institute

Speakers

Peter Adshead, University of Illinois at Urbana-Champaign
Yacine Ali-Haïmoud, Johns Hopkins University
Francois Bouchet, Institut d'Astrophysique de Paris
Kipp Cannon, Research Center for the Early Universe
William East, SLAC National Accelerator Laboratory
Bryan Gaensler, University of Toronto
Vera Gluscevic, Institute for Advanced Study
Stephen Green, Perimeter Institute
Gil Holder, McGill University
Justin Khoury, University of Pennsylvania
Jean-Luc Lehners, Max Planck Institute for Gravitational Physics
Steve Liebling, Long Island University
Eugene Lim, King's College London
Marilena LoVerde, Stony Brook University
Frans Pretorius, Princeton University
Leonardo Senatore, SLAC National Accelerator Laboratory
Jon Sievers, University of KwaZulu-Natal
Neil Turok, Perimeter Institute
Nicolas Yunes, Montana State University
Aaron Zimmerman, Canadian Institute for Theoretical Astrophysics

Program

14 June 2016

Yacine Ali-Haimoud
Dark matter phenomenology across cosmic times

Justin Khoury
A Dark Matter Superfluid

Jean-Luc Lehners
The Classicality Puzzle

Leonardo Senatore
Inhomogeneous Anisotropic Cosmology

Vera Gluscevic
A new probe of primordial magnetic fields at high redshift

15 June 2016

Stephen Green
Turbulent gravity in asymptotically AdS spacetimes

Aaron Zimmerman
Black hole ringdown and quasinormal modes

Frans Pretorius
The Dynamical Strong-field Regime of General Relativity

Nicolas Yunes
What does the Advanced LIGO detection say about gravity?

Kipp Cannon

16 June 2016

William East
Spacetime Dynamics of the Higgs Instability and the Fate of the Early Universe

Eugene Lim
Can inflation really begin with inhomogeneous initial conditions?

Steve Liebling
Compact Objects in the Era of GW Astronomy

Francois Bouchet
Latest cosmological news from the Planck satellite Project

Gil Holder
Mapping dark matter on the largest and smallest scales

17 June 2016

Peter Adshead
Asymmetric reheating and chilly dark sectors

Marilena LoVerde
Structure Formation in a ν CDM Universe

Jon Sievers

Neil Turok
Shocks in the Early Universe

Bryan Gaensler
Cosmology and Fundamental Physics with the Square Kilometre Array



International Workshop on “Fundamental Science and Society”

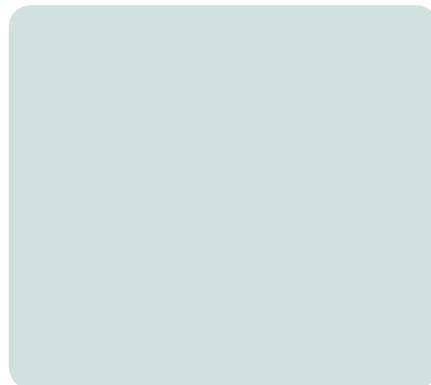
International Center for Interdisciplinary Science
and Education (ICISE), Quy Nhon, Vietnam

7 - 8 July 2016

On the occasion of the 50th anniversary of the prestigious “Rencontres de Moriond”, the Ministry for science and technology of Vietnam, the Popular Committee of the Province of Binh Dinh, the “Rencontres du Vietnam” and the “Rencontres de Moriond” organized a workshop on the theme “Fundamental Science and Society”, with the high patronage of UNESCO and the support and labels of the International Solvay Institutes and CERN. The workshop benefited from the sponsorship of H.E. Vu Duc Dam, Vice Prime minister and H.E. Nguyen Quân, Minister of Science and Technology of Vietnam. The two-day event took place in Vietnam, at the new International Conference Center in Quy Nhon, during the first week of July 2016 (7 and 8 of July).

The new International Conference Center in Quy Nhon constitutes a focal intellectual center in South-East Asia devoted to high-level education and curiosity-driven research, in the heart of one of the most dynamical and future-oriented regions on the planet. The topics addressed by the workshop are relevant to all fundamental sciences. This was reflected in the invitation of leading figures not only from physics, but also from mathematics, economics, chemistry and biology.

It was very natural that the International Solvay Institutes, which shares the same values of pursuing curiosity-driven research and promoting high-level education, sponsored the event.



Program

7 July 2016

Opening and greeting speeches

J. Tran Thanh Van, President of the Rencontres du Vietnam

S.E. Chu Ngoc Anh, Minister of Science and Technology

Leaders of the province of Binh Dinh

Nguyen Van Hieu, Academician, Russian Academy of Science

Celebration of the 50th anniversary of the Rencontres de Moriond

Etienne Augé, Vice-President of Paris South University

Jean-Marie Frère, Professor, Free University of Brussels

Jean Audouze, Astrophysicist, Former Advisor of President François Mitterrand, France

Kok Khoo Phua, President of the Institute of Advanced Studies, Nanyang Technical University, Singapore

J. Tran Thanh Van, President of the Rencontres

Science in Vietnam

Vu Duc Dam, Vice-Prime Minister of Vietnam

Conference Keynotes

David Gross, Nobel laureate in Physics 2004

Koji Omi, Founder and Chairman, Science and Technology in Society forum (STS forum)

Jean-Marie Solvay, President of the International Solvay Institutes and Administrator of Solvay Group, Brussels

Frederick Bordry, Director for Accelerators and Technology of CERN

Round Tables

The importance of pursuing Basic Science in Emerging countries

Moderator

Lars Brink, former president of the Nobel Committee for Physics

Keynote

Kurt Wüthrich, Nobel laureate in Chemistry 2002

Panelists

Yu Lu, Tate Medal in 2007, The Chinese Academy of Science

K. K. Phua, Director of the Institute of Advanced Studies and President of World Scientific Publishing, Singapore

Fernando Quevedo, Director of ICTP, Trieste

Ngô Bao Châu, Field Medal in 2010, Chicago

Pierre Darriulat, Director of VATLY Institute, Hanoi

Basic Science and Sustainable Development

Moderator

Maurizio Bona, Head of Relations with International Organisations, CERN, Geneva

Keynote

Finn Kydland, Nobel laureate in Economy 2004

Panelists

Nikhil Seth, Executive Director of the United Nations Institute for Training and Research (UNITAR)

Dominique Guellec, Director of Science and Technology, OCDE, Paris

Ton Nu Thi Ninh, Former Vietnam Ambassador in Belgium and European Union

Grammenos Mastrojeni, Coordinator for eco-sustainability and science policy, Italian Development Cooperation

Nguyễn Quang Liêm, Director of the Institute of Material Science, VAST, Hanoi

8 July 2016

Basic Science and Peace

Moderator

Herwig Schopper, Former CERN General Director

Keynote

David Gross, Nobel laureate in Physics, 2004

Panelists

Finn Kydland, Nobel laureate in Economy 2004

V. Matveev, Russian Academy of Science, General Director of JINR

E. Rabinovici, Vice-President of SESAME (Middle East countries)

R. Thakur, Director of the Centre for Nuclear Non-Proliferation and Disarmament, Canberra

Science and Climate

Moderator

J. Jouzel, vice-president of GIEC-Peace Nobel laureate 2007

Keynote

John Church, Expert in sea rise, CSIRO, Australia

Panelists

Fredolin Tangang, Professor, Malay Academy of Science, National University of Malaysia

Tran Thuc, Institute of Meteorology, Hydrology and Climate Change

Trinh Xuân Thuận, Professor, University of Virginia, Charlottesville, USA

Basic Science and Health

Moderator

Christine Clerici, President of University Paris Diderot

Keynote

Jean-François Bach, Perpetual secretary of the French Academy of Sciences

Panelists

Sean Hill, Director of Neuroinformatics of the "Human Brain Project"

Socorro Escalante, Advisor at the World Health Organization in Vietnam

Frederick Bordry, Chairman of "CERN Medical Applications Steering Committee"

Robert Sebbag, Vice President of SANOFI-AVENTIS

Basic Science and Education, Knowledge and Technology Transfer

Moderator

Jean Audouze, former Science Advisor
of President Mitterrand

Keynote

P. Léna, Professor, Academy of Science,
France

Panelists

J. Friedman, Nobel laureate in Physics 1990,
MIT

Phan Thanh Binh, President of VNU Ho Chi
Minh, Vietnam

Dam Thanh Son, Professor, American
Academy of Science, University of Chicago

Hesheng Chen, Director of IHES, Beijing,
The Chinese Academy of Science

Yves Demay, Directeur de l'Ecole Polytechnique

Basic Science, Open Innovation and Collaborative Economy

Moderator

Maurizio Bona, Head of Relations with
International Organisations, CERN, Geneva

Keynote

Jovan Kurbalija, founding director
of DiploFoundation, Geneva

Panelists

Ang Beng Wah, Professor at National
University of Singapore

Bruce McKellar, President of IUPAP
(International Union of Pure & Applied
Physics)

Dominique Guellec, Director of Science
and Technology, OCDE, Paris

Nicolas Cudré-Mauroux, Director of Research
and Innovation, Solvay group

Sebastien Remy, Senior Vice-Président
d'Airbus, Director of Innovation, Airbus group

Conclusions and End of the conference

Michel Spiro, President, French Physical
Society, Paris





Science Days
2016

Science Days 2016

29 - 30 April
27 November



The Solvay Institutes organized two activities for secondary school students in 2016, the first one was held on 29-30 April for the “WetenschapsEXPO” of the VUB and the second one on 27 November as part of the yearly Science Day, also of the VUB.

Both activities had regular polyhedra, or Platonic solids as they are sometimes called, as heroes of the day. The five of them form one of the summits of the classical space geometry. They have fascinated

Homo sapiens since centuries. Their first extant appearance comes from the Scottish Neolithic, around 2800 BCE as carved balls. The dodecahedron, the nicest of the five, was used as rolling dice by the Etruscans in the 6th century BCE, 200 years before Plato could philosophize about its merits.

The icosahedron, the dual of the dodecahedron, is less glamorous but still interesting. It is the starting point for constructing a shape; this was the subject of the first of our activities the ‘C60 fullerenes and footballs’. The semi-regular polyhedron behind these two objects was found by Archimedes. It is the truncated icosahedron, so that what remains of the triangular faces of the icosahedron are regular hexagons. It is precisely the shape of the smallest of the big carbon molecules with sixty carbon atoms. It is sometimes called a bucky-ball. Larger carbon molecules, the so-called nanotubes, are tubes with two half bucky-balls at their ends. Using Zometools it is possible to construct these polyhedra. It is an appropriate way to exercise one’s intellectual capacity and develop one’s spatial insight.

A participant at WetenschapsEXPO showed the projection of regular hyperpolyhedra in a four dimensional Euclidean space with dodecahedra or icoshedra as hyperfaces. This was an interesting complement, because only in three and four-dimensional Euclidian spaces does there exist polyhedra with pentagonal symmetry.



The November activity had again the regular polyhedra as subject but was more oriented towards their symmetry properties.

Let us number the summits of a tetrahedron from 1 to 4. Any of his symmetries (an isometry mapping the tetrahedron on itself) defines a permutation of the set $\{1, 2, 3, 4\}$. It is easy to see that you get all of them once. But Evariste Galois showed that the solution of a fourth degree equation depended on the properties of the group of all these permutations.

These properties are easy to find on the tetrahedron and so one proves that every algebraic equation of degree four is solvable by radicals. What happens for degree 5? A good candidate to look at is the dodecahedron, since it has symmetries of order 5. What can we number from 1 to 5? Kepler, who was fascinated by polyhedra, gave us the answer: one can fit exactly five cubes in a dodecahedron. So the group of symmetries of the dodecahedron is isomorphic to a subgroup of the permutations of $\{1,2,3,4,5\}$. The construction of the 5 cubes in a dodecahedron with Zometools is a real challenge for any good student. The advantage of working with Zometools (or any other proper geometrical set) is that it is more concrete than a drawing in a book.

The Institutes received a grant of the Flemish Community to contribute to the financing of these two activities. We are very thankful for this assistance.





Seminars

The list below gives the joint inter-university weekly seminars co-organized by the Theoretical Particle Physics Group of the VUB, the Service de Physique Théorique and the Service de Physique Théorique et Mathématique, both of the ULB, the High Energy Physics and Relativistic Field Theory group of the KUL, the Groupe de Mécanique et Gravitations at UMons, and the International Solvay Institutes.

The list also gives the group seminars of the research team of the Director.

February

A topological gauge theory for entropy and the emergence of hydrodynamics
Felix Haehl | Durham

Gauged Supergravity for AdS and Flat Space
Alessandra Gnechchi | KUL

Resuming instantons in $N = 2$ SCFT
Marco Billo | INFN Turin

Non-relativistic Hydrodynamics and Lifshitz Black Branes | Jelle Hartog | ULB

Pure Lovelock holographic superconductor
Olivera Miskovic | Pontificia Universidad Católica de Valparaiso

Black resonators & geons: evading black hole theorems and the path to cosmic censorship violation | Oscar Dias | Southampton

Supersymmetric AdS backgrounds and their moduli spaces | Jan Louis | DESY

March

Field Theory Description of Topological States of Matter | Andrea Cappelli | INFN Florence

A Monotonicity Theorem for Two-dimensional Boundaries and Defects
Andy O'Bannon | Southampton

Scrambling of locally perturbed thermal states | Joan Simon | Edinburgh

Correlation Functions of Coulomb Branch Operators | Zohar Komargodski

Resolved Gravity Duals of $N=4$ Quiver Field Theories in $2+1$ d
William Cottrell | Wisconsin

Old and new scaling laws in quantum quench
Sumit Das | Kentucky

An exact result for vacuum decay
Guilherme Pimentel

Relating DFT to $N=2$ gauged supergravity
Erik Plauschinn

April

Bootstrapping the S-matrix
Miguel Paulos | CERN

A goldstino at the bottom of the cascade
Matteo Bertolini | SISS, Trieste

On non-extremal smooth geometries and gravitational instantons | Bidisha Chakrabarty

Causality in 3D massive gravity theories
Carolina Gomez

Higher-Spin Symmetries: from quantum gravity to boiling water
Evgeny Skvortsov | LMU Munich

Defects and universality in applications of AdS/CFT to condensed matter physics
Johanna Erdmenger | MPI Munich

A few algebraic surprises in Anti-de Sitter space
Oleg Evnin | Chulalongkorn University and VUB

Poles in three-point functions
Joseph Minahan | Uppsala

May

Tunneling into Microstate Geometries
Daniel Mayerson | Michigan

The Information Paradox revisited
Malcolm Perry | Cambridge

June

Hexagons and Three-Point Functions

Benjamin Basso | ENS Paris

Relating Double Field Theory to $N=2$ gauged supergravity | Erik Plauschinn | LMU Munich

Some lessons from the connection between asymptotic symmetries and soft theorems

Eduardo Conde | Seoul National University

Scalling regime beyond the BPS bound

Guillaume Bossard

Conformal Higher Spins and Twistor Actions

Tristan McLoughlin

July

The Cosmological Slavnov-Taylor Identity

from BRST Symmetry in Single-Field Inflation

Andrea Quadri

September

From Conformal to Einstein Gravity

Rodrigo Olea

Hypersymmetry | Javier Matulich

October

The $N=2$ superconformal bootstrap

Pedro Liendo | DESY

The Power of Supergravity Solutions

Bert Verhocke | KU Leuven

T-branes and 3d Mirror Symmetry

Roberto Valandro | Trieste

Hydrodynamics and its destruction

Saso Grozdanov | Leiden

Black Holes and Random Matrices

Masanori Hanada

Black holes at large D : Things we've learned

so far | Roberto Emparan | Barcelona

Hexagons and Three-Point Functions

Benjamin Basso | ENS Paris

T-Duality and scattering of stringy states

Jnan Maharana

BGG sequences, metric projective geometry

and partially massless gauge theories

Emanuele Latini | University of Bologna

Higher Spins and Strings

Matthias Gaberdiel | ETH Zurich

November

Hilbert Series and aspects of the moduli

space of instantons on CP^2

Alessandro Pini

Codimension-2 Microstates of Black Holes

Masaki Shigemori | Queen Mary

Black hole instabilities and the formation

of singularities in general relativity

Pau Figueras | Queen Mary

Automorphic String Amplitudes

Hendrik Gustafsson

Relative entropy of excited states in

conformal field theories | Gábor Sárosi | VUB

Out of equilibrium steady states in conformal

field theories | Amos Yarom | Technion

A causality in Massive Gravity: another brick

in the wall? | Gustavo Lucena

Classicalization and Dual Theory

Cesar Gomez | Madrid

M5-branes on an elliptic fibration

Benjamin Assel | CERN

Holography in Two-Dimensional Dilaton

Gravity | Jakob Salzer

Internal structure of black holes

Amitabh Virmani

E theory | Peter West

Segmented strings | David Vegh | Utrecht

The primordial universe as a particle detector

Guilherme Pimentel | Amsterdam

December

Causality, Non-Locality and Negative

Refraction | Davide Forcella

Non-AdS Higher Spin Gravity

Stefan Prohazka

String theory on AdS₃ and Higher Spins

Juan Jottar | ETH Zurich

Deforming the web of generalized free CFTs

Anastasios Petkou | Aristotle University of

Thessaloniki

Research

$\mu = 20000$ $\sigma = 2$
 $N(\mu, \sigma)$

Research

These sections describe successively:

- the research carried in the groups of Professors Marc Henneaux, Director, and Alexander Sevrin, Deputy-Director for Physics and Scientific Secretary of the International Scientific Committee for Physics (Research on gravitation, strings and cosmology)
- the research carried in the group of Professor Anne De Wit, Scientific Secretary of the International Scientific Committee for Chemistry
- research in Chemistry carried out in the group of Professor Jan Steyaert and Professor Emeritus Lode Wyns, Deputy-Director for Chemistry
- the research highlights of other scientists connected with the Institutes

Research on Gravitation, String Theory and Cosmology

Groups of Professors Marc Henneaux | ULB
and Alexander Sevrin | VUB

Researchers

Permanent Members

Riccardo Argurio | ULB
Vijay Balasubramanian (10 %) | VUB
Glenn Barnich | ULB
Andrés Collinucci | ULB
Geoffrey Compère | ULB
Ben Craps | VUB
Stéphane Detournay | ULB
Oleg Evnin (10 %) | VUB
Frank Ferrari | ULB
Marc Henneaux | ULB
Laura Lopez Honorez (10 %) | VUB
Alberto Mariotti | VUB
Kentarou Mawatari (10 %) | VUB
Alexander Sevrin | VUB
Daniel Thompson (10 %) | VUB

Visiting Professor

Gastón Giribet | Sabbatical, Buenos Aires

Postdoctoral Members

Jay Armas | ULB
Tatsuo Azeyanagi | ULB
Rudranil Basu | ULB
Chris Blair | VUB
Andrea Campoleoni | ULB
Simone Giacomelli | ULB
Adolfo Guarino | ULB
Jelle Hartong | ULB
Michael Kay | ULB
Alexey Koshelev | VUB | Universidade da Beira Interior, Portugal
Laetitia Leduc | ULB
Jiang Long | ULB
Christoffer Petersson | ULB
Charles Rabideau | VUB joint postdoc with UPenn
Max Riegler | ULB
Gábor Sárosi | VUB joint postdoc with UPenn
Charlotte Sleight | ULB
Massimo Taronna | ULB
Hongbao Zhang | VUB

Graduate Students

Dries Coone | VUB
Karen De Causmaecker | VUB
Tim De Jonckheere | VUB
Saskia Demulder | VUB
Laura Donnay | ULB
Sibylle Driezen | VUB
Anxo Fariña Biasi | VUB visiting PhD student
U. de Santiago de Compostela, Spain
Marco Fazzi | ULB
Paolo Gregori | ULB
Victor Lekeu | ULB
Amaury Leonard | ULB
Jonathan Lindgren | ULB-VUB
Vincent Luyten | VUB
Pujian Mao | ULB
Andrea Marzolla | ULB
Daniel Naegels | ULB
Kévin Nguyen | VUB
Blagoje Oblak | ULB
Roberto Oliveri | ULB
Pablo Pais | ULB
Arash Ranjbar | ULB
Romain Ruzziconi | ULB
Guillaume Valette | ULB
Matthias Vereecken | VUB
Céline Zwickel | ULB

Master Students

John Bekx | VUB
Alain Buisseret | ULB
Marine De Clerck | VUB
Thomas Evrard | ULB
Adrien Fiorucci | ULB
Antoine Pasternak | ULB
Jeriek Van Den Abeele | VUB
Jonas Verhellen | VUB

Research Summary

Of all the fundamental forces (electromagnetism, gravitation, weak and strong nuclear forces), gravity remains the most mysterious. In spite of its remarkable successes, Einstein's general theory of relativity, which has led to an unprecedented geometrization of physics, is an unfinished revolution. A major challenge of modern physics is to reconcile quantum mechanics and Einstein's gravity. This will undoubtedly need new developments that will go beyond Einstein's revolution. Fully unravelling the mysteries of the gravitational force is a long-term research goal.

The group has a long-standing interest and a demonstrated expertise in quantum gravity, quantum field theory, string theory and M-theory, black holes, cosmology, the cosmological constant problem ("dark energy") and the novel mathematical structures underlying these questions. These challenging areas raise many of the most profound issues in theoretical physics.

A central thread in the study of gravity and the fundamental interactions is the concept of symmetry (global and local). Some of the general background is given below.

General Framework

The standard model of particle physics is based on quantum field theory, a framework that reconciles Poincaré invariance with quantum mechanics and allows one to understand the electromagnetic and the two types of nuclear interactions. The fourth fundamental interaction, gravitation, is described by Einstein's theory of general relativity. Experiments as well as theoretical arguments indicate that neither the standard model, nor general relativity can be complete.

Purely theoretical attempts at generalizations are constrained, of course, by mathematical consistency and the need to incorporate the previous theories in the domains where they have been successful. Additional guiding principles are needed, though. Symmetry is such a principle and pervades most of the research carried out in theoretical high energy physics.

The Yang-Mills type theories for the three microscopic forces of elementary particle physics are invariant under Poincaré symmetries, the symmetry group of flat space-time. These theories admit in addition certain internal symmetries known as gauge symmetries. In general relativity, gravitation arises when going from a flat to a curved spacetime, and Poincaré symmetries become part of the gauge group of diffeomorphisms.

In models that go beyond the existing theories, other symmetries can come to the front.

(i) Supersymmetry

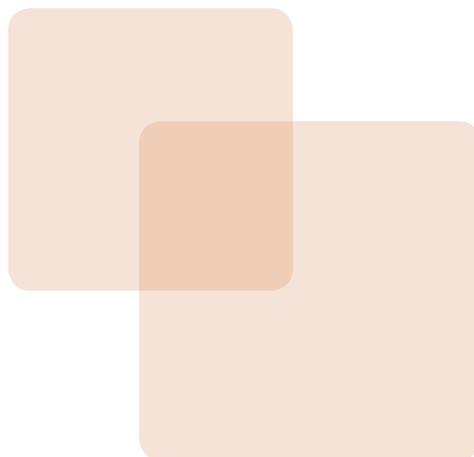
Supersymmetry is a natural extension of Poincaré symmetry in the presence of fermionic matter fields. One objective of the Large Hadron Collider at CERN in Geneva is to test supersymmetric extensions of the standard model.

Supersymmetry is also an important ingredient of string theory, a model for unification of the four fundamental interactions and for a microscopic formulation of gravity. At low energy, higher dimensional theories of gravitation emerge that include supersymmetry as part of their gauge group together with supersymmetric extensions of Yang-Mills gauge theories.

(ii) Dualities

One of the first theoretical extensions of Maxwell's theory of electromagnetism has been the inclusion of magnetic sources. The introduction of such sources is motivated by the desire to preserve invariance under duality rotations, a symmetry of the source-free equations. The solution that is dual to the Coulomb solution describing a static point-particle electron is a magnetic monopole. In some sense, black hole solutions in gravitational theories are the analog of the Coulomb solution to Maxwell's theory.

In nonlinear theories like Yang-Mills theories, dualities relate a strongly coupled regime to one at weak coupling, where standard perturbative computations may be performed. In supersymmetric situations, these dualities become tractable. Finally, dualities between different string theories as well as holographic duality between gauge and gravity theories feature prominently in most of the recent developments in string theory.



(iii) Hidden symmetries

Hidden symmetries in gravity and string theory arise in compactifications of supergravity theories and among the string duality groups. The algebraic structure of these symmetries is related to infinite-dimensional Lorentzian Kac-Moody algebras, in particular the algebras E10 and E11.

(iv) Higher spin symmetries

Higher spin gauge fields (massless fields with spins greater than the spin 2 of the graviton) play a central role in many searches for a quantum-mechanically consistent formulation of gravity. For instance they appear in the zero tension limit of string theory. High spin gauge field theories are described by a huge “higher spin symmetry”.

The symmetries described in (i)-(iv) have strong but still somewhat mysterious connections with each other.

Many questions outlined above constitute central themes of three ERC grants (Advanced Grants SyDuGraM and High-Spin-Grav of Marc Henneaux, and Starting Grant HoloBHC of Geoffrey Compère).

Research carried out in 2016

We have continued our research along the general directions outlined above. This has led to 134 published papers and preprints submitted for publication. These are listed on pages 160-167. Specific achievements by some researchers from the group are described in the subsequent pages.

Support to the research of the Director

The research of the director and of his group has benefited, as in the previous years, of gifts from the Solvay family and the Solvay Group. This support was extended by additional gifts from Messrs. Collen, de Selliers de Moranville and Jaumotte. This generous support was precious to cover international collaborations, the organization of workshops as well as doctoral and postdoctoral grants to researchers. It is most gratefully acknowledged.

Marina Solvay Fellowship

Thanks to a special gift of Mrs. Marina Solvay, the “Marina Solvay Fellowship” was created in 2012. The fellowship enables a brilliant young researcher to pursue her or his career as a postdoctoral fellow in the group of “physique théorique et mathématique” of the ULB.

List of Marina Solvay fellows

Waldemar Schulgin (2012-2014)

David Tempo (2015)

Jelle Hartong (2016)

Dr. Jelle Hartong was the third holder of the Marina Solvay fellowship, in 2016. He got his PhD degree at the University of Groningen in 2008. After postdoctoral stays at the Albert Einstein Center for Fundamental Physics (AEC) at the University of Bern (Switzerland), and at the Niels Bohr Institute in Copenhagen (Denmark), he joined the UBL group.

As explained in his research description, his work deals with holography in new non relativistic contexts, where he has become one of the world leading experts.



Researchers who directly benefited from the support to the research of the Director

Holography and strongly coupled fluid dynamics

Jelle Hartong

Postdoctoral Member | ULB

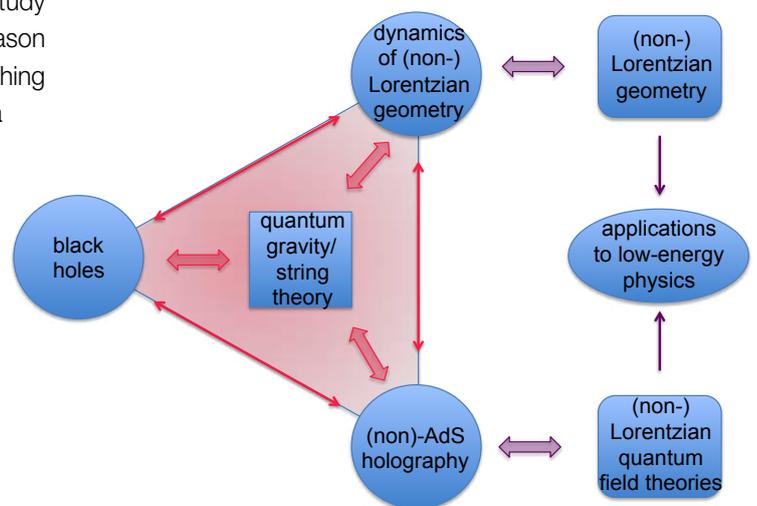
One of the key problems in theoretical physics concerns the description of systems where the interactions between the various parts are strong. When the interactions are weak there exist many mathematical methods that allow one to compute physical quantities to any desired accuracy. However for strong coupling no mathematical tools are available and one is forced to resort to numerical methods, very crude approximations or some ad hoc phenomenological model.

Some of the important strong coupling problems of current interest appear in low-energy physics and have to do with the so-called strange metals in condensed matter physics. Strange metals are phases of quantum matter that are not described by any existing techniques. An example of such a phase is high- T_c superconductivity.

My research uses modern techniques from high-energy theory that can be used to study strong coupling problems better. The reason this works is because there is something very universal about the physics of a quantum critical phase of matter and it is through this universality that new techniques from high-energy theory can be applied to strange metals. These new techniques are known as holography, a subject that can be viewed as an approach to quantum gravity and that has strong relations with string theory.

Holography is an equivalence between a theory containing gravity and a theory describing matter without gravity. Further it maps the strong coupling phase of the matter theory to classical gravity theories such as Einstein's theory of general relativity. For example it has been shown that certain black holes behave similarly to superconductors.

Until recently we only knew how to do holography in detail for so-called anti-de Sitter (AdS) space-times. In my research I have developed a new set of mathematical tools, that go under the general name of non-Lorentzian geometry, that allow one to study a wider range of holographic dualities.



Jelle Hartong

For applications to condensed matter physics we need to understand holography for specific non-AdS space-times such as the so-called Lifshitz space-times. The techniques that I developed allow one to do exactly that.

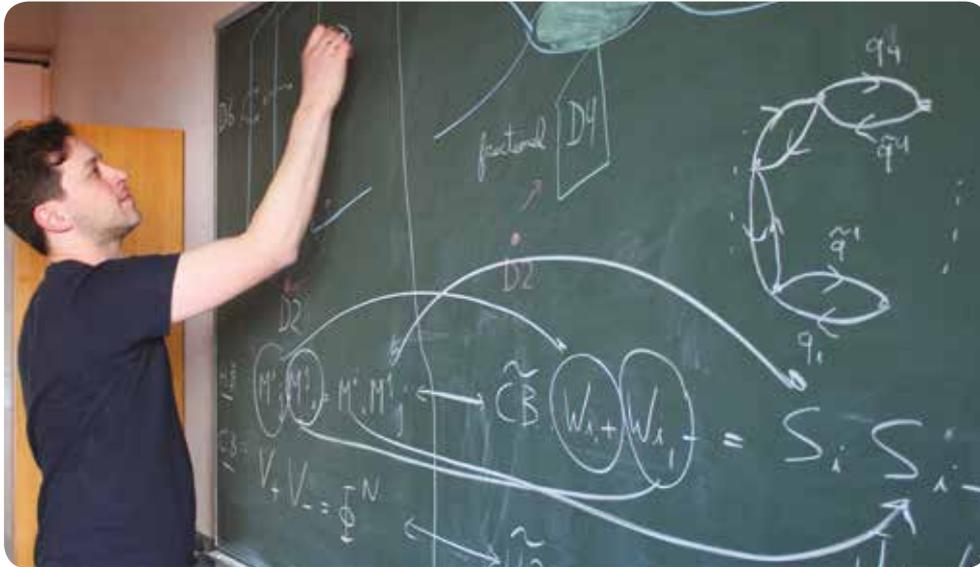
An important regime in which we understand holography well, is the so-called fluid/gravity correspondence. This concerns moving black hole type objects on the gravitational side of the correspondence and strongly coupled fluid dynamics on the other side of the correspondence. At the same time there is good theoretical motivation to expect that strange metals should have a regime in which the transport of electrons can be described by a fluid model. This fluid model should provide an effective description of the theory (some non-Lorentzian quantum field theory) describing the strange metal phase. The various topics and their interrelations are shown in the figure. The goal of my research is thus to construct the general theory of such fluids using input from various holographic models.

Arash Ranjbar
Graduate Student I ULB

Arash Ranjbar is doing research towards his PhD degree under the supervision of Marc Henneaux (ULB). He is working on gauged supergravity models and string theory. He is expected to defend his thesis in 2018.

Research Interests of some other members

Andrés Collinucci
Permanent Member I ULB



One of the greatest insights into nature was Einstein's realization that answers to deep questions come from geometry.

Geometry makes its entrance

Before the inception of the theory of General Relativity, gravity was thought to be a force of nature similar to electromagnetism. However, Einstein showed that the language of Riemannian geometry truly captures its essence. By treating space and time as different directions, differently directed threads in the fabric of the universe, the laws of nature were recast into a form that not only clarified what we knew, but predicted unexpected phenomena, such as the bending of light when it shoots past a star, or the formation of black holes.

The missing piece

As great as this discovery was, it turned out to be only a piece of the puzzle. There are other forces of nature: electromagnetism, the weak interaction and the strong interaction. The latter, which is responsible for the binding of nuclei (which would otherwise repel electrically), is poorly understood. The difficulty comes from the fact that this force acts strongly (as the name suggests) between minuscule objects: Quarks. It falls deeply into the realm of quantum mechanics, a world where classical intuition and classical computational methods fall short.

The fact that the strong interaction between quarks is so notoriously intractable is one of the longstanding problems in physics.

Geometry triumphantly returns

In the 1990s, two prominent physicists, Seiberg and Witten, discovered once again the motto: “Geometry is the natural language for physics”. They took a simplified version of the problem, known as $N=2$ gauge quantum field theory, and recast it into a geometric formalism. One way to think of what they did is via a simpler example. Suppose you are studying water. One thing you might want to do is explore what happens to it when you fiddle with its temperature and its pressure independently. After taking data samples, you would make a two-dimensional plot, one axis for each parameter, and you would discover that there are lines separating the plot into sectors according to the various phases of water (liquid, gas, etc.).

Seiberg and Witten studied what happens when the “fields” describing the strong force take on various background values. But, instead of a simple flat two-dimensional plot, their analysis led them to a rich variety of intricate geometries. These fall in the category of “complex algebraic geometry”. Once the appropriate geometry is assigned to a given theory, its quantum equations are magically solved, providing incredibly detailed information about what is going on physically.

String theory as an all-encompassing framework

My current research is in the field of “string theory”. This is a candidate framework for understanding both gravity and quantum field theory together in a consistent way. Einstein’s theory of General Relativity teaches us how to study massive objects such as stars or black holes. On the other hand, quantum field theory, and the various versions solved by Seiberg and Witten’s methods, teach us about the tiniest constituents of matter. However, ultimately, even stars and black holes are made of these tiny constituents, so it doesn’t make sense to have two separate sets of laws. So far, the only viable framework at unifying the laws of gravity with those of quarks and leptons is string theory. Its main postulate is that particles of matter are actually very tiny vibrating strings. As innocent as this assumption sounds, the theoretical ramifications pretty quickly take epic proportions. For instance, we learn that our universe would actually have not four, but ten dimensions. Notions of size become fuzzy, as predicted by “T-duality”. Models describing seemingly different physical situations turn out to have correspondences with each other known as “dualities”. Many weird phenomena pop up in string theory. But one common thread persists: Geometry is *almost* always the right language to understand things.

A couple of years after “Seiberg-Witten theory” saw the light of day, Cumrun Vafa, a prominent physicist at Harvard, invented “F-theory”. This is in a way the culmination of all of the ideas I have described so far. F-theory is a version of string theory that combines Einstein’s geometric description of our universe, with Seiberg and Witten’s geometrization of gauge theories. In Vafa’s description, spacetime is combined with the space of parameters in an elegant way, into what is known in algebraic geometry as an “elliptic fibration”. This combined space exhibits a family of tori (the surfaces of donuts), one for each point of our spacetime. The important physical information is encoded in how this family of tori varies over spacetime. As you move along spacetime, this torus changes shape slightly, until something snaps, and one of its handles pinches off. This signals the presence of interesting physical objects, known as 7-branes, which are key ingredients of string theory.

What is amazing about this way of phrasing the laws of physics, is that it is simple in its inception, but very powerful and detailed in its output. It allows us to exploit the techniques of algebraic geometry, a field developed over centuries by mathematicians, to make concrete calculations about physical quantities.

But this whole compelling story I have been describing is far from settled. F-theory is still in its infancy, and we have barely understood all the rules. We are now at the same stage as someone who is learning the allowed moves in chess, with the goal of winning a major competition in the future. It is precisely the missing pieces of the puzzle that I find fascinating. For instance, as I have written, geometry encodes important physical

information about a system. This mantra is so deeply seeded in string theorists and has become so ordinary, that interesting research usually contains phrases such as “non-geometric” in the title, to highlight the urge to go beyond this paradigm.

Going beyond the geometric

My current research is rooted in this urge to go beyond purely geometric methods. The picture painted by F-theory, of a theory of gravity and of the other forces of nature described by geometry, needs to be supplemented with a much richer story. Since my arrival at the ULB, I have been working on devising a new formalism, which uses what are known as Eisenbud’s “matrix factorizations”, to give a new perspective on these issues. The motivation for this is that F-theory only captures a small part of the interesting physical data, leaving out many interesting phenomena, and very generic expected features in gauge theories.

Most of the information captured geometrically encodes the positions of 7-branes: These are basic heavy objects in string theory that may be key ingredients in explaining particle physics.

Relative displacements of 7-branes are translated into deforming the F-theory geometry by stretching or bending the space. In technical gauge theory terms, this corresponds to giving vacuum expectation values to adjoint scalars along a Cartan subalgebra of the gauge group.

However, a lot of information is not captured by this formalism. For instance, when gauge theories have adjoint scalar fields that acquire vacuum expectation values, these are always assumed to be diagonalizable. Yet, we all learn in linear algebra that a general matrix need not be diagonalizable. When a scalar takes an upper triangular form, known in the physics literature as a “T-brane”, we are in uncharted waters. In string theory terms, a bound state between 7-branes is created. All of the beautiful geometric data from F-theory becomes incomplete and misleading, unless we shift our perspective. For instance, it is usually thought that gauge groups and the matter contents of the gauge theory sector are entirely encoded by the singularities of the F-theory space. As soon as non-Abelian effects come into play, such as T-branes, this goes out the window. A gauge group could be completely broken by a T-brane, even though the geometry is highly singular.

In works conducted with Raffaele Savelli, a physicist from Saclay in Paris, I have seen hints that Matrix factorizations, as discovered by Eisenbud, might bring about the right paradigm shift. This is a subfield in algebraic geometry that adds natural structures on complex algebraic spaces that have certain singularities. Precisely the types of singularities of interest to physicists, Gorenstein singularities, often admit descriptions as hypersurfaces in an ambient space. The hypersurface equation can be written as the product of two matrices, and each such pair of matrices is called a matrix factorization. The various matrix factorizations have an

interlinked structure that can be packaged as a quiver. In physical terms, one is enhancing the information about the singularity by adding probe D-branes to it.

In recent work with physicists abroad (R. Savelli, and Roberto Valandro from ICTP and the University of Trieste), and a collaborator at the ULB, (Simone Giacomelli), we pushed this point of view by studying what D2-branes “see” when they probe T-brane bound states between D6-branes. We found that this corresponds in M-theory to deforming the UV Lagrangian of the probe M2-brane by a monopole operator. We have only initiated the investigation, but our initial results have raised new interesting questions about N=2 gauge theories in three dimensions. For instance, how are quantum enhanced flavor symmetries seen in theories that do not enjoy N=4 supersymmetry?

Can we understand what an M2-brane probing an isolated threefold or even fourfold singularity sees?

Can we understand more complex T-branes in theories with exceptional gauge groups?

Finally and most importantly, can this help us find new definition of F-theory as a non-perturbative formulation of string theory?

If we can answer this last question, we will have a chance at describing UV complete theories of matter that can be combined with quantum gravity.

Sibylle Driezen
PhD Student | VUB

One of the most miraculous achievements of physics is that, over centuries, we have gained great insights in very diverse phenomena by explaining them through only four fundamental forces. Still there are several aspects, such as dark matter, black holes and the big bang, that remain unresolved by the two celebrated pillars of modern physics: the Standard Model and general relativity. Therefore, theoreticians were confronted with the difficult task to find a theory that goes beyond the Standard Model and, in the end, might even unify it with general relativity. With this in mind, theoretical developments such as supersymmetry, supergravity and string theory received a great deal of attention. One of the most promising fields is a supersymmetric string theory, where it is assumed that the elementary particles behave like tiny strings. This simple premise will lead to several dramatic consequences: the theory automatically describes gravity together with gauge theories and introducing supersymmetry also ensures full quantum consistency.

In the meanwhile, however, string theory predicts that the number of spacetime dimensions has to exceed four and its key characteristics will only come at play at experimentally inaccessible energies, making the theory's credibility quite small. Encouraged by its excellent properties, research in string theory has not been disregarded, and a number of ways have been found to circumvent the mentioned problems. For example, we can recover our four-dimensional world by making the extra dimensions too small (and thus compactified) or too dark (i.e. weakly interacting with our world) to be observed.

Perseverance lead to numerous new insights also in other scientific fields, for instance, in strongly coupled physical systems using the AdS/CFT correspondence or in fundamental mathematics due to the discovery of mirror symmetry.



“ My personal research focusses on other peculiar theoretical concepts in string theory. In particular, I study the connections between various manifestly supersymmetric extensions of string theory, the existence of a special duality called T-duality and the geometrical structure of spacetime. Recently, I also became interested in how these ideas relate to the field of (deformed) integrable models.”

T-duality

Duality symmetries are extremely important symmetries in theoretical physics. They relate seemingly very different theories that, however, describe the same physics. In this way, phenomena which are hard to understand in one framework, could be formulated very easily in the other framework, which greatly helps in unravelling the mysteries. String theory exhibits many different duality symmetries. A famous example is the so called AdS/CFT correspondence which relates a weakly coupled quantum gravity (formulated as a string theory) to a strongly coupled conformal field theory and vice versa. In my research, I study the presence of T-duality in string theory. In general, this duality tells us that the strings do not notice any physical distinction when they are propagating in certain completely different spacetimes. The existence of T-duality is due entirely to the extended nature of the string and the possibility of compactified extra dimensions predicted by string theory. Closed strings especially can - in contrast to ordinary point particles - wind around these compact dimensions, as illustrated by figure 1.

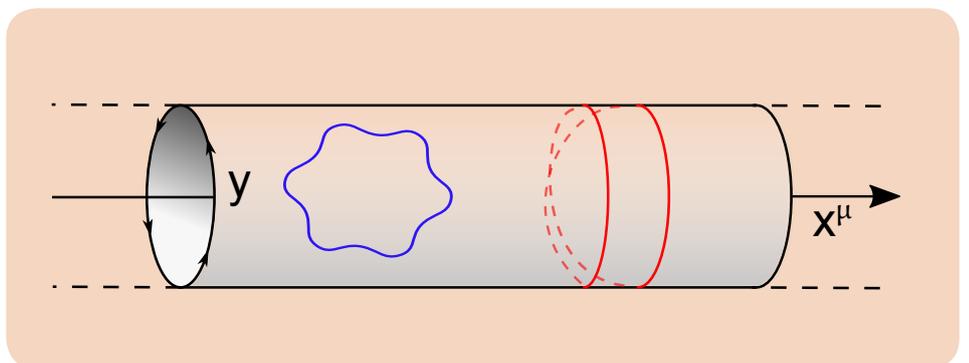


Fig. 1 Illustration of a closed string which is (blue) not wound or (red) wound twice around the compact dimension y

This possibility has a direct consequence to the mass spectrum of the string states, where T-duality was first observed. Explicitly, the duality exchanges the string winding modes for its momentum modes while exchanging a small compact spacetime for a large compact spacetime (or vice versa) to render the mass spectrum invariant. In later years it was shown that T-duality is indeed a true symmetry of the full theory.

It is clear that the strings experience the geometry of spacetime in a very different way compared to point particles. T-duality is however reminiscent of the Lorentz symmetry in special relativity. There, our notions of space and time were scrambled into each other, and in order to understand the physics better, we introduced the concept of spacetime. In the same spirit, we can try to treat the momentum and winding modes of the string on an equal footing. In such a description, T-duality would be a manifest symmetry and the strings would be understood in a very different geometrical language. Together with Chris Blair, Alexander Sevrin and Daniel Thompson, my research consists of making a manifest T-dual and consistent description of various supersymmetric extensions of a string model. We developed a different approach to this question in the case where there are no supersymmetries present and applied this successfully to the $N=(0,1)$ supersymmetric string. When more supersymmetries are included, however, a lot of puzzles remain.

Supersymmetric string models in superspace

In addition, I perform research in string-inspired models where the number of supersymmetries is manifest by formulating the model in superspace. The advantage of these formulations is that the model's geometrical properties become fully transparent. On the other hand, the number of explicit examples of such models is rather scarce. Using also the ideas of T-duality, we have been able to unravel certain parts of the unknown superspace-lagrangian of a new model formulated on a group manifold with a high number of dimensions. Nowadays, one of my new interests lies within another direction of these models, namely: their integrability. This new research focusses on deforming the known superspace-models using the ideas of integrability while preserving the number of supersymmetries. The interesting aspects of these deformations is that one could in principle find a large class of new, exactly solvable, superspace-models and as a consequence novel supergravity solutions as well.

Gábor Sárosi

VUB joint Postdoc with UPenn

The 20th century brought unprecedented advances in our understanding of natural phenomena. The Standard Model of particle physics – a quantum field theory – accurately describes every known particle and almost all observed forces among them down to the scale of 10^{-19}m under a unifying principle called gauge symmetry. However, this beautiful model fails to incorporate the force known to mankind for the longest time, the gravitational force. The current state of the art description of this force is Einstein's general relativity, a classical field theory, describing celestial dynamics with a very high precision. However, when we consider spacetimes varying on the Planck scale ($\sim 10^{-35}\text{m}$), quantum effects become important and we need a quantum theory of gravity.

Since gravity itself shows a certain kind of gauge symmetry, it is a natural idea to promote it to a quantum field theory, just like the Standard Model. However, this naive approach does not work due to the heavy dependence of such an 'effective field theory' on the details of its UV completion. On one hand this is our luck, as gravitational phenomena provide a window to the dynamics of degrees of freedom with the highest possible energies, but on the other hand observation of quantum gravitational effects in accelerators seems way out of reach of current experimental technology and there is no reason to believe that this will change in the upcoming centuries.



Black holes and the information problem

Our task to understand quantum gravity then might seem hopeless. However, one such window to the physics of the ultraviolet that gravity provides is the existence of black holes. These objects are predicted by general relativity, and they are realized in nature as was recently confirmed by the LIGO experiment. A very important feature of black holes is the so called information problem. When coupled to quantum fields, a classical black hole is predicted to evaporate into perfectly thermal radiation, thus leading to a breakdown of unitary time evolution, a basic principle of quantum mechanics. This signals that quantum effects are fundamental in the description of black holes and they are not just confined to regions with curvature singularities, where they are naively expected to become important. Moreover, a fundamental discovery from the seventies is that black holes have a thermodynamical entropy. Any theory of quantum gravity must therefore be able to account for this entropy by counting microstates and must also provide a mechanism for unitarity restoration in the evaporation process. In this sense, black holes are our 'theoretical laboratories' to test our models of quantum gravity.

String theory and AdS/CFT

We are in possession for some time now of a particular theoretically consistent model incorporating gravitation – and a lot else – called string theory. While this theory is yet to make direct contact with experimental high energy physics, nevertheless one can ask how the theory resolves the above questions about black holes and how in general classical gravitation arises in the appropriate limit of the quantum theory. These are very difficult questions to answer and they form the basis of a significant part of string theory research of the last couple of decades, over which a lot of progress has been made. A particularly concrete and successful setup is the AdS/CFT correspondence, which states that string theory in asymptotically Anti de Sitter (AdS) spacetime in $d + 1$ dimensions is described by ordinary conformal field theory (CFT) on its d dimensional boundary, according to a – still incomplete – dictionary. Recent insights into this dictionary suggest that the classical spacetime is an effective description of a large number of strongly interacting non- gravitational quantum degrees of freedom, and that the structure of quantum entanglement in the states of the CFT play a prominent role in this effective description.

Entanglement in conformal field theories

One of the goals of my research is to understand more this relation between entanglement and geometry. For this reason, with my collaborator Tomonori Ugajin (KITP, Santa Barbara), we study and calculate certain entanglement related quantities in generic states of conformal field theories. An object of central importance is the so called modular Hamiltonian, which encodes information about the entanglement structure of the state, moreover, it can be used to quantify distinguishability of states under restricted quantum measurements. This latter property is also related to the information problem. We have already calculated the modular Hamiltonian of small ball shaped regions for generic states of a CFT and we hope to extend the validity of these calculations and understand them in terms of gravitational variables in present research.

Energy spectra of black holes and chaos

A particularly sharp version of the black hole information problem is the eternal decay of two point functions in an asymptotically AdS black hole background. Such a behaviour is forbidden for unitary quantum mechanical systems with a finite entropy. The question is then how quantum gravity restores unitarity at late times in the two point function. There is a great deal of evidence that the microscopic dynamics of a black hole must be highly chaotic, from which the general expectation is that two point functions display erratic fluctuation at late times, with a mean value changing very slowly in time according to random matrix theory, showing a linear rise after the departure from the classical gravity result, followed by a saturation at very late (exponential in the entropy) times.

This picture was confirmed recently in a tractable toy model of black holes, the Sachdev-Ye-Kitaev model. In order to gain more insight for the black holes of string theory, in a recent work, my collaborators V. Balasubramanian (UPenn/VUB), B. Czech (IAS), B. Craps (VUB) and I have studied the two point function in the background of particular stringy black holes, which are bound states of D1 and D5 branes wrapping five extra dimensions. Presently, we only have access to this two point function in the tensionless limit, which corresponds to an integrable field theory rather than a chaotic one, and therefore a highly non-geometric limit of the gravitational theory.

Nevertheless, the two point function in question reproduces the gravitational answer for early times and shows a qualitatively similar behaviour as the one expected from random matrix theory at very late times, with the relevant time scales modified due to integrability. Our present research focuses on turning on interactions perturbatively and hence moving closer to black holes of classical gravity. The ultimate goal here is to understand the late time behaviour of these two point functions in terms of bulk string theory.

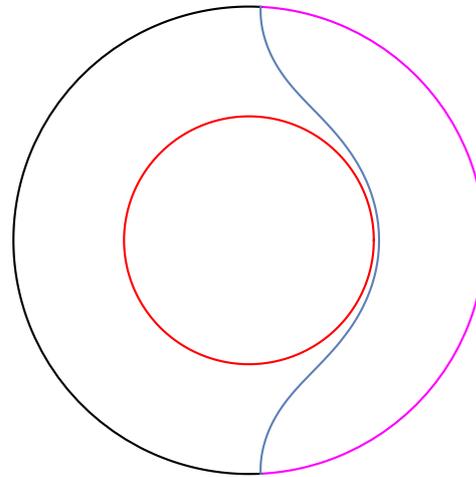
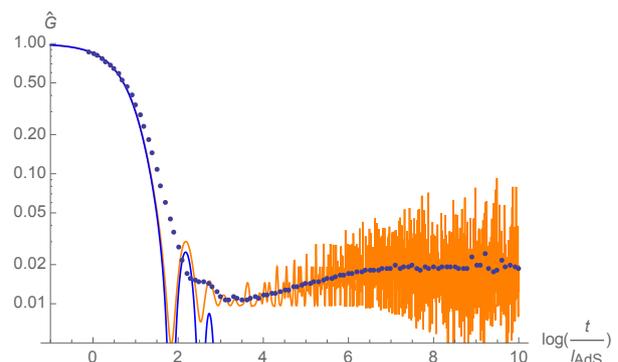


Fig. 1: Conformal diagram of a spatial slice of a black hole spacetime in three dimensional asymptotically AdS space. The union of the black and purple curves is the boundary where the dual two dimensional CFT lives. The red curve is the horizon of the black hole. A famous result of Ryu and Takayanagi shows that the von Neumann entropy of the purple region in the CFT can be computed by the area (here length) of the minimal surface (blue) anchored at the boundaries of the region. Knowledge of the modular Hamiltonian of the purple region contains this information and in addition it can be used to quantify the distinguishability of the different microstates creating the geometric background under measurements restricted to the region between the blue and the purple curve.

Fig. 2: Log-log plot of a two point function of a typical two charge D1D5 black hole microstate (orange) versus the corresponding gravitational two point function (blue). The latter shows an eternal decay while the former displays erratic fluctuations at late times. An appropriate time average of the orange curve (blue dots) displays qualitatively similar behaviour to the one following from a random matrix spectrum, with modified time scales due to integrability.



Appraisals and Prizes | Thesis defended in 2016

Appraisals and Prizes

Saskia Demulder | VUB won a 2016 Solvay Award.

Saskia Demulder | VUB received the 2016 prize for the best Master Thesis from the Belgian Physical Society.

Sibylle Driezen | VUB received the 2016 prize for the best Master Thesis from the Belgian Physical Society.

Romain Ruzziconi | ULB received the 2016 Robert Brout Prize.

Thesis defended in 2016

Karen De Causmaecker | VUB – “Unconventional Signatures of Supersymmetry” – 22 August 2016 (thesis advisor: Prof. Jorgen D’Hondt).

Laura Donnay | ULB – “Symmetries and dynamics for non-AdS backgrounds in three-dimensional gravity” – 11 May 2016 (thesis advisor: Prof. Glenn Barnich).

Marco Fazzi | ULB – “Higher-dimensional field theories from type II supergravity” – 4 July 2016 (thesis advisor: Prof. Andrés Collinucci).

Pujian Mao | ULB – “New Applications of Asymptotic Symmetries Involving Maxwell Fields” – 28 September 2016 (thesis advisor: Prof. Glenn Barnich).

Blagoje Oblak | ULB – “BMS Particles in Three Dimensions” 24 June 2016 (thesis advisor: Prof. Glenn Barnich).

Fellowships

Chris Blair received an FWO postdoctoral fellowship.

Tim De Jonckheere obtained a 2-year extension of his FWO “aspirant” PhD fellowship.

Sibylle Driezen received an FWO “aspirant” PhD fellowship.

Laura Lopez Honorez obtained a permanent FNRS research position at the ULB, she keeps her 10 % professorship at the VUB (she was also awarded with a 3-year extension of her FWO postdoctoral fellowship which she did not accept).

Daniel Thompson received a prestigious Royal Society University Research Fellowship at the University of Swansea, he keeps his 10 % professorship at the VUB.

Matthias Vereecken obtained a 2-year extension of his FWO “aspirant” PhD fellowship.

Talks at conferences, seminars and schools

Riccardo Argurio

A Holographic Perspective on Symmetry Breaking
University of Amsterdam, The Netherlands
November 22

Vijay Balasubramanian

The Maps Inside Your Head - Diversity and Self-Organization of Neural Circuits
ICTP-SAIFR, Sao Paolo, Brazil
January 25-29 (5 lectures)

Is there a limit to human knowledge
New York Academy of Sciences, USA
April 10

Novel forms of entanglement and spacetime
YITP, Kyoto University, Japan – June

Adaptive molecular sensing in the olfactory and immune systems
Solvay Institutes, Brussels, Belgium – July

Poster: *Disorder and compressive sensing in the olfactory system*
Statphys2016, Lyon, France – July

Tensor Networks
Perimeter Institute, Waterloo, Canada – July

Public lecture: *What is time?*
Aspen Center for Physics, USA – August

Circuit organization in the brain (5 lectures)
Göttingen Summer School on Computational Neuroscience, Germany – September 14-16

Adaptive Molecular Sensing
Monell Chemical Sciences Institute, Philadelphia, USA – September

Entwinement in discretely gauged theories
Princeton University, USA – September

Public lecture: *Decoding your mental GPS: transcendental numbers in the brain*
University of Pennsylvania, Philadelphia, USA
September

Interpreting the Function of Neural Circuits in The Brain
University of Pennsylvania, Philadelphia, USA
October

New form of quantum entanglement in discretely gauged theories
University of Pennsylvania, Philadelphia, USA
October

Bulk reconstruction
Princeton University, USA – October

Colloquium: *The maps inside your head*
University of Pennsylvania, Philadelphia, USA
November

New forms of quantum entanglement
ICTP, Trieste, Italy – November

Jam packed: optimal molecular sensing in the immune and olfactory systems
PCTS, Princeton University, USA – December

Glenn Barnich

Finite BMS transformations
Ecole Normale Supérieure, Paris, France
January 12

Finite BMS transformations
The Joint Meeting on Quantum Fields and Nonlinear Phenomena, University of Craiova, Sinaia, Romania – March 12

Organizer: Workshop on Topics in Three Dimensional Gravity
International Center for Theoretical Physics, Trieste, Italy – March 21-24

Organizer: Workshop on Flat Holography
Simons Center, Stony Brook, USA
April 4-8

PhD thesis opponent
Chalmers University Gothenburg, Sweden
April 28

Lectures on *BMS symmetry*
IMPRS PhD school. Albert-Einstein-Institute, Golm, Germany – May 4

Finite BMS transformations

- Programme on Higher-Spin Theory and Duality. Munich Institute for Astroparticle Physics, Germany – May 16-27
- Workshop on recent developments in symmetries and (super)gravity theories. Bosphorus University, Istanbul, Turkey
June 13

- Mathematics and Physics at the Crossroads. University of Rome, Italy
June 8

Lectures on *BV quantization*
Saalburg Summer School. Wolfersdorff,
Germany – September 5-8

Finite BMS transformations
VII Tuscan Meeting on Theoretical Physics.
Scuola Normale Superiore, Pisa, Italy
October 4

Invited participant at “Conférence sur
l’analyse asymptotique en relativité générale”
University of Brest, Roscoff, France
October 5-7

Lecture course: Advanced GR
Amsterdam-Brussels-Geneva-Paris Doctoral
School, Quantum Field Theory, Strings
and Gravity, International Solvay Institutes,
Brussels, Belgium – October 10-14

Lecture course on *BMS current algebras*
University of Edinburgh, UK – October 17-21

- Finite BMS transformations*
- University of Prague, Czech Republic
November 14
 - University of Oxford, UK – November 29
 - Gravity colloquium: Southampton, UK
December 1
 - Quantum mechanics of Fundamental
Systems X. Centro d’Estudios Científicos,
Valdivia, Chile – December 12-16

Chris Blair

*The $SL(2) \times R^+$ exceptional field theory
and F-theory*
Pohang University of Science and Technology
(Duality and Novel Geometry in M-theory
workshop), South Korea – February 3

*The odd and exceptional geometries of string
theory and M-theory*
Theory at Sea meeting, Oostende, Belgium
May 26

*Introduction to string theory (10 hours of
lectures)*
Nesin Mathematics Village, Turkey
September 12-17

*Black hole thermodynamics, T-duality and
double field theory*
Max Planck Institute for Gravitational Physics,
Potsdam, Germany – October 24

Andrea Campoleoni

*Higher-spin gauge theories in $D=2+1$ and
their lessons for higher dimensions*
University of Tours, France – February 10

*Higher spins in three dimensions and BMS
symmetry*

- University Paris Diderot, France – March 15
- XXII Conference “Current Problems in
Theoretical Physics”, Vietri sul Mare, Italy
March 18

Higher spins in 3D: going from AdS to flat
ICTP workshop on Topics in Three
Dimensional Gravity, Trieste, Italy – March 24

Hamiltonian derivation of higher-spin charges
Munich Institute for Astro- and Particle
Physics; topical workshop of the programme
“Aspects of Higher Spin Theory”, Germany
May 24

*Higher-spin theories from a Hamiltonian
viewpoint*
University of Vienna, Austria – October 18

*Hints on Quantum BMS symmetries from
three dimensions*
Scuola Normale Superiore, Pisa, Italy
November 9

Andrés Collinucci

T-branes through 3d mirror symmetry
Universiteit van Amsterdam, The Netherlands
March 1

Probing T-branes with 3d mirror symmetry
Ludwig-Maximilians-Universität München,
Germany – June 2

Geoffrey Compère

Supertranslations and superrotations
ICTP, Trieste, Italy – March 22

BMS Holography
Niels Bohr Institute, Copenhagen, Denmark
April 26

BMS Vacua and Black Holes

- CECS Valdivia, Chile – December 12
- Beijing, China – August 4
- Nordita Institute, Stockholm, Sweden
August 17
- LMU, Munich, Germany – October 20

Dries Coone

Inflation and the 750 GeV resonance

VUB, Brussels, Belgium – May 9

Inflation with a random nonminimal coupling to gravity

Theory at Sea, Oostende, Belgium – May 25

Ben Craps

AdS (in)stability: an analytic approach

- APC Paris, France – January 19
- University of Turin, Italy – March 8

AdS (in)stability: an analytic approach and its interplay with numerics

University of Santiago de Compostela, Spain
June 27

Entwinement in discretely gauged theories

Nordita, Stockholm, Sweden – August 15

Snaartheorie

Ghent University, Belgium – November 3

Het Brout-Englert-Higgsdeeltje

Elcker-ik, Antwerp, Belgium – November 29

Saskia Demulder

How non-perturbative physics can resurge from perturbation Theory

BPS Meeting, Gent, Belgium – May 18

Stéphane Detournay

Asymptotic Symmetries and Non-Conformal Field Theories

ICTP - Workshop on tropics in three-dimensional gravity. Trieste, Italy – March 23

Soft Heisenberg Hair on Black Holes

Institut Henri Poincaré, Paris, France
May 26

Oleg Evnin

A few algebraic surprises in AdS

- KU Leuven, Belgium – April 27
- Perimeter Institute, Waterloo, Canada
June 2

Weak fields and effective integrability in AdS

- Wigner Institute Budapest, Hungary
September 23
- LPTHE and ENS Paris, France
September 27

Frank Ferrari

Black Hole Horizon and Bose-Einstein Condensation

String Theory Seminar, CERN, Genève, Switzerland – January 26

The Analytic Renormalization Group

Workshop Advances in transport and response properties of strongly interacting systems, ECT (European Center for Theoretical Studies in Nuclear Physics and Related Areas) Trento, Italy – May 5

Series of lectures and seminars

Institute for Basic Science, Center for Theoretical Physics of the Universe, Fields, Gravity and Strings Group, Seoul National University, Seoul, South Korea:

General Overview of Toy Models for Quantum Black Holes

November 15

SYK, Random Hermitian Matrices and Chaos

November 16

Introduction to the Physics of Spin Glasses and Replica Symmetry Breaking

November 23

A Simple Model for a Probe Particle Entering a Black Hole: Bose-Einstein Condensation, Infinite Redshift and Entanglement Entropy

November 24

The Analytic Renormalization Group Seminar. Institute for Basic Science, Center for Theoretical Physics of the Universe, Fields, Gravity and Strings Group, Seoul National University, Seoul, South Korea
November 28

A Simple Model for a Probe Particle Entering a Black Hole: Bose-Einstein Condensation, Infinite Redshift and Entanglement Entropy Seminar. Institute of Physics, University of Amsterdam – December 13

Simone Giacomelli

Superconformal theories from M5 branes

- ICTP, Trieste, Italy – February 4
- Imperial College London, UK – March 7

T-branes through 3d mirror symmetry

- University of Salerno, Vietri sul mare, Italy
March 19
- University of Prague, Czech Republic
June 16
- University of Bern, Switzerland – July 4

Adolfo Guarino

Mass deformations and $SL(2)$ angles from exceptional field theory
Galileo Galilei Institute, Florence, Italy
October 28

Jelle Hartong

Geometry at Infinity and Physics on the Boundary of a Space-Time
Vienna University of Technology, Austria
January 14

Carrollian Geometry and Flat Space Holography
KU Leuven, Belgium – January 26

Non-relativistic Hydrodynamics and Lifshitz Black Branes

- University of Leiden, The Netherlands
February 11
- KU Leuven, Belgium – February 17
- Niels Bohr Institute Copenhagen, Denmark
April 26

Non-Relativistic Field Theory and Hydrodynamics
Bogazici University, Istanbul, Turkey
June 13

Newton-Cartan and Carrollian geometry in holography and hydrodynamics
Nordita, Stockholm, Sweden – August 11

Non-relativistic holography, Newton-Cartan geometry and hydrodynamics (review)
University of Crete, Heraklion, Crete – September 9

Non-Lorentzian field theory and hydrodynamics
Chalmers University of Technology, Gothenburg, Sweden – October 3

Marc Henneaux

Black holes in 2+1 anti-de Sitter hypergravity
University of Buenos Aires, Argentina – 7 January

Electric-magnetic $SO(2)$ duality for higher spin gauge fields
Universidad Andrés Bello, Santiago, Chile
13 January

Hyperbolic Coxeter Groups and Hidden Symmetries of Gravity
Conference “Quantum Field Theory, String Theory and Beyond”, Institute for Advanced Studies, Jerusalem, Israel – 29 February

Twisted Self-Duality and $SO(2)$ Electric-Magnetic Duality for Gravity and Higher Spin Gauge Fields Seminar. Penn State University, University Park/State College, USA – 25 March

Asymptotically flat spaces in D spacetime dimensions: a review of the Hamiltonian approach
Workshop “Flat Holography”, Simons Center for Geometry and Physics, Stony Brook, NY, USA
5 April

Twisted Self-Duality and $SO(2)$ Electric-Magnetic Duality for Gravity and Higher Spin Gauge Fields Workshop “Aspects of Higher Spin Theory”, MIAPP, Germany – 25 May

Twisted Self-Duality for Gravity and Higher Spin Gauge Fields

- Seminar. Ecole Normale Supérieure and the IHP, Paris, France – 14 June
- Seminar. Niels Bohr Institute, Copenhagen, Denmark – 7 December

Alexey Koshelev

Non-local Starobinsky Inflation

QUARKS-2016, Pushkin, Russia – June 2

Introduction to non-local gravity

Heidelberg University, Germany – July 6

Infinite derivative operators in field theory

New trends in Theoretical physics, Steklov Math Institute, Moscow, Russia
September 28

Is non-local gravity UV complete?

University of Aveiro, Portugal – October 24

Are there Black holes in non-local gravity

X Black Hole Workshop, University of Guimaraes, Portugal – December 20

Jonathan Lindgren

Holographic thermalization in confining gauge theories

Utrecht University, the Netherlands
February 4

Collisions of pointlike particles in three-dimensional anti-de Sitter space

Stockholm University, Sweden – April 21

Black hole formation from pointlike particles in three dimensions

Theory at Sea, Oostende, Belgium – May 25

Holographic thermalization in confining gauge theories

VUB, Brussels, Belgium – June 16

Collisions of pointlike particles in three-dimensional anti-de Sitter space

Nordita, Stockholm, Sweden – August 17

Black hole formation from pointlike particles and emerging thin shell spacetimes in AdS3

Leiden University, the Netherlands
November 10

Laura Lopez Honorez

DM annihilation and 21cm cosmology

- RWTH Aachen University, Germany
April 14
- Planck conference, Valencia, Spain
May 25
- LAPTH Annecy, France – June 21
- Dark side of the Universe conference, Bergen, Norway – July 29
- VUB-Kobe symposium Brussels, Belgium
November 8
- IBS-Multidark-IPPP workshop, Lumley, UK
November 22

Alberto Mariotti

The diphoton excess interpretation

Louvain University (CP3), Louvain-la-Neuve, Belgium – January 8

Diphoton excess illuminates dark matter

- Planck Conference 2016, Valencia, Spain
May 24
- Durham University, UK – June 10

The diphoton excitement at the LHC

IAP Meeting, Louvain-la-Neuve, Belgium
June 17

Beyond Standard Model signatures at the LHC

VUB-Kobe symposium Brussels, Belgium
November 8

Twin Higgs meets SUSY

GDR Terascale Workshop Paris, France
November 23

Andrea Marzolla

On-Shell Amplitudes in spinor/helicity formalism

XII Modave Summer School in Mathematical Physics, Belgium – September 11-12

Poincaré invariance shapes the massive 3- point amplitude

- INFN Roma Tor Vergata, Rome, Italy
October 5
- University of Copenhagen, Denmark
November 9

- University of Oviedo, Spain – November 17
 - Humboldt-University Berlin, Germany
November 23
 - École Polytechnique Fédérale de
Lausanne, Switzerland – November 30
- Holographic Ward identities of symmetry breaking*
University of Durham, UK – December 5

Kentarou Mawatari

NLO QCD predictions for DM production at the LHC
LAPTh, Annecy, France – January 26

Monte Carlo tools
LPSC Grenoble, France – April 13

750 GeV scalar? or something else?
KIAS, Seoul, Korea – April 25

Higher-order QCD predictions for DM production at the LHC
KIAS, Seoul, Korea – April 27

Latest developments in Monte Carlo simulations
Subatech, Nantes, France – May 23

A comprehensive approach to dark matter studies: exploration of top-philic models

- CERN, Geneva, Switzerland – June 17
- MITP, Mainz, Germany – July 11

Monte Carlo overview
IHEP, Beijing, China – July 20

Higgs characterization
BCTP, Bonn, Germany – December 2

Blagoje Oblak

BMS Particles in Three Dimensions
Columbia University, New York, USA
April 14

Roberto Oliveri

Near-horizon extreme Kerr magnetospheres
University of Oviedo, Spain – November 17

Mass of Kerr-Newman black holes in an external magnetic field
Charles University Prague, Czech Republic
December 13

Pablo Pais

Thermodynamics equilibrium conditions and non-perturbative Propagators
Universidade do Estado do Rio de Janeiro, Brazil – May 17

Gábor Sárosi

Relative entropy of excited states in conformal field theories

- University of Pennsylvania, Philadelphia, USA – October 31
- KU Leuven, Belgium – November 16
- University of Amsterdam, The Netherlands
December 3

Late time behavior of two point functions in the D1D5 CFT
It from Qubit annual meeting of the Simons Foundation, New York, USA – December 8

Alexander Sevrin

The Third Way for Gauge Theories
Niels Bohr Institute, Copenhagen, Denmark
February 25

Massa? Massa!
Probus, Antwerp, Belgium – March 10

Massa? Massa!
Sint-Jozefscollege, Aalst, Belgium – April 24

Some comments on supersymmetry and the doubled formalism from a worldsheet perspective
Simons Center for Geometry and Physics, Stony Brook, New York, USA – May 13

De ouroboros van de fysica
Sint-Jan Berchmanscollege, Westmalle, Belgium – May 23

Charlotte Sleight

Interactions in Higher-Spin Gauge Theories: a Holographic Perspective
University of Amsterdam, The Netherlands
November 15

Massimo Taronna

Cubic Interactions in Higher-Spin Theory from CFT

- Conference “Current Problems in Theoretical Physics”, Vietri, Italy – March 18
- University of Mons, Belgium – April 21
- MIAPP Munich, Germany – May 25
- Quark Conference. St. Petersburg, Russia
June 3
- Tomsk State University, Russia – August 3

Higher-Spin Holography, Cubic Interactions and Beyond

- Trinity College, Dublin, Ireland
November 2
- University of Naples, Italy – November 17
- University of Bologna, Italy – November 20

Higher-Spin Algebra, Holography & Flat Space

Lebedev Institute, Moscow, Russia
November 30

Methods in Higher Spin Holography

Lebedev Institute, Moscow, Russia
December 1

Daniel Thompson

Generalised T-duality and Integrable Deformations

Asia Pacific Center for Theoretical Physics,
Pohang, Korea – February 1

Resurgence!

Theory by the sea workshop, Oostende,
Belgium – May 25

Generalised T-duality and Integrable Deformations and Resurgence

- ENS de Lyon, France – May 23
- LMU Munich, Germany – June 16

Generalised Duality in String Theory: New Approaches and Applications

Durham, UK – April 20

Generalised T-duality and Integrable Deformations and Resurgence

Institut Henri Poincaré, Paris, France
October 27

Generalized Geometry & T-dualities

Workshop organizer, Simons Center for
Geometry and Physics, Stony Brook, USA
May 9

Céline Zwikel

BTZ black holes, warped AdS3 black holes and flat space cosmologies in higher gravity theories

- Technische Universität Wien, Austria
October 20
- Oviedo University, Spain – November 17

List of Publications

- [1] H. Afshar, S. Detournay, D. Grumiller, W. Merbis, A. Perez, D. Tempo and R. Troncoso, “Soft Heisenberg hair on black holes in three dimensions,” *Phys. Rev. D* 93 (2016) no.10, 101503 [arXiv:1603.04824 [hep-th]].
- [2] H. Afshar, S. Detournay, D. Grumiller and B. Oblak, “Near-Horizon Geometry and Warped Conformal Symmetry,” *JHEP* 1603 (2016) 187 [arXiv:1512.08233 [hep-th]].
- [3] R. Argurio, A. Marzolla, A. Mezzalana and D. Musso, “Analytic pseudo-Goldstone bosons,” *JHEP* 1603 (2016) 012 [arXiv:1512.03750 [hep-th]].
- [4] R. Argurio, N. Bobev, N. Boulanger, B. Craps, M. Henneaux, T. Hertog, A. Sevrin, A. Van Proeyen and T. Van Riet, “Proceedings, The String Theory Universe, 21st European String Workshop and 3rd COST MP1210 Meeting : Leuven, Belgium, September 7-11, 2015,” *Fortsch. Phys.* 64 (2016) no.4-5, pp.269.
- [5] C. Arina et al., “A comprehensive approach to dark matter studies: exploration of simplified top-philic models,” *JHEP* 1611 (2016) 111 [arXiv:1605.09242 [hep-ph]].
- [6] J. Armas, J. Gath, V. Niarchos, N. A. Obers and A. V. Pedersen, “Forced Fluid Dynamics from Blackfolds in General Supergravity Backgrounds,” *JHEP* 1610 (2016) 154 [arXiv:1606.09644 [hep-th]].
- [7] J. Armas, “Membrane Hydrodynamics and Black Soap Bubbles,” *Fortsch. Phys.* 64 (2016) 408.
- [8] J. Armas, N. A. Obers and M. Sanchioni, “Gravitational Tension, Spacetime Pressure and Black Hole Volume,” *JHEP* 1609 (2016) 124 [arXiv:1512.09106 [hep-th]].
- [9] J. Armas, J. Bhattacharya and N. Kundu, “Surface transport in plasma-balls,” *JHEP* 1606 (2016) 015 [arXiv:1512.08514 [hep-th]].
- [10] A. S. Arvanitakis and C. D. A. Blair, “Black hole thermodynamics, stringy dualities and double field theory,” *Class. Quant. Grav.* 34 (2017) no.5, 055001 [arXiv:1608.04734 [hep-th]].
- [11] M. Astorino, G. Compère, R. Oliveri and N. Vandevorde, “Mass of Kerr-Newman black holes in an external magnetic field,” *Phys. Rev. D* 94 (2016) no.2, 024019 [arXiv:1602.08110 [gr-qc]].
- [12] J. P. Babaro, G. Giribet and A. Ranjbar, “Conformal field theories from deformations of theories with W_n symmetry,” *Phys. Rev. D* 94 (2016) no.8, 086001 [arXiv:1605.01933 [hep-th]].
- [13] M. Backovic, S. Kulkarni, A. Mariotti, E. M. Sessolo and M. Spannowsky, “Cornering diphoton resonance models at the LHC,” *JHEP* 1608 (2016) 018 [arXiv:1605.07962 [hep-ph]].
- [14] M. Backovic, A. Mariotti and D. Redigolo, “Di-photon excess illuminates Dark Matter,” *JHEP* 1603 (2016) 157 [arXiv:1512.04917 [hep-ph]].
- [15] I. Bakhmatov, A. Kleinschmidt and E. T. Musaev, “Non-geometric branes are DFT monopoles,” *JHEP* 1610 (2016) 076 [arXiv:1607.05450 [hep-th]].
- [16] V. Balasubramanian, A. Bernamonti, B. Craps, T. De Jonckheere and F. Galli, “Entwinement in discretely gauged theories,” *JHEP* 1612 (2016) 094 [arXiv:1609.03991 [hep-th]].
- [17] G. Barnich and C. Troessaert, “Finite BMS transformations,” *JHEP* 1603 (2016) 167 [arXiv:1601.04090 [gr-qc]].
- [18] G. Barnich, C. Troessaert, D. Tempo and R. Troncoso, “Asymptotically locally flat spacetimes and dynamical nonspherically-symmetric black holes in three dimensions,” *Phys. Rev. D* 93 (2016) no.8, 084001 [arXiv:1512.05410 [hep-th]].

- [19] D. S. Berman, C. D. A. Blair, E. Malek and F. J. Rudolph, "An action for F-theory: $SL(2)R+$ exceptional field theory," *Class. Quant. Grav.* 33 (2016) no.19, 195009 [arXiv:1512.06115 [hep-th]].
- [20] J. Bernon, A. Goudelis, S. Kraml, K. Mawatari and D. Sengupta, "Characterising the 750 GeV diphoton excess," *JHEP* 1605 (2016) 128 [arXiv:1603.03421 [hep-ph]].
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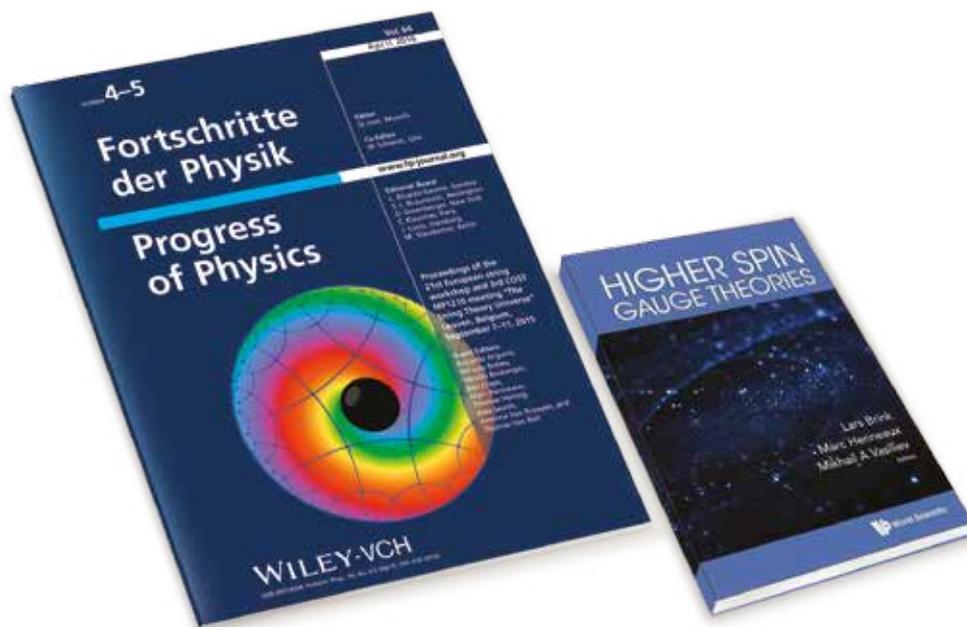
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Group of Professor Anne De Wit | ULB

Researchers

Permanent Members

Fabian Brau
Yannick De Decker
Anne De Wit
Laurence Rongy

Postdoctoral Members

Igal Berenstein
Marcello Budroni
Jorge Carballido-Landeira
Shyam Gopalakrishnan
Ceri Middleton
Chinar Rana
Gábor Schuszter
Virat Upadhyay
Aurore Woller

PhD Students

Jean-François Derivaux
Alexis Grau Ribes
Lorena Lemaigre
Vanessa Loodts
Rachel Lucena
Alexia Papageorgiou
Carelle Thomas
Reda Tiani
Valérie Voorluis

Master Students

Théa Gutmacher
Nathalie Ruth
Hind Saghou

Research Summary

CO₂ sequestration

Upon dissolution of carbon dioxide (CO₂) into deep saline aquifers, various chemical reactions are likely to take place between dissolved CO₂ and reactants dissolved in the brine, which may drastically impact the mixing of stored CO₂ in the reservoir. We have

analyzed by combined theoretical and experimental approaches to what extent the nature of the dissolved chemical reactants affects the convective dynamics generated by the dissolution of CO₂ into the host phase. We find that some reactions are able to accelerate the dissolution of CO₂ in water (see Fig. 1) while others refrain it. Our results suggest that, in the context of CO₂ sequestration, the details of the chemical composition of the storage site should be taken into account for more accurate modeling of the reactive transport of dissolved CO₂.

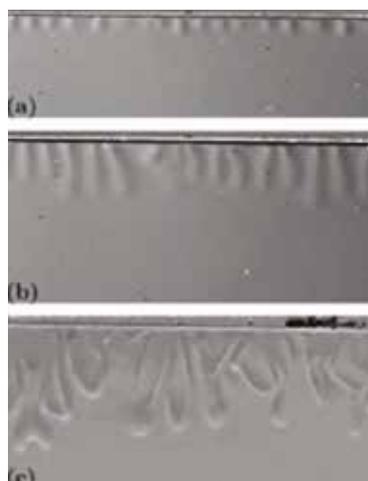


Fig. 1: Experimental comparison of convective dissolution of CO₂ in pure water after 6 min (a) and 13 min (b) with dissolution in an alkaline solution of LiOH after 13 min (c).

Convection in sea ice

To understand the important action of sea ice systems on the Earth's climate and global warming, it is crucial to analyze the various transport processes that can help transfer greenhouse gases from the atmosphere to the ocean via the intermediate ice layer. In this context, convective processes during sea-ice growth have been studied experimentally by cooling salt water from above in a Hele-Shaw cell. It has been observed that brine is rejected from the ice layer by interfacial convection from an enhanced salinity boundary layer while internal convection develops through brine drainage channels. Estimates of relative mass fluxes through the ice-water interface by the two mechanisms suggest that, when brine channels are active, the mass of salt they reject is higher than the finger pathway. However, due to the episodic nature of rejection from brine channels, there are certain periods where the mass flux from the two mechanisms is equal, or even periods where the interfacial flux becomes dominant.

Fingering dynamics induced by a precipitation reaction

When a precipitation reaction occurs in a porous medium, the solid phase can block the pores and induce a local decrease of the permeability. This can perturb flows in the porous matrix and lead to non homogeneous transport. We have analyzed numerically the influence of a simple precipitation reaction on the properties of flow in a model porous medium. We have shown that a fingering instability can occur by which the interplay between the flow and the reaction can lead to a deposit of the solid precipitate in a fingered pattern (Fig.2). This spatially structured solid deposit has a shape that varies with the diffusion coefficient of the mineral formed. These results contribute to understand the properties of mineralisation reactions in soils, important among others for underground sequestration of CO_2 .

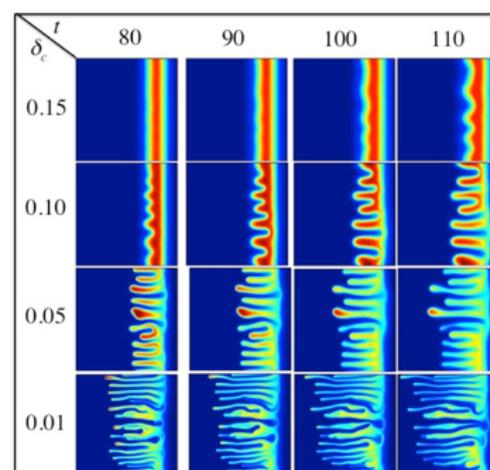


Fig.2: Temporal evolution (from left to right) of the spatial distribution of a solid precipitate for various values of the dimensionless diffusion coefficient δ_c of the solid particles.

Localized patterns around a chemical oscillator

When two gels, each loaded with a different set of reactants of an oscillatory reaction, are brought into contact, reaction–diffusion patterns such as waves or stationary Turing patterns can develop in the reactive contact zone. The initial condition which separates the reactants at the beginning leads to a localization in space of the different dynamical regimes accessible to the chemical oscillator. We have classified both numerically and experimentally the composite traveling structures that can result in this geometry from the interaction between chemical fronts and localized waves.

Chemical fronts in microgravity:

In collaboration with European research teams (European Space Agency network focusing on chemo-hydrodynamic instabilities), we have characterized the dynamics of autocatalytic reactions in microgravity. The microgravity condition was achieved on board of the MASER-13 sounding rocket. Self-organized surface tension-driven flows have been observed to travel with reaction fronts, which we have explained with the help of numerical simulations.

Marangoni-driven flows in reactive systems:

Simple $A + B \rightarrow C$ reactions can induce complex flow dynamics when they occur in thin horizontal aqueous layers in contact with air. If the three chemical species diffuse at different rates and affect the surface tension differently, we have proposed a general classification of the surface tension profiles as a function of the Marangoni numbers quantifying the effect of each species on the surface tension, the ratio of initial concentrations of reactants and the ratios of diffusion coefficients. Such a classification allows to study the resulting structure of the convective rolls as well as the nonlinear dynamics of the reaction front.

Reaction-diffusion layers at electrodes:

In collaboration with Prof. T. Doneux (CHANI, ULB), we study the coupling between electrochemical reactivity and mass transport processes, which occurs during the proton reduction reaction. To obtain spatial information about the processes taking place in the diffusion layer, cyclic voltammetry is coupled with confocal fluorescence microscopy. The experimental results are compared to theoretical pH profiles obtained by integrating a numerical model describing diffusive mass transport coupled to the electrochemical reaction.

Pattern formation in elastic thin sheets:

Twisted ribbons under tension exhibit a remarkably rich morphology depending on the applied twist and tension. This complexity emanates from the instability of the natural, helicoidal symmetry of the system, which generates both longitudinal and transverse stresses, thereby leading to buckling of the ribbon. We focused on the tessellation patterns made of triangular facets and have described experimental observations within an “asymptotic isometry” approach that brings together geometry and elasticity. The geometry consists of parametrized families of surfaces, isometric to the undeformed ribbon in the singular limit of vanishing thickness and tensile load. Energy minimization selects then the favored structure among those families. This framework allows to determine the domain of existence of faceted structures which compares well with experiments.

Research Interests of some other members

Fabian Brau

Associate Professor | ULB



“ Despite their nonchalant appearance, chameleons are formidable predators, capturing their prey by whipping out their tongues with incredible precision. They can even capture preys weighting much more than their own weight. In collaboration with colleagues from the National Museum of Natural History in Paris and the Université de Mons (UMons), I have studied this amazing sticky weapon. This work has been published this year in Nature Physics.”

How chameleons capture their prey

Chameleons are fascinating creatures with amazing characteristics. Their feet have opposable toes, giving them a tongs-like appearance, to firmly grip branches (*Fig.1*). Their eyes move independently of each other to provide 360 degree vision. Their skin changes colour via the active tuning of a lattice of nanocrystals contained in some cells. But their most outstanding characteristic is probably their ballistic tongue, allowing the capture of distant preys.

Thanks to this tongue, chameleons are very efficient predators, leaving little chance to their prey. During a capture, their tongue whips out with an acceleration up to 1500 m/s^2 and extends to reach a length twice that of the chameleon's body. They are also able to capture preys weighting up to 30% of their own weight. Sufficient adhesion between the prey and the tongue is therefore necessary to catch such preys.

We have demonstrated that the mucus secreted at the tip of a chameleon's tongue has a viscosity 400 times larger than the one of human saliva.

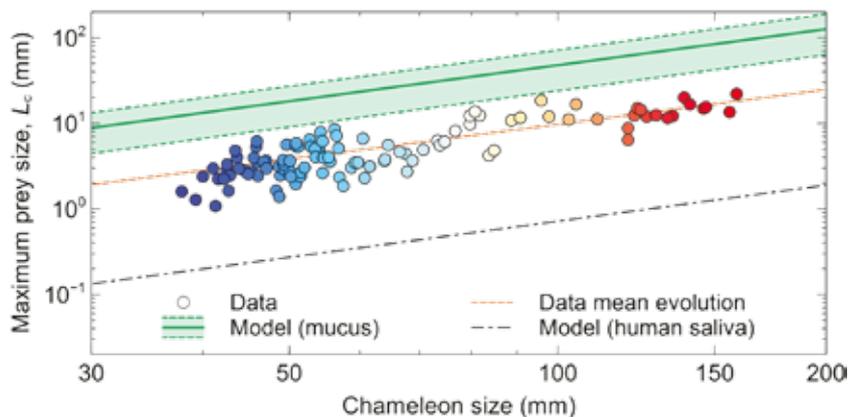
However, the viscosity alone does not allow to determine the adhesion force between the tongue and the prey. Indeed, this force results from the resistance to deformation of the mucus film during a sudden stretch.



Fig.1: One of the chameleons (Chamaeleo calytratus) used for measuring mucus viscosity and prey prehension kinetics (courtesy of A. Maillard).

It is therefore necessary to know the speed at which the mucus between the prey and the tip of the tongue is stretched during a capture to determine the adhesive force. Mechanical tools combined with measurements of the morphology of the tongue allowed to develop a dynamic model of prey capture. This model shows that beyond a critical value of the prey size, L_c , the mucus film breaks releasing the prey from the deadly trap. This critical size, which depends on the size of the chameleon, describes well the evolution of the biggest prey caught by these predators while being large (Fig. 2).

Fig. 2 : Comparison between the maximum prey size measured in vivo and the one derived from the model. The influence of the viscosity of the fluid is also shown.



This “safety factor” allows chameleons to capture preys even when conditions are not optimal (partial contact with the prey or prey firmly gripped to its support).

The deformability of the tongue during the projection, producing a large contact area with the prey, combined with the high viscosity of the mucus, thus constitutes a particularly effective adhesive trap.

This interdisciplinary study provides a new methodology for studying the capture of prey by other predators, such as salamanders or toads, also feeding themselves in this way.

Reference:

F. Brau, D. Lanterbecq, L.-N. Zghikh, V. Bels and P. Damman
Dynamics of prey prehension by chameleons through viscous adhesion, Nature Physics 12, 931 (2016).

Gábor Schuszter
Postdoctoral Member I ULB



“ During my postdoc at ULB, I worked on chemical reactions in non-equilibrium conditions to study how hydrodynamic flows influence precipitation reactions. I focused essentially on carbonate mineralization in a confined geometry to investigate how the injection of one reactant into another one alters the amount of product generated.”

This type of reaction in such confined conditions can be viewed as a model system for the underground sequestration of carbon dioxide (CO_2) in depleted oil, gas reservoirs or saline aquifers. In practice, this storage is performed by injecting supercritical CO_2 in geological formations (porous media) where it will, depending on the *in situ* conditions, partially or entirely transform into carbonate minerals. This process could offer a long term solution to offset the increasing emission of greenhouse gas in the atmosphere since a large amount of mineralized CO_2 can be stored underground. However, the conditions under which such a transformation of a fluid into a solid phase can be successfully and effectively performed without clogging the reservoir pores are still not well characterized.

In laboratory-scale experiments, a model system consisting in two horizontal Plexiglas plates separated by a tiny interstice (a so-called Hele-Shaw cell) is used as the equivalent of a porous medium. The cell is filled by a calcium chloride solution mimicking the solution present in geological formations which contain among others dissolved calcium and magnesium ions. A sodium

carbonate solution is injected into the cell to simulate the injection of dissolved CO_2 . When the calcium and the carbonate solutions mix, a white calcium carbonate precipitate appears. I have investigated experimentally to what extent the values of the concentrations of the reactants, their stoichiometric ratio, and the injection flow rate influence the yield and the spatial distribution of the precipitate.

For small reactant concentrations and low flow rate, the precipitate distribution is uniform and spreads radially (*Fig. 1a*). The amount of precipitate does not depend on the angular direction. However, in such conditions, only a small part of the injected CO₂ can be mineralized on small time scales. If one of the reactant concentrations or the injection rate is increased, the mineralization is significantly more efficient. However, this leads at the same time to the formation of spatial precipitation patterns with preferred directions (*Fig. 1b*).

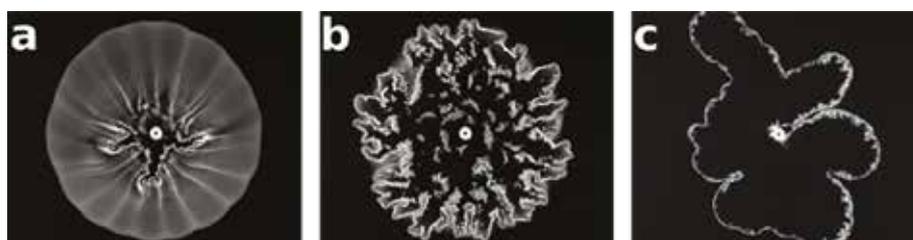


Figure 1: Calcium carbonate precipitation patterns at different reaction concentrations and flow rate.

It is thus difficult in this case to predict where the precipitation will occur. I have also shown that the amount of precipitate does not vary monotonically with the concentration of the reactants and the flow rate (which enhances mixing). There exists critical values of these parameters beyond which the production of precipitate decreases. Indeed, for large reactant concentrations and flow rates, a large amount of precipitate is produced but only in a small area where the reactants meet. The precipitate is then so dense and cohesive that it forms a wall with low permeability – basically a membrane – which hinders further convective mixing. The reaction proceeds next only thanks to further transport by diffusion (*Fig. 1c*). These results thus show that some optimization is needed to reach an effective precipitate production in porous media, such as in underground reservoirs.

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Calcium Carbonate Mineralization in a Confined Geometry,
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Phys. Chem. Chem. Phys. 18, 25592 (2016).

Appraisals and Prizes | Thesis defended in 2016

Appraisals, Prizes and Fellowships

Fabian Brau has been appointed as Associate Professor at ULB.

Marcello Budroni has obtained a F.R.S.-FNRS Chargé de Recherches position and has received the “Best Talk” Award of the Conference WIVACE 2016, 4-7/10/2016, Salerno, Italy.

Jean-François Derivaux has been awarded a Solvay Award for his Master’s Thesis.

Anne De Wit has become member of the Editorial Advisory Board of the Journal Physical Review Fluids and has obtained a new Prodex research grant. She was also member of the jury of the “Fluid Dynamics Prize” of the American Physical Society.

Alexia Papageorgiou and Alexis Grau Ribes both received a FRIA PhD fellowship.

Laurence Rongy has been promoted Associate Professor at ULB.

Thesis defended in 2016

- PhD thesis

Lorena Lemaigre – “Convective patterns triggered by chemical reactions, dissolution and cross-diffusion: an experimental study”
13 May 2016 (thesis advisor: Prof. A. De Wit).

Vanessa Loodts – “Influence of chemical reactions on convective dissolution: a theoretical study”
21 December 2016 (thesis advisor: Prof. A. De Wit).

- Master Thesis

Alexia Papageorgiou – “Approches expérimentale et numérique pour l’étude spatiale de couches de réaction-diffusion aux électrodes : application à la réaction de réduction des protons”
20 June 2016 (advisors: Profs T. Doneux and L. Rongy).

Talks at conferences, seminars and schools

Anne De Wit

Precipitation patterns in flows

Talk at the Workshop on chemo-hydrodynamic pattern formation at interfaces, Brussels, Belgium – March 21

Chemical control of hydrodynamic instabilities,

Department seminar in Prof. Lee Cronin's laboratory, Glasgow, UK – May 26

Chemo-hydrodynamic patterns and instabilities

European Space Agency, ESTEC, The Netherlands – September 30

Fabian Brau

Elastic instability: Surface structuration through auto-organization

Experimental Polymer Physics, Freiburg University, Germany – March 7

Structures périodiques et localisées dans des plaques minces élastiques

IRPHE, Marseille, France – May 27

Laurence Rongy

Marangoni-driven deformation of Iodate-Arsenous Acid reaction fronts in microgravity: numerical simulations

Workshop on chemo-hydrodynamic pattern formation at interfaces, Brussels, Belgium March 21

Influence of Marangoni-driven flows on $A + B \rightarrow C$ reaction fronts

Workshop on chemo-hydrodynamic pattern formation at interfaces, Brussels, Belgium March 22

Chemically-induced Marangoni convection around autocatalytic fronts in microgravity conditions

Gordon Research Seminar on Oscillations and Dynamic Instabilities in Chemical Systems, Stowe, Vermont, USA – July 17

Marcello Budroni

Scale-free networks out of multifractal chaos

WIVACE 2016, Salerno, Italy – October 04

Classification of cross-diffusion-driven convection in three-component double-layer systems: Theory and Experiments

630th WE-Heraeus Seminar, Bayreuth, Germany October 10

Jorge Carballido-Landeira

Talk at the 9th Chaotic modeling and simulations international conf. (CHAOS2016), London, UK May 23-26

Jean-François Derivaux

Towards an alternative approach to stochastic thermodynamics

Workshop Modeling of chemically powered nanomotors, Leuven, Belgium – April 12

Chinar Rana

Effect of adsorption and viscous fingering instability on the dispersion and form of peaks in liquid chromatography

Séminaire à l'ESPCI, Paris, France October 21

Gábor Schusztér

Calcium Carbonate Mineralization in a Confined Geometry

- XXXVI Dynamics Days Europe, Corfu, Greece June 6-10
- Gordon Research Seminar on Oscillations and Dynamic Instabilities in Chemical Systems, Stowe, Vermont, USA – July 16-17

Flow-controlled precipitation patterns for carbon dioxide sequestration

- 630th WE-Heraeus Seminar, Bayreuth, Germany October 9-12
- Department Seminar, Université Paul Sabatier, Toulouse, France – October 15

Reda Tiani

Influence of Marangoni-driven flows on $A + B \rightarrow C$ reaction-diffusion fronts
IMA 8 Conference, Bad Honnef, Germany
June 12-16

Chemically-driven Marangoni flows across $A + B \rightarrow C$ reaction fronts
MicroMAST conference, Brussels, Belgium
September 5-8

Marangoni flows induced by $A + B \rightarrow C$ reaction fronts with arbitrary diffusion coefficients
69th APS-DFD conference, Portland, USA
November 20-22

Aurore Woller

Stochastic thermodynamics of biological processes
10th European Conference on Mathematical and Theoretical Biology, Nottingham, UK
July 11-15

Scientific stays

Fabian Brau

Visiting professor in the physics department of University of Massachusetts, USA from 03/10 to 02/11/2016.

Jorge Carballido-Landeira

Research stay in the group of Prof. A.P. Muñuzuri, Facultad de Fisica, Universidad de Santiago de Compostela, Spain from 14/8 to 21/9/2016.

Organized Conferences

Fabian Brau

Co-organization of a thematic session "Instabilities and bifurcations in Solids, Structures and Soft Materials" at the "Engineering Mechanics Institute (EMI) international conference" (American Society of Civil Engineers), Université de Lorraine, France 25-27 October 2016.

Jorge Carballido-Landeira

Member of the organizing committee of the 2nd BCAM Workshop on Nonlinear dynamics in Biological Systems, Bilbao, Spain 1-2 September 2016.

List of Publications

- C. Barroo, Y. De Decker, T. Visart de Bocarmé and N. Kruse
Emergence of Chemical Oscillations from Nanosized Target Patterns,
Phys. Rev. Lett. 117, 144501 (2016).
- I. Berenstein and J. Carballido-Landeira
Back and forth invasion in the interaction of Turing and Hopf domains in a reactive microemulsion system,
RSC Adv. 6, 56867 (2016).
- I. Berenstein, C. Beta and Yannick De Decker
Comment on “Flow-induced arrest of spatiotemporal chaos and transition to a stationary pattern in the Gray-Scott model”,
Phys. Rev. E 94, 046201 (2016).
- F. Brau, D. Lanterbecq, L.-N. Zghikh, V. Bels and P. Damman
Dynamics of prey prehension by chameleons through viscous adhesion,
Nature Physics 12, 931 (2016).
- M.A. Budroni and A. De Wit
Localized stationary and traveling reaction-diffusion patterns in a two-layer $A + B \rightarrow$ oscillator system,
Phys. Rev. E 93, 062207 (2016).
- M.A. Budroni, J. Carballido-Landeira, A. Intiso, L. Lemaigre, A. De Wit, and F. Rossi
From Microscopic Compartmentalization to Hydrodynamic Patterns: New Pathways for Information Transport.
Communications in Computer and Information Science, Book Series 587, p. 171-183 (2016).
- M.A. Budroni, L. Lemaigre, D.M. Escala, A. Perez-Munuzuri and A. De Wit
Spatially Localized Chemical Patterns Around an $A + B \rightarrow$ Oscillator Front,
J. Phys. Chem. A 120, 851 (2016).
- P. Bunton, D. Martin, S. Stewart, E. Meiburg, A. De Wit
Schlieren imaging of viscous fingering in a horizontal Hele-Shaw cell,
Exp. Fluids 57, 28 (2016).
- J. Carballido-Landeira, B. Escibano (Eds.),
Nonlinear Dynamics in Biological Systems,
Springer, ISBN 978-3-319-33053-2 (2016).
- Y. De Decker, J.-F. Derivaux and G. Nicolis
Stochastic thermodynamics of reactive systems: An extended local equilibrium approach,
Phys. Rev. E 93, 042127 (2016).
- A. De Wit
Chemo-hydrodynamic patterns in porous media, Philos. Trans. Roy. Soc. A 374, 20150419 (2016).
- F. Haudin, F. Brau, J. Cartwright, et A. De Wit
Les nouvelles variétés de jardins chimiques confinés, La Recherche 512, 52 (2016).
- F. Haudin, M. Callewaert, W. De Malsche, and A. De Wit
Influence of nonideal mixing properties on viscous fingering in micropillar array columns, Phys. Rev. Fluids 1, 074001 (2016).
- V. Loodts, P.M.J. Trevelyan, L. Rongy, and A. De Wit
Density profiles around $A + B \rightarrow C$ reaction-diffusion fronts in partially miscible systems: A general classification,
Phys. Rev. E 94, 043115 (2016).

- C.A. Middleton, C. Thomas, A. De Wit and J.-L. Tison
Visualizing brine channel development and convective processes during artificial sea-ice growth using Schlieren optical methods, *J. Glaciol.* 62, 1 (2016).
- H. Pham Dinh, V. Démercy, B. Davidovitch, F. Brau and P. Damman
From Cylindrical to Stretching Ridges and Wrinkles in Twisted Ribbons
Phys. Rev. Lett. 117, 104301 (2016).
- G. Schuszter, F. Brau, and A. De Wit
Calcium Carbonate Mineralization in a Confined Geometry,
Environ. Sci. Technol. Lett. 3, 156 (2016).
- G. Schuszter, F. Brau and A. De Wit
Flow-driven control of calcium carbonate precipitation patterns in a confined geometry,
Phys. Chem. Chem. Phys. 18, 25592 (2016).
- G. Schuszter and A. De Wit
Comparison of flow-controlled calcium and barium carbonate precipitation patterns,
J. Chem. Phys. 145, 224201 (2016).
- P. Shukla and A. De Wit
Fingering dynamics driven by a precipitation reaction: Nonlinear simulations,
Phys. Rev. E 93, 023103 (2016).
- C. Thomas, V. Loodts, L. Rongy and A. De Wit
Convective dissolution of CO₂ in reactive alkaline solutions: Active role of spectator ions,
Int. J. of Greenhouse Gas Control 53, 230 (2016).
- R. Tiani and L. Rongy
Influence of Marangoni flows on the dynamics of isothermal $A + B \rightarrow C$ reaction fronts,
J. Chem. Phys. 145, 124701 (2016).
- V. Voorluijs and Y. De Decker
Emergence of chaos in a spatially confined reactive system, *Physica D* 335, 1 (2016).

Press releases

Fabian Brau (press releases related to the article in Nature Physics 12, 931 (2016))

- Interview for RTBF radio « midi première » on 22/06/2016
- Interview for RTBF TV news on 23/06/2016
- The Washington Post:
<https://www.washingtonpost.com/news/speaking-of-science/wp/2016/06/21/super-sticky-spit-helps-chameleons-snag-their-prey/>
- The New-York Times:
<http://www.nytimes.com/2016/06/21/science/chameleons-sticky-spit.html>
- Los Angeles Times:
<http://www.latimes.com/science/sciencenow/la-sci-sn-chameleon-tongue-20160622-snap-story.html>
- The Times of India:
<http://www.gadgetsnow.com/tech-news/Slip-of-the-tongue-Chameleons-sticky-secret-revealed/articleshow/52837321.cms>
- New-Zealand Herald:
http://www.nzherald.co.nz/world/news/article.cfm?c_id=2&objectid=11661306
- The Japan Times:
<http://www.japantimes.co.jp/news/2016/07/09/world/science-health-world/chameleons-mysterious-tongue-prowess-revealed/>
- National Geographic:
<http://news.nationalgeographic.com/2016/06/chameleon-tongue-mucus-sticky-animals/>
- Science:
<http://www.sciencemag.org/news/2016/06/chameleon-spit-400-times-thicker-humans>
- Nature 534, 438 (2016):
<http://www.nature.com/nature/journal/v534/n7608/full/534438a.html>
- Le Point:
http://www.lepoint.fr/science/le-coup-de-langue-collant-du-cameleon-10-07-2016-2053404_25.php
- Le Monde:
http://www.lemonde.fr/sciences/article/2016/06/27/langue-visqueuse-langue-tueuse_4959143_1650684.html
- Le Soir: édition du 21/06/2016, page 6.
<http://plus.lesoir.be/node/46602>
- Pour La Science:
http://www.pourlascience.fr/ewb_pages/a/actu-comment-la-langue-du-cameleon-colle-sa-proie-37181.php
- Science & Avenir:
https://www.sciencesetavenir.fr/animaux/reptiles-et-amphibiens/video-comment-fonctionne-la-langue-des-cameleons_103592
- Scientific American:
<https://www.scientificamerican.com/espanol/noticias/los-camaleones-capturan-grandes-presas-gracias-a-su-viscosa-saliva-con-video/>



Laboratory Structural Biology Brussels | VUB

Group of Professor Jan Steyaert

Former head: Emeritus Professor Lode Wyns

Prof. em. Lode Wyns is former head of the laboratory Structural Biology Brussels at the Vrije Universiteit Brussel (VUB) and former director of the Flanders Institute for Biotechnology (VIB) Structural Biology department. His group and department have a long history as national and international excellence center in protein structural biology and biophysics, with topics ranging from

enzyme kinetics, protein signaling, protein conformational stability and functional disorder, and glycan-binding proteins.

The VUB laboratory is now headed by Prof. Jan Steyaert who also serves as Science Director to the VIB-VUB Center for Structural Biology together with Prof. Han Remaut.

The mission of the center is to study the structure and dynamics of macromolecular complexes to explain their mode of action in health and disease. The center integrates structural biology work with genetic and cellular studies, aiming to bridge molecular and cellular resolution, and actively translates these findings into biotechnological and medical applications.

2016 has proven another successful year for the center, with five graduated PhD students, 73 papers in leading international peer-reviewed journals, 2 patent applications and with research highlights in the molecular mechanisms

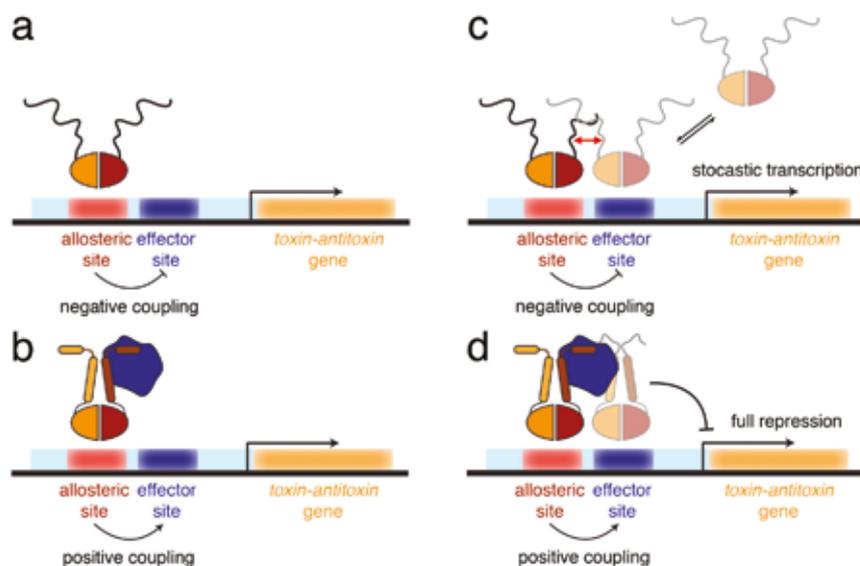
underlying allosteric regulation through protein order-disorder transitions, neurological disorders and infectious disease processes. The center is also proud to announce the successful bid by a VIB-VUB consortium for the installation of a state-of-the-art cryo electron microscopy center on the VUB campus, equipped with a 300 kV cold FEG and direct electron detector for the structural study of biological samples and 3D reconstruction of macromolecular complexes. A 4M euro investment by the FWO-Hercules foundation ensures that the Belgian life science community will have direct local access to this empowering technology that is revolutionising our ability to image dynamic and complex biological macromolecules in unprecedented detail.

We also look forward to welcome Prof. Richard Henderson (Cambridge University) as the 2017 International Solvay Chair in Chemistry. Prof. Henderson has pioneered the development of biological cryo-electron microscopy and serves as an authority in the field.

Highlights

Protein function from structural disorder

The classic view in protein science is the function of a protein is intrinsically linked to its three-dimensional structure. Nevertheless, it has become clear that many proteins do not fold into a well-defined three-dimensional structure and function as an intrinsically disordered ensemble. Despite the abundance of such intrinsically disordered proteins in proteomes, how they can carry out their cellular tasks is poorly understood. We unraveled one such mechanism by studying the regulation of the *phd/doc* module, an operon involved in bacterial persistence. We found that intrinsic disorder in the prokaryotic transcription factor Phd acts as a regulatory switch between negative and positive co-operativity. In absence of its partner Doc, intrinsic disorder in Phd prevents two molecules to bind at adjacent sites on the operator due to physical overlap of two disordered ensembles. Binding of Doc rigidifies the C-terminal region of Phd and bridges two Phd dimers together, resulting in coincident binding and efficient repression of the operon.

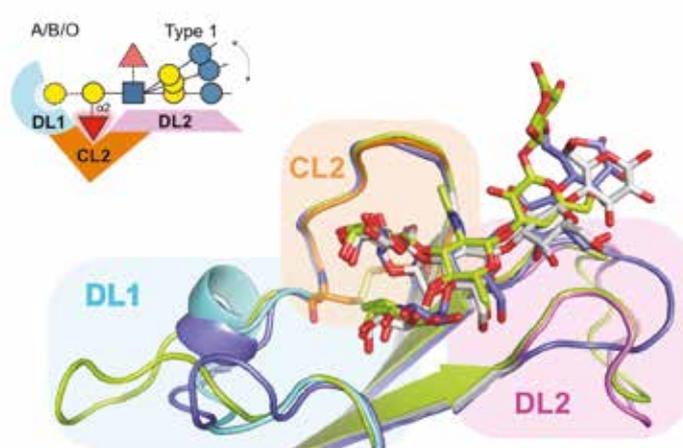


Ref: Garcia-Pino A., De Gieter S., Talavera A., De Greve H., Efremov R.G., Loris R. (2016) An intrinsically disordered entropic switch determines allostery in Phd/Doc regulation. *Nat. Chem. Biol.* 12, 490-496.

Structural Insights into Polymorphic ABO Glycan Binding by *Helicobacter pylori*

Helicobacter pylori is a common human pathogen associated with gastric cancer and peptic ulcers. The bacterium lives in the stomach mucosa, a few hundred microns away from the noxiously acidic gastric lumen, and does so by a select group of specialised adhesins. The BabA binds mucosal ABO and Lewis b blood group carbohydrates with exceedingly high affinity. A remarkable characteristic of *Helicobacter pylori* is its extremely high and fast evolving genetic diversity, to the point where each infected person carries its individualised “quasispecies”. This sequence diversity is particularly prevalent in surface-associated proteins such as the BabA adhesin. Indeed, from one clinical isolate to another, BabA share on average shares as little as 60% amino acid sequence identity. In collaboration with the group of Prof. Thomas Borén at Umeå university, Sweden, we analysed the structure – function relationship of the adhesins.

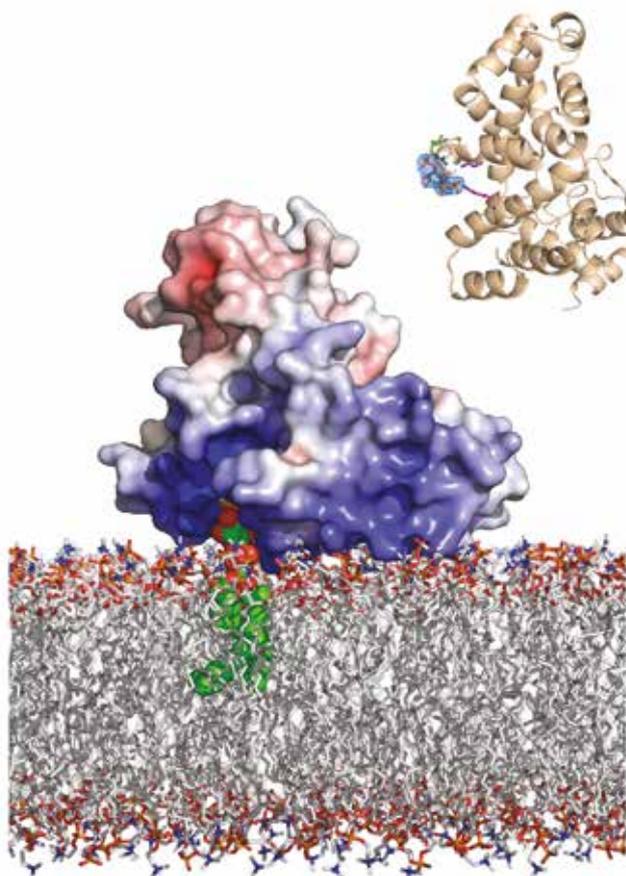
X-ray structures of representative clinical isolates reveal a polymorphic, three-pronged carbohydrate binding site. Remarkably, two high diversity loops, DL1 and DL2, are located directly inside the glycan binding pocket, and provide adaptive control to binding affinity, notably the adhesins’ generalist ABO versus specialist O blood group preference. We find that *H. pylori* strains can switch blood group preference with single DL1 amino acid substitutions, and can co-express functionally divergent BabA isoforms. *H. pylori* appears to use the DL1 and DL2 loops to tune blood group preference and affinity in accord with the prevalence of blood group antigens in different human populations. Inside the highly structurally diverse carbohydrate binding site, the embrace of a specific ABO fucose residue by a disulfide-clasped loop provides the anchor point for receptor binding. As a result, receptor binding is redox-sensitive and treatment with the redoxactive pharmaceutical N-acetylcysteine abolishes BabA activity and lowered gastric mucosal neutrophil infiltration in *H. pylori* – infected Leb⁻-expressing mice, providing perspectives on possible non-antibiotic *H. pylori* eradication therapies.



Ref: Moonens K, Gideonsson P, Subedi S, Bugaytsova J, Romaõ E, Mendez M, Nordén J, Fallah M, Rakhimova L, Shevtsova A, Lahmann M, Castaldo G, Brännström K, Coppens F, Lo AW, Ny T, Solnick JV, Vandenbussche G, Oscarson S, Hammarström L, Arnqvist A, Berg DE, Muyldermans S, Borén T, Remaut H. (2016) Structural Insights into Polymorphic ABO Glycan Binding by *Helicobacter pylori*. *Cell Host Microbe* 19:55-66.

Phosphoinositol phosphate signaling in neurological synapses

Research into the molecular mechanisms underlying epilepsy pathology has revealed that increasing the concentration of a specific lipid (Phosphatidylinositol 4,5-bisphosphate, PI(4,5)P₂) in the membrane of neurons could suppress epileptic seizures. This finding is the result of a cross-disciplinary collaboration between the groups of Patrik Verstreken (KU Leuven), specialised in the nervous system research and Wim Versées, specialised in structural biology. Earlier research involving fruit flies had already demonstrated that a protein known as 'Skywalker' plays a crucial role in maintaining communication between neurons. Mutations in the human homologous gene named 'TBC1D24' cause severe epilepsy and DOORS syndrome, but the molecular mechanisms underlying these pathologies are unresolved.



By combining forces, the scientists were able to solve the three-dimensional structure of Skywalker, making it possible to study the protein in atomic detail and giving them completely new insights into the function of this protein. They thus discovered that a pocket of Skywalker binds specific lipids (named phosphoinositides) phosphorylated at the 4 and 5 positions. And more importantly, this binding is impaired in over 70% of patients with a specific TBC1D24 mutation. Based on this discovery, the scientists were able to completely suppress the epileptic seizures of the mutant fruit flies by increasing the concentration of PI(4,5)P₂ in the neuronal membranes. This means that increasing specific lipids at the synapses of patients with a TBC1D24 mutation is a possible strategy for preventing epileptic seizures. And although this research focuses on people with TBC1D24 mutations, one can assume that these findings could be relevant to various forms of epilepsy.

Ref: Fischer, B., Lüthy, K., Paesmans, J., De Koninck, C., Maes, I., Swerts, J., Kuenen, S., Uytterhoeven, V., Verstreken, P., and Versées, W. (2016) Skywalker-TBC1D24 has a lipid-binding pocket mutated in epilepsy and required for synaptic function. *Nat. Struct. Mol. Biol.* 23(11):965-973.

Nanobodies to Study G Protein–Coupled Receptor Structure and Function

Since 20 years, the Wyns lab has been developing Nanobodies as tools to study the structure and function of the highest hanging fruits in structural biology including amyloidogenic proteins and IDPs. Recent work with top labs worldwide has been focusing on the use of Nanobodies to study GPCR structure and function.

Nanobodies, the recombinant antigen-binding fragments of camelid heavy-chain-only antibodies, have emerged as important research tools to lock GPCRs in particular conformational states. The first active-state stabilising nanobodies produced in Brussels have elucidated several agonist-bound structures of hormone-activated GPCRs and have provided insight into the dynamic character of key receptors including adrenergic, muscarinic and opioid receptors. Nanobodies have also been used to stabilise transient GPCR transmembrane signaling complexes, yielding the first structural insights into GPCR signal transduction across the cellular membrane. This work was conducive in awarding the 2012 Nobel Prize in Chemistry to Robert Lefkowitz and Brian Kobilka. Beyond their *in vitro* uses, nanobodies have also served as conformational biosensors in living systems and have provided novel ways to modulate GPCR function. Confo Therapeutics, the latest spin off of the lab exploits the conformational complexity of GPCRs to innovate drug discovery.

Ref: Manglik, A., Kobilka, B. K. & Steyaert, J. (2017) Nanobodies to Study G Protein-Coupled Receptor Structure and Function. Annu Rev Pharmacol Toxicol 57: 19-37.

List of Publications

Group Steyaert

- Hariharan, P., Jiang, X., Pardon, E., Steyaert, J., Kaback, H. R. & Guan, L. (2016) Thermodynamics of nanobody binding to lactose permease. *Biochemistry* 55, 5917-5926.
- Jianga, X., Smirnovab, I., Kashob, V., Wua, J., Hiratae, K., Kea, M., Pardon, E., Steyaert, J., Yan, N. & Kaback, R.H. (2016) Crystal Structure of a LacY/Nanobody Complex: the periplasmic-open conformation, *Proc Natl Acad Sci USA* 133, 12420-12425.
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- Figuroa, M., Sleutel, M., Vandevenne, M., Parvizi, G., Attout, S., Jacquin, O., Vandenameele, J., Fischer, A., Damblon, C., Goormaghtigh, E., Valerio-Lepiniec, M., Urvoas, A., Durand, D., Pardon, E., Steyaert, J., Minard, P., Maes, D., Matagne, A., Martial, J., Van de Weerd, C. (2016) The unexpected structure of the designed protein octarellin V. 1 forms a challenge for protein structure prediction tools. *Journal of Structural Biology* 195, 19-30.
- Wijckmans, E., Nys, M., Debaveye, S., Brams, M., Pardon, E., Bertrand, D., Steyaert, J. & Ulens, C. (2016) Functional and Biochemical characterization of *Alvinella pompejana* Cys-loop receptor homologues. *Plos One* 11, e0151183.
- Peyrassol, X., Laeremans, T., Lahura, V., Steyaert, J., Parmentier, M. & Langer, I. (2016) Development by genetic immunization of monovalent antibodies (nanobodies) behaving as antagonists of the human ChemR23 receptor. *Journal of immunology* 196, 2893-2901.

Group Remaut

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Javaheri A, Kruse T, Moonens K, Mejías-Luque R, Debraekeleer A, Asche I, Tegtmeier N, Kalali B, Bach NC, Sieber SA, Hill DJ, Königer V, Hauck CR, Moskalenko R, Haas R, Busch DH, Klaile E, Slevogt H, Schmidt A, Backert S, Remaut H*, Singer BB* and Gerhard M* (2016) *Helicobacter pylori* adhesin HopQ engages in a virulence-enhancing interaction with human CEACAMs. *Nature Microbiol.* - DOI: 10.1038/NMICROBIOL.2016.189.

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Group Versées

Fischer, B., Lüthy, K., Paesmans, J., De Koninck, C., Maes, I., Swerts, J., Kuenen, S., Uytterhoeven, V., Verstreken, P. and Versées, W. (2016) Skywalker-TBC1D24 has a lipid-binding pocket mutated in epilepsy and required for synaptic function. *Nat. Struct. Mol. Biol.* 23(11):965-973.

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the dimeric Parkinson's Protein LRRK2 reveals a highly compact folding. *Proc Natl Acad Sci U S A.* 113(30): E4357-66.

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Fislage, M., Wauters, L., Versées, W. (2016) MnmE, a GTPase that drives a complex tRNA modification reaction. *Biopolymers* 105(8):568-79. Invited review.

Group Loris

Garcia-Pino A., De Gieter S., Talavera A., De Greve H., Efremov R.G., Loris R. (2016) An intrinsically disordered entropic switch determines allostery in Phd/Doc regulation. *Nat. Chem. Biol.* 12, 490-496.

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- Group Messens**
- Kerchev, P., Waszczak, C., Lewandowska, A., Willems, P., Shapiguzov, A., Li, Z., Alseekh, S., Muhlenbock, P., Hoeberichts, F. A., Huang, J., Van Der Kelen, K., Kangasjarvi, J., Fernie, A. R., De Smet, R., Van de Peer, Y., Messens, J., and Van Breusegem, F. (2016) Lack of GLYCOLATE OXIDASE1, but Not GLYCOLATE OXIDASE2, Attenuates the Photorespiratory Phenotype of CATALASE2-Deficient Arabidopsis. *Plant Physiol* 171, 1704-1719.
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Research Highlights of other scientists connected with the Institutes

ALGC Research Group | VUB

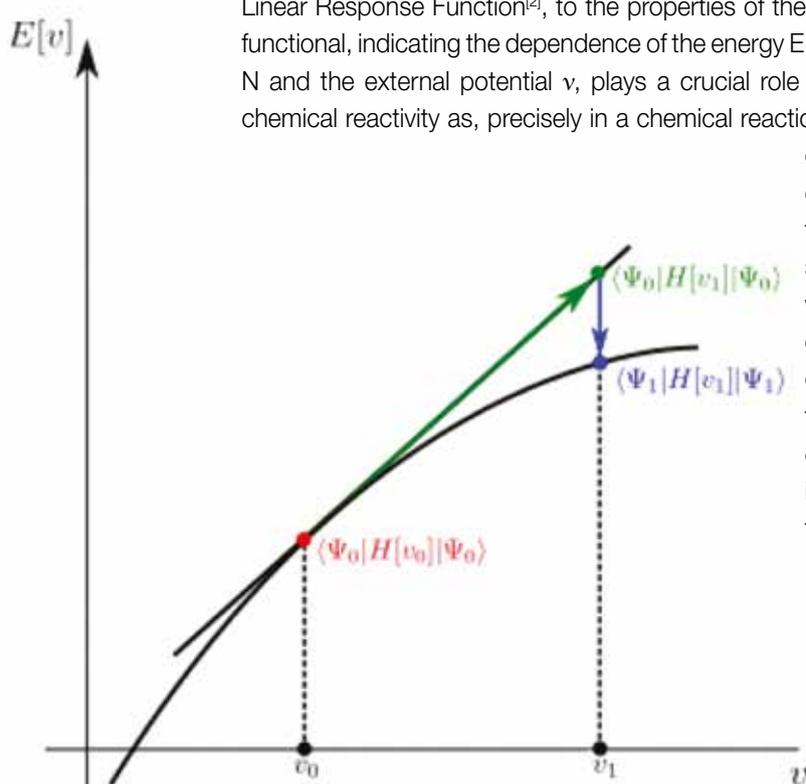
Group of Professor Frank De Proft and Emeritus Professor Paul Geerlings

The ALGC Research Group (Prof. Frank De Proft and Em. Prof. Paul Geerlings) has been extending its long-standing research interest in Conceptual Density Functional Theory^[1] in a natural way to several new research lines on the basis of the experience gained in various aspects of Density Functional Theory. Research Lines have been launched on Molecular Electronics, on Molecular Switching Properties, on Inverse Design and on the study of molecular behaviour in the molecules' real environment upon reactions, i.e. in most cases a solution, necessitating ab initio Molecular Dynamics and Metadynamics Simulations. Beyond and along these lines various applied quantumchemical studies are performed applying DFT based concepts on a variety of substrates most often carried out in direct interaction with experimentalists.

Conceptual DFT

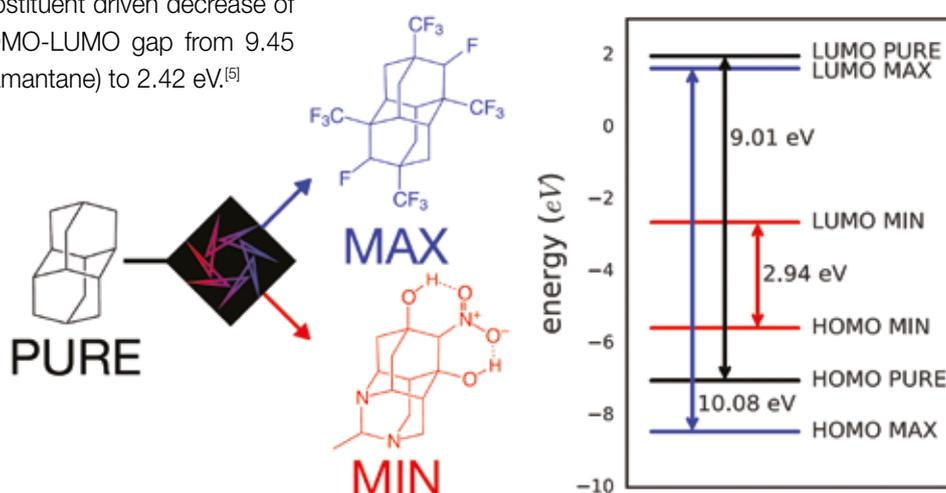
Concerning the Conceptual DFT part particular attention was paid, as part of Zino Boisdenghien's PhD Thesis and Dr. Stijn Fias' fundamental research on the Linear Response Function^[2], to the properties of the $E=E[N, v]$ functional. This functional, indicating the dependence of the energy E on the number of electrons N and the external potential v , plays a crucial role in predicting / interpreting chemical reactivity as, precisely in a chemical reaction, perturbations in N and/

or v are omnipresent. The concavity of the $E=E[v]$ functional has been scrutinized and connected with the negative values of the diagonal elements of the linear response function $\chi(r, r') = (\delta\rho(r)/\delta v(r'))_N$ for which a physical interpretation has been put forward^[3].



Inverse design

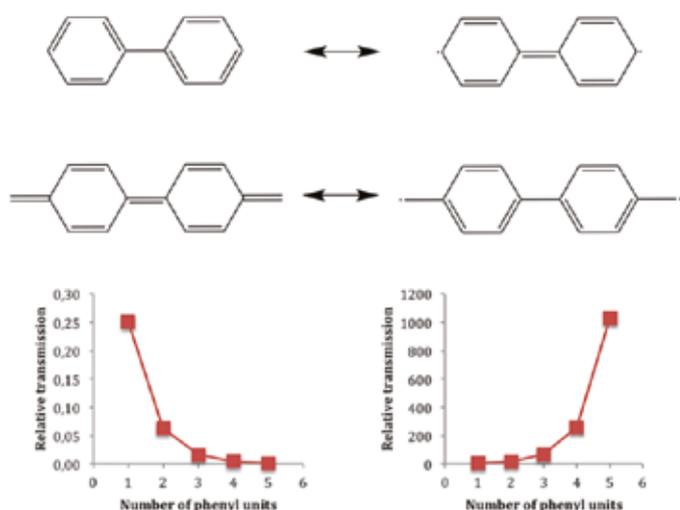
Inverse design is a quickly developing field with the ultimate aim to help experimental chemists when exploring the huge Chemical Space looking for molecules with optimal properties. On the basis of the experience built up in recent years (collaboration with Profs. W. Yang and D. N. Beratan from Duke University, USA)^[4] Dr. Freija De Vleeschouwer and her Doctoral Student Jos Teunissen explored chemical space to look for functionalized diamondoids (adamantane and diamantane derivatives) showing great potential as building blocks for various new optoelectronic applications. In this endeavour the HOMO-LUMO energy gap was optimized systematicall using a home made inverse design code, resulting e.g. in a substituent driven decrease of the HOMO-LUMO gap from 9.45 eV (adamantane) to 2.42 eV.^[5]



Molecular Electronics

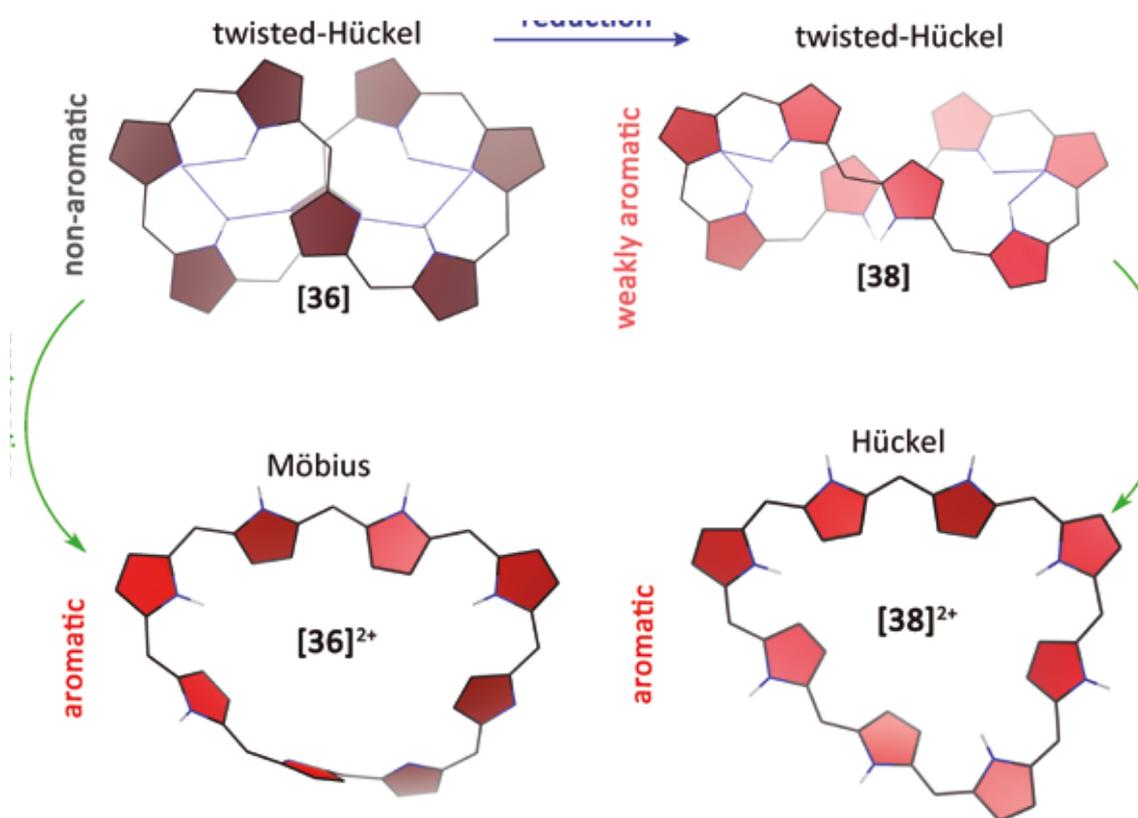
In the Molecular Electronics research line, started by PhD student Thijs Stuyver and Dr. Stijn Fias^[6], a collaboration with Nobel Laureate Roald Hoffmann (Cornell University), resulted in an in depth study on the conductivity of conjugated π -

electron molecular chains leading to the conclusion that conductivity of molecules can be tuned by “pushing” them towards more or less diradical character. These new insights enable the rationalization of a variety of experimental and theoretical results for π conjugated alternant hydrocarbons, especially the striking difference between extended oligophenylenes and related quinoid chains^[7].



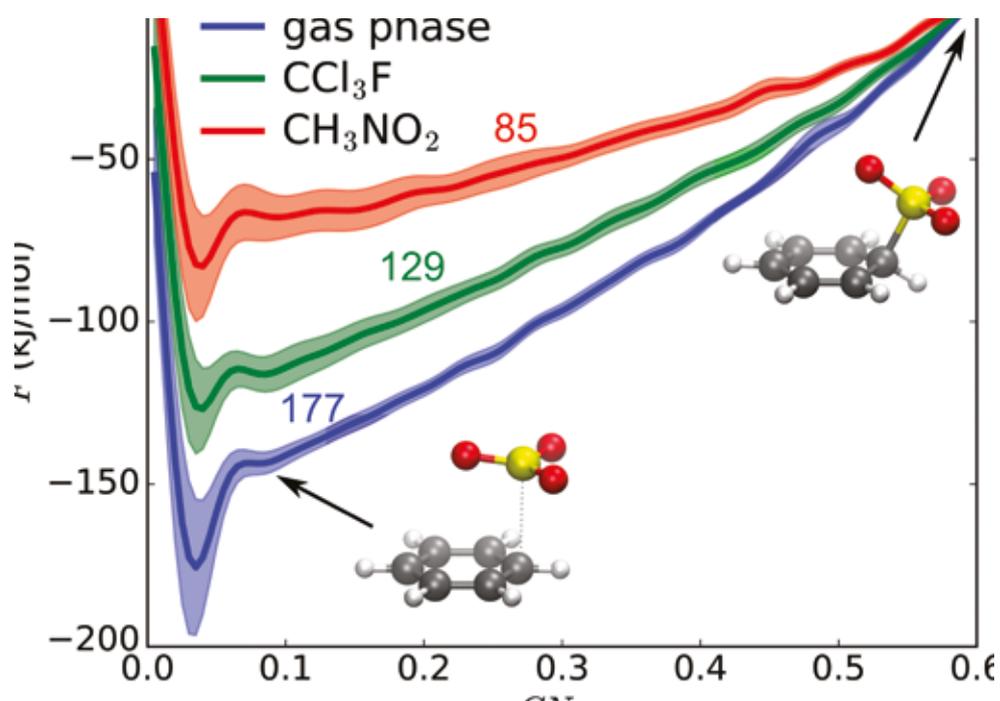
Molecular Switches

Molecular Switches have recently been explored in ALGC in the case of extended porphyrins under the impetus of Prof. Mercedes Alonso^[8], with particular attention to topological switches from Hückel to Möbius rings under the influence of external stimuli. Together with her PhD student Tatiana Wöller and in collaboration with Dr. Contreras Garcia from Paris VI, octaphyrins were scrutinized for their behavior under external stimuli such as protonation and reduction. A non aromatic figure-eight conformation upon protonation turns out to be preferable for neutral octaphyrins that switches to a Möbius aromatic conformation upon protonation. The consequences for Non Linear Optical and Conductivity properties were analyzed thus linking two of the new research lines^{[9] [10]}.



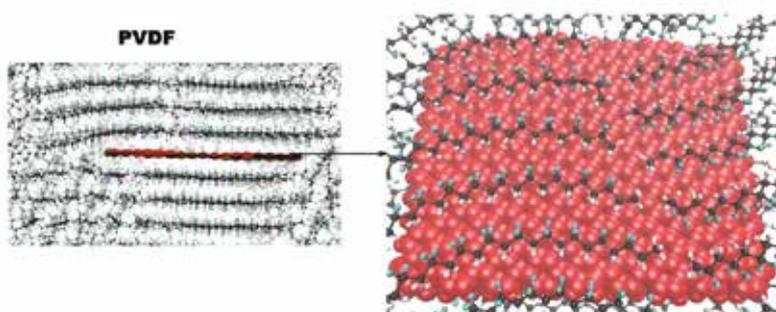
Dynamics

In the “Dynamics” tree of research a classical organic textbook reaction, the aromatic sulfonation with sulfur trioxide, has been reconsidered in view of recent theoretical work by Schleyer and co-workers putting question marks on the long standing “kinetics and mechanism” of this reaction. In a detailed simulation of the reaction in gasphase and different solvents, Dr. Sam Moors presented a new sequence of elementary reaction steps and kinetic model compatible with all experimental data, leading to publication in the influential *Chemical Science*^[11].



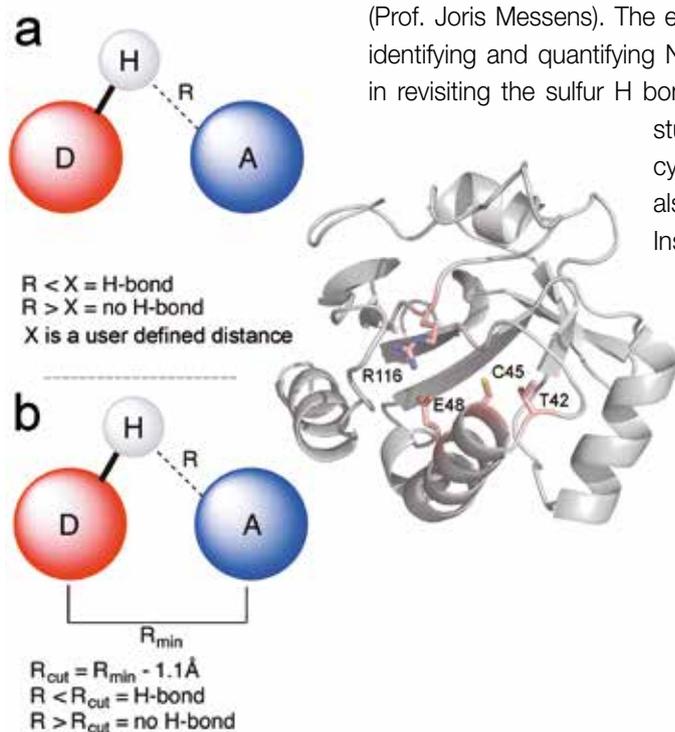
Molecular Dynamics Simulation

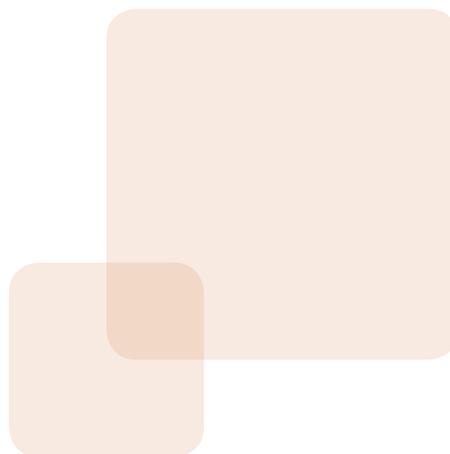
Molecular Dynamics Simulation have also been at stake in a study by PhD Student Songül Güryel who, in a collaboration with Dr. M. Walker and Prof. M. Wilson from Durham (UK), investigated the structure and morphology of graphene / polymer nanocomposites. The results indicate that graphene induces order in both polystyrene and polvinylidene fluoride systems by providing a nucleation site for crystallization whereas polystyrene remains disordered in the presence of graphene.^[12] In the figure the first layer of PVDF polymer on the graphene surface is shown (side view and top view). These results are in line with the recent results of a quantummechanical study by ALGC in the context of a joint venture with Solvay SA.^[13]



Applied quantumchemistry

Finally, as a prototype example of applied quantumchemistry in direct interaction with experimental chemists, the work by PhD student Laura Van Bergen should be highlighted with members from the experimental Redox Biology group of the VUB/VIB (Prof. Joris Messens). The electron density based NCI index for identifying and quantifying Non Covalent Interactions was used in revisiting the sulfur H bonding network in proteins, the case studied being the active site of single-cysteine peroxiredoxine. (collaboration also with Prof. L. Nilsson, Karolinska Institute)^[14]





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Laboratory of Polymer Chemistry | ULB

Group of Professor Yves Geerts

Organic semiconductors are carbon-based materials used in field-effect transistors. They hold great promises to fabricate elementary electronic circuits over large area at low economical and environmental costs. This generates numerous fundamental and applied research initiatives. However, one important question remains unanswered: what is the mechanism of transport of electric charges¹. In particular, the role of dynamic disorder is not well-established. In close collaboration with the team of Prof. Shu Seki at Kyoto University, the group of Prof. Yves Geerts has made some decisive progress towards a better understanding of charge transport mechanism. An unprecedented charge carrier mobility of $170 \text{ cm}^2/\text{V}\cdot\text{s}$ has been measured by Field-Induced Time Resolved Microwave Conductivity.^[2,3] This value, obtained at short time- and length-scales, i.e. 10^{-10} s and 10^{-7} m , respectively, validates the transient localization scenario for charge transport.^[4] In simple terms, electrical charges are delocalized over short time- and length-scales and can move very fast. At longer time- and length-scales, charges are forced to slow down and hop as schematically depicted in the figure 1.

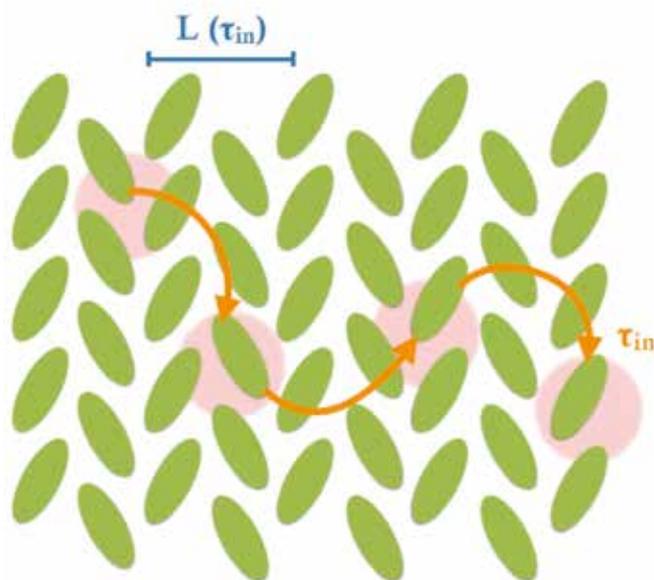


Figure 1. Schematic picture of charge transport in organic semiconductors. Charge are delocalized over a certain length-scale, $L(\tau_{in})$, below a given time-scale, τ_{in} .

The value of $170 \text{ cm}^2/\text{V}\cdot\text{s}$ is the largest ever reported for molecular semiconductors, but not all organic semiconductors are capable of such performance. The group of Prof. Sirringhaus, at the University of Cambridge, has recently developed a powerful experimental technique to determine the amplitudes of molecular lattice fluctuations based on analysing diffuse scattering streaks in electron diffraction. It has been established that thermal lattice fluctuations are a key factor in the charge transport physics, a significant and widely-recognised breakthrough. Using this technique, a recent collaboration between Prof. Sirringhaus and Prof. Geerts has demonstrated that some semiconductors exhibits an exceptionally low degree of dynamic disorder and hence, they tend to exhibit higher values of charge carrier mobility.^[5,6]

^[1] "What Currently Limits Charge Carrier Mobility in Crystals of Molecular Semiconductors?" G. Schweicher, Y. Olivier, V. Lemaury, Y. H. Geerts, *Isr. J. Chem.* **2014**, *54*, 595-620.

^[2] Charge carrier mobility μ ($\text{cm}^2/\text{V}\cdot\text{s}$) is defined as the drift velocity of the charge carrier (cm/s) per unit applied electric field (V/cm). Silicon widely used in computers chips exhibits a mobility on the order of $1000 \text{ cm}^2/\text{V}\cdot\text{s}$ whereas organic semiconductors have generally a lower mobility, up to $20 \text{ cm}^2/\text{V}\cdot\text{s}$, at most.

^[3] "Unraveling Unprecedented Charge Carrier Mobility through Structure Property Relationship of Four Isomers of Didodecyl [1] benzothieno [3,2-b] [1] benzothiophene", Y. Tsutsui, G. Schweicher, B. Chattopadhyay, T. Sakurai, J.-B. Arlin, C. Ruzié, A. Aliev, A. Ciesielski, S. Colella, A. R. Kennedy, V. Lemaury, Y. Olivier, R. Hadji, L. Sanguinet, F. Castet, S. Osella, D. Dudenko, D. Beljonne, J. Cornil, P. Samori, S. Seki, Y. H. Geerts, *Adv. Mater.* **2016**, *28*, 7106-7114.

^[4] "The Transient Localization Scenario for Charge Transport in Crystalline Organic Materials", S. Fratini, D. Mayou, S. Ciuchi, *Adv. Funct. Mater.* **2016**, *26*, 2292-2315.

^[5] "Reducing dynamic disorder in small-molecule organic semiconductors by suppressing large-amplitude thermal motions" S. Illig, A. S. Eggeman, A. Troisi, L. Jiang, C. Warwick, M. Nikolka, G. Schweicher, S. G. Yeates, Y. H. Geerts, J. E. Anthony, H. Sirringhaus, *Nature Communication* **2016**, *7*, 10736.

^[6] This important insight was enabled by the support from the Wiener Anspach Foundation that has generously funded the post-doctoral stay at Cambridge of Dr. Guillaume Schweicher, a former Ph.D. student of Prof. Geerts.

New S stars model atmospheres

S-type stars are evolved giant stars whose atmospheres are enriched in carbon and elements heavier than iron produced by the s-process of nucleosynthesis. The s-process consists in neutron captures on iron-seed elements, such that beta-decay rates dominate over neutron-capture rates. It is responsible for the production of ~50% of the elements heavier than iron.

S stars are therefore key-objects to understand heavy-element nucleosynthesis and mixing processes within evolved stars.

However, S-star atmospheres are notoriously difficult to investigate because of their non-standard chemistry associated to the cool temperature of their atmospheres; this is why no dedicated model atmospheres existed until now to perform surface abundance determinations.

A grid of MARCS model atmospheres has been computed at ULB for S stars, well-covering their parameter space: effective temperatures between 2700 and 4000K, carbon-to-oxygen ratio (C/O) between 0.50 and 0.99, surface gravity $0 < \log g < 5$, solar and subsolar metallicities, and various levels of s-process overabundances. The MARCS models make use of a new ZrO line list. Synthetic spectra computed from these models are used to derive photometric indices, as well as TiO and ZrO band strengths. A method is proposed to select the model best matching any given S star, a non-trivial operation since the grid contains more than 3500 models covering a five-dimensional parameter space. The method is based on the comparison between observed and synthetic photometric indices and spectral band strengths, and has been applied on a vast subsample of the Henize sample of S stars.

Our results reveal that ZrO bands in warm S stars ($T_{\text{eff}} > 3200$ K) are not caused by the C/O ratio being close to unity, as traditionally believed, but rather by some genuine Zr overabundance.

More generally, it is found that, at $T_{\text{eff}} = 3200$ K, a change of C/O from 0.5 to 0.99 has a strong impact on V-K (2 mag). Conversely, a range of 2 magnitudes in V-K corresponds to a 200 K shift along the (T_{eff} , V-K) relationship (for a fixed C/O value). Hence, the use of a (T_{eff} , V-K) calibration established for M stars will yield large errors for S stars, so that a specific calibration must be used, as provided in the present investigation.

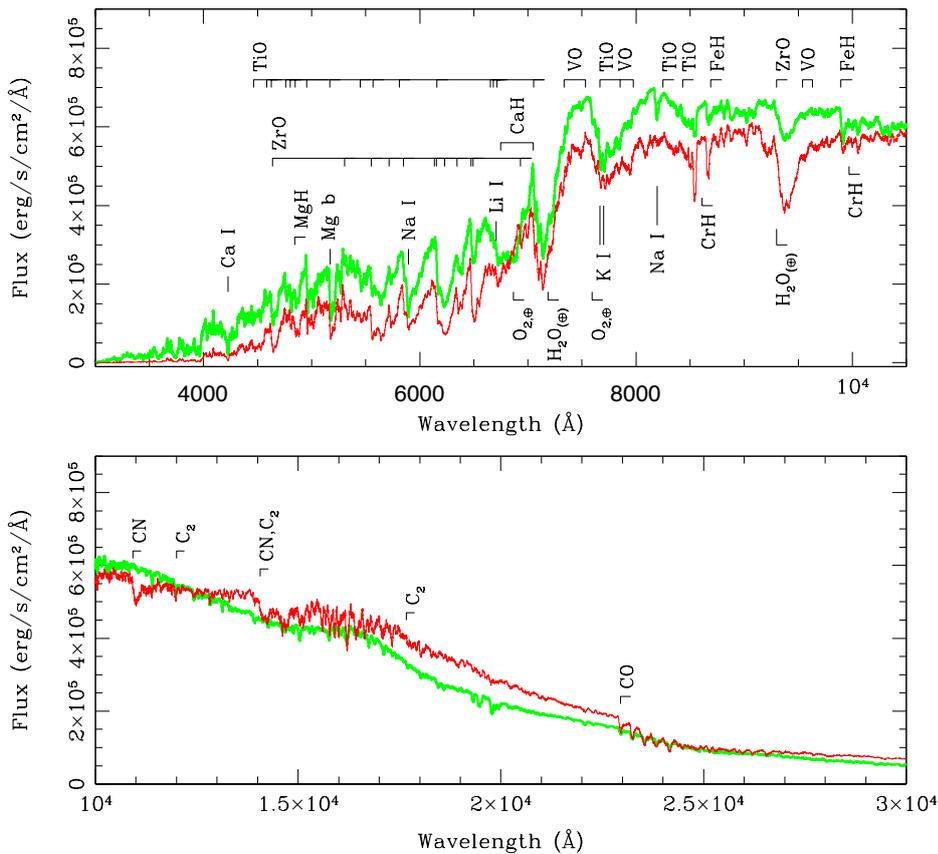
The defining spectral features of dwarf S stars are outlined, but none is found among the Henize S stars.

Actually S-star surface over-abundances can be due either to intrinsic nucleosynthesis and dredge-up of processed material at the stellar surface during an advanced phase of stellar evolution (the so-called thermally-pulsing asymptotic giant branch or TPAGB), or to an extrinsic pollution by a companion star, that was a TPAGB star in the past, and that is now an extinct white dwarf.

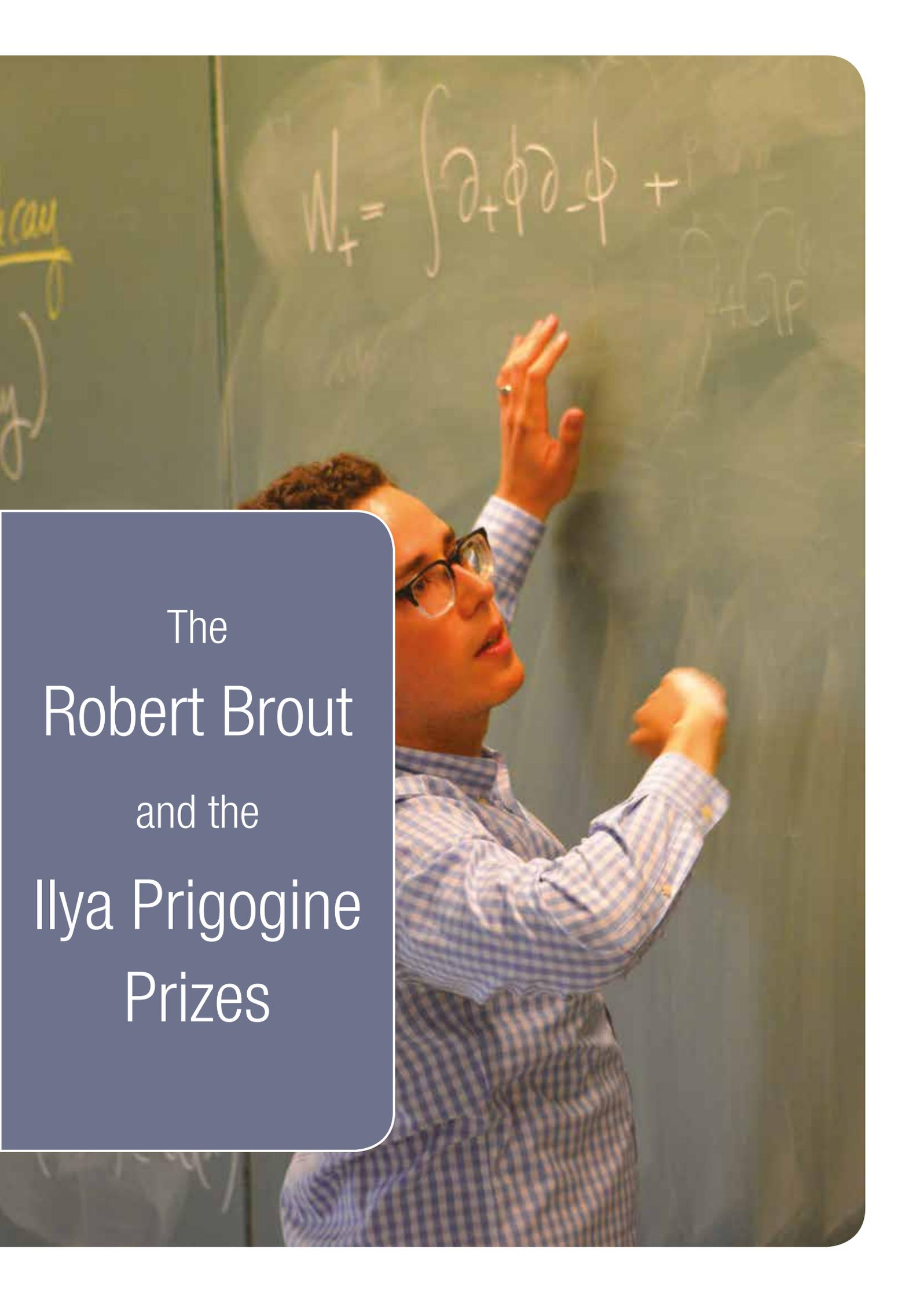
Using the atmospheric parameters derived by our method for the sample of Henize S stars, we show that the extrinsic-intrinsic dichotomy among S stars reveals itself very clearly as a bimodal distribution in the effective temperatures.

Moreover, the increase of s-process element abundances with increasing C/O ratios and decreasing temperatures is apparent among intrinsic stars, confirming theoretical expectations.

This paper is accepted in Astronomy and Astrophysics (Van Eck S., Neyskens P., Jorissen A., Plez B., Edvardsson B., Eriksson K., Gustafsson B., Jørgensen U.G., Nordlund Å., 2017, in press).



Comparison between modelled spectra of a giant S star (thin red line) and a dwarf S star (thick green line). Dwarf S stars have never been observed but are doomed to exist according to current stellar evolution models. These modelled spectra are the first attempt to identify their characterizing spectral features. Both stars have an effective temperature of 3500 K, C/O = 0.75, [s/Fe] = 1, [Fe/H] = 0, they only differ by their surface gravity value ($\log g = 0$ and $\log g = 4$). Some spectral features are identified (those identified with a circled « + » are however telluric bands, caused by the Earth atmosphere).

A man with glasses and a blue and white checkered shirt is pointing at a chalkboard. The chalkboard has several mathematical equations written on it. The most prominent equation is $W_+ = \int \partial_+ \phi \partial_- \phi + \dots$. There are other faint equations and symbols on the board, including $\frac{d}{dt}$ on the left and $\frac{d}{dt} \phi$ on the right.
$$W_+ = \int \partial_+ \phi \partial_- \phi + \dots$$

The
Robert Brout
and the
Ilya Prigogine
Prizes



The Robert Brout and the Ilya Prigogine Prizes

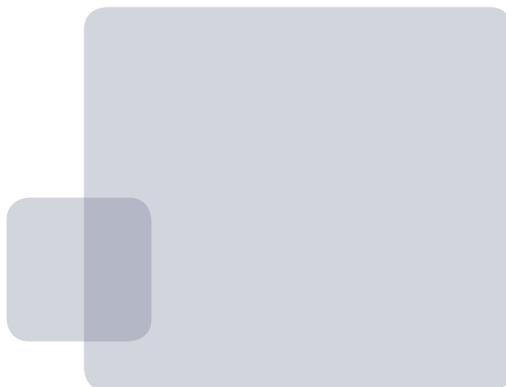
In order to commemorate the memory of two exceptional scientists from the University of Brussels, the juries of the masters in chemistry and in physics of the ULB and the VUB have created:

- the Ilya Prigogine Prize, to be awarded to the best students finishing their master studies in chemistry, provided they have a brilliant curriculum (one prize at the ULB, one prize at the VUB).
- the Robert Brout Prize, to be awarded to the best students finishing their master studies in physics, provided they have a brilliant curriculum (one prize at the ULB, one prize at the VUB).

Given the close ties of these two personalities with the Institutes, the International Solvay Institutes are associated with this initiative.

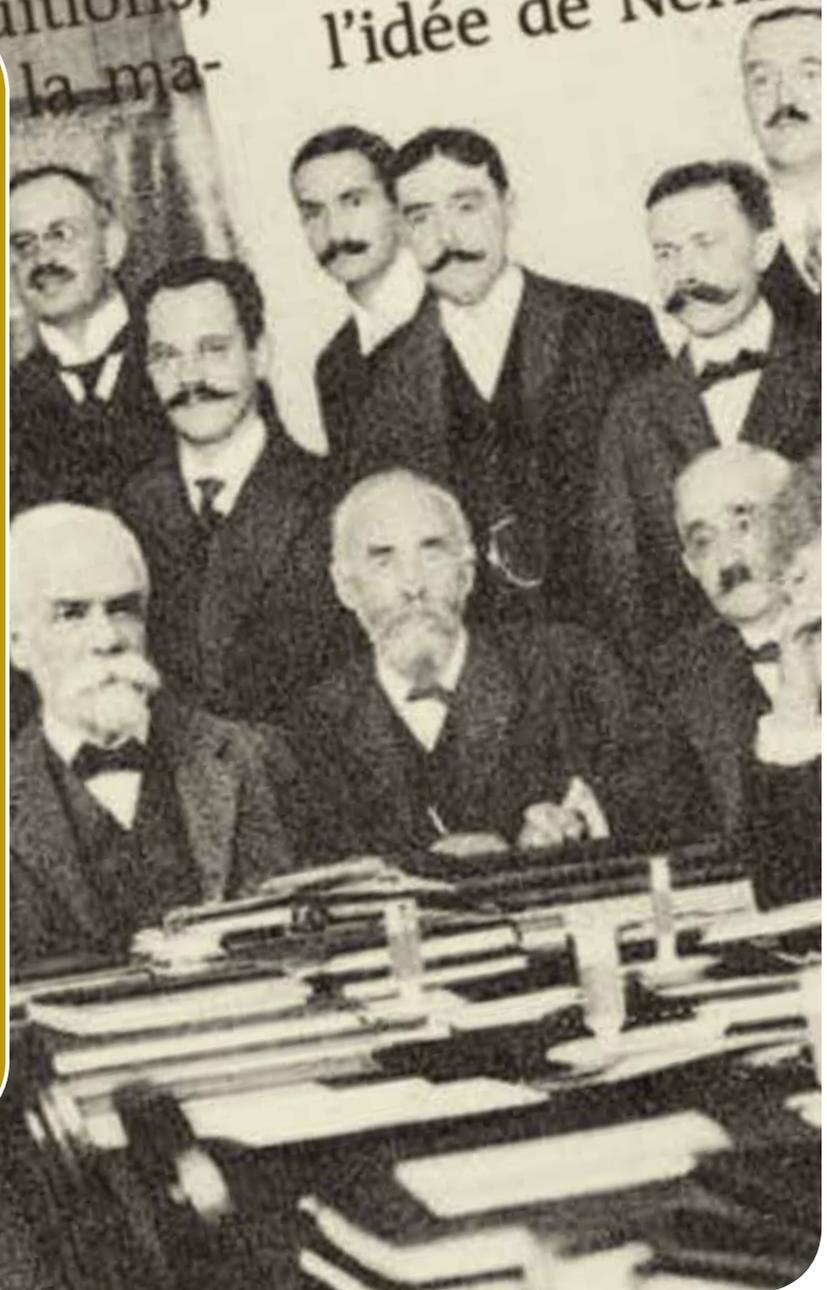
In 2016, the prizes were awarded to:

- Benjamin Claessens (Ilya Prigogine Prize VUB)
- Diego Beghin (Robert Brout Prize ULB)
- Romain Ruzziconi (Robert Brout Prize ULB)



Nernst s'est
industriel de la chimie, patron
e, passionné de sciences,
s mécènes de son temps
il a découvert un procédé
soude et a fondé, en 1863 la
son nom. Elle est toujours,
ni plus tard, l'un des plus
de la chimie européenne.
un savant dans l'âme, lui-
stitutions,
la ma-
nomènes et la
pas le consensus.
même la réalité de
à sa résolution », e
son arrière-arrière
Instituts Solvay q
jusqu'à aujourd'h
de la physique et
Solvay reprend
l'idée de Nernst

Appendix



Einstein avait raison : les ondes gravitationnelles

SCIENCES Une équipe de chercheurs a saisi la première photo

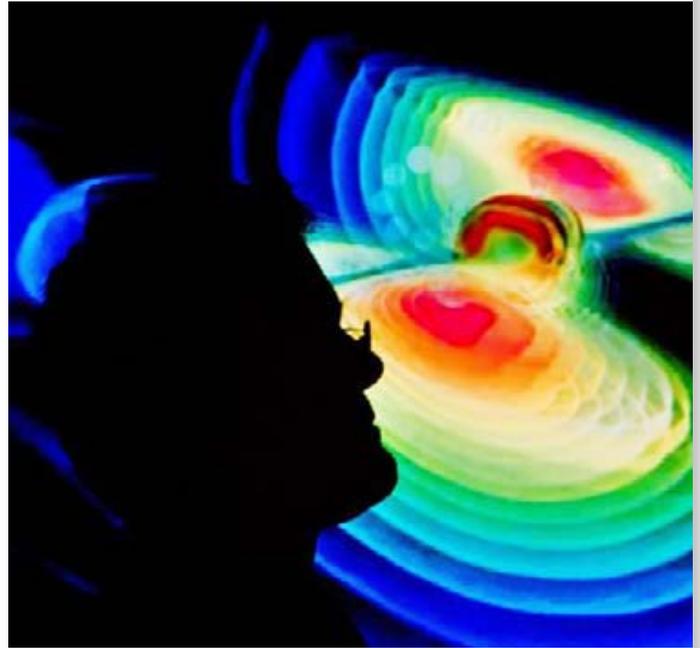
- ▶ L'existence des ondes gravitationnelles vient d'être démontrée.
- ▶ Elles résultent de la fusion de deux trous noirs.
- ▶ Cette découverte majeure ouvre la porte sur un monde jusqu'alors inconnu.

C'est un grand jour ! Pile 100 ans après la prédiction théorique formulée par Albert Einstein, l'existence des ondes gravitationnelles vient d'être démontrée de façon directe par l'expérience. L'une des idées fondatrices de sa théorie de la relativité générale est que la géométrie de l'espace-temps est élastique. Alors même que l'espace-temps est vide, des vibrations s'y propagent depuis les confins de l'Univers à la vitesse de la lumière. Ces vagues, ce sont les ondes gravitationnelles. Lors de leur passage, l'espace-temps s'étire ou se contracte avant de reprendre sa configuration normale.

L'empreinte gravitationnelle mesurée par les scientifiques du projet LIGO (Laser Interfero-

meter Gravitational-Wave Observatory) correspond exactement à l'allure du signal prédite par les simulations informatiques. Elles reproduisaient la fusion de deux trous noirs de bonne taille : l'un de 36 fois la masse du Soleil, l'autre un peu moins gros (29 masses solaires). Autrement dit, « leur masse est environ 10 millions de fois celle de la Terre mais concentrée dans un rayon de ... 150 km, précise Stéphane Detournay, chercheur qualifié FNRS spécialiste des trous noirs (ULB). En tournant l'un autour de l'autre à une vitesse proche de la moitié de celle de la lumière (soit 300 tours par seconde) jusqu'à leur fusion en une seule entité en énorme "boom", les deux trous noirs ont perdu 3 masses solaires. Cette masse s'est dissipée en un premier jet d'ondes gravitationnelles. Un second jet a été mesuré lorsque le trou noir fraîchement né s'est peu à peu relaxé, passant d'un état hors d'équilibre à une forme statique. On voit cela via les pics de fréquence mesurés. Aucun doute n'est possible : le même signal a été observé par deux détecteurs très éloignés (l'un dans l'état de Washington, l'autre en Louisiane). »

Quant à l'amplitude des pics



Un infime signal correspondant à l'empreinte laissée par la fusion de deux trous noirs a été détecté pour la première fois. © EPA/JULIAN STRATENSCHULTE

(leur hauteur, qui correspond à la quantité d'énergie reçue sur la Terre), elle nous indique que cette coalescence de trous noirs s'est déroulée il y a quelque 1,3 milliard d'années-lumières. C'est-à-dire que les scientifiques internationaux travaillant sur LIGO ont pris la photo d'un événement qui s'est déroulé il y

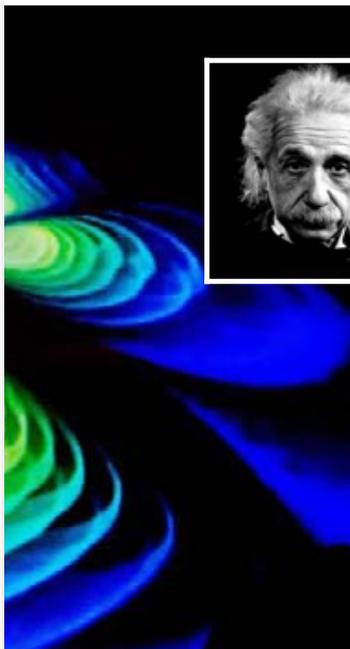
a 1,3 milliard d'années. Et quel événement ! C'est la première fois que l'humanité observe (certes de façon indirecte) la fusion de deux trous noirs.

Une nouvelle trousse à outils

Jusqu'alors, nous n'avions que le rayonnement de la gamme des ondes électromagnétiques

existent !

Photo de la fusion de trous noirs



celui de l'astronomie gravitationnelle», s'enthousiasme le Pr. Jean-Marie Frère, physicien théoricien (ULB).

Mais cette fusion de deux trous noirs, où s'est-elle déroulée ? On ne le sait pas encore précisément. « Grâce à l'écart de quelques millisecondes entre la détection du signal au niveau du premier détecteur puis du second, on a pu identifier une surface située entre les deux détecteurs et s'étendant à l'infini. Mais on ignore à quelle distance de la Terre s'est déroulé cet événement », indique le Pr Frère. Pour affiner le résultat en une localisation plus précise, il faudrait réaliser une triangulation et donc se munir d'un troisième détecteur.

Bonne nouvelle : la version améliorée de l'interféromètre Virgo (basé à Pise, Italie) devrait entrer en action courant de l'année. Elle sera plus sensible encore que les deux interféromètres, désormais stars, de LIGO.

De quoi ouvrir les yeux sur un monde jusqu'alors inconnu. Et peut-être remonter jusqu'à l'empreinte du Big Bang. ■

LÆTITIA THEUNIS

deux trous noirs

pour sonder l'Univers. Depuis hier, notre trousse à outils s'est enrichie des ondes gravitationnelles. « On ouvre donc la porte à l'observation de toute une gamme de nouveaux objets et de nouveaux phénomènes auxquels nous étions aveugles jusqu'ici », poursuit-il. « On a démarré un nouveau pan de l'astronomie :

Englert « Une avancée remarquable »

ENTRETIEN

Le professeur François Englert est prix Nobel de physique 2013. Il est le codécouvreur du fameux boson scalaire ou boson BEH (Brout-Englert-Higgs).

Comment jugez-vous cette observation ?

C'est une remarquable avancée dans l'expérience astronomique. D'un point de vue théorique, on n'avait pas de doute que ces ondes existaient. On ne pouvait pas avoir de doute raisonnable de l'existence de ces ondes, même si on peut évidemment douter de tout dans la vie. On peut croire que l'autre face de la Lune est fondamentalement différente de la face qu'on observe en permanence ou supposer qu'elle sera similaire à la face que l'on observe. Ce qui aurait donc été très surprenant, c'est que l'expérimentation en démente l'existence ! Il n'en demeure pas moins que c'est une expérience extraordinaire, parce que c'est un phénomène très difficile à débusquer, que la distance rend terriblement faible. Vous m'apprenez que les chercheurs annoncent que la variation enregistrée mesure cent-millionième de la taille d'un atome et que l'onde est déglagée par deux trous noirs qui tournent l'un autour de l'autre. C'est une expérience en soi remarquable, même si elle n'est pas révolutionnaire du point de vue théorique.

Cette découverte vaut-elle un Nobel ?

Je ne suis pas compétent pour les donner ni les prédire. Juste pour en recevoir un. Il est difficile de jauger dans quelle mesure sera estimée la réalisation de cette expérience extraordinaire mais qui n'établit pas de principe théorique neuf. Cela dépend beaucoup de ceux qui l'estimeront. Le plus surprenant,



« Une expérience extraordinaire », pour le Prix Nobel François Englert. © LE SOIR/GARRIGOS

nant, c'est que ces résultats n'ont jamais été obtenus à plus courte distance. Cela démontre le poids des études expérimentales en astrophysique. En fait, et ce n'est pas de l'humilité mal placée, je ne suis pas compétent pour l'estimer. Il y a une différence essentielle entre le boson scalaire et les ondes gravitationnelles sur des objets macroscopiques. Le premier était entouré d'un doute raisonnable et opposé à d'autres théories. L'expérience a permis de confirmer que ce boson existait et a eu un impact théorique direct. Cette expérience-ci n'ouvre pas d'impact théorique direct.

Question classique, face à ce genre d'annonce : cela va changer quoi dans ma vie ?

Si vous ne vous intéressez qu'à la structure des broses à dents, cela ne changera rien dans votre existence. Mais toutes les connaissances que nous pouvons accumuler sur la structuration du monde répondent à cette curiosité fondamentale sans laquelle l'humanité serait un bien triste chose. On peut vivre sans se poser de questions. Ou, comme c'est mon cas, croire que la curiosité humaine est une des choses les plus importantes à développer. ■

Propos recueillis par FRÉDÉRIC SOUMOIS

Il veut comprendre les premiers instants après le Big Bang: Marc Henneaux (ULB) distingué comme «leader dans son domaine» - 10/05/2016 14:09:00

Ixelles -

Marc Henneaux, professeur au service de physique théorique et mathématique de la faculté des sciences de l'ULB, a reçu un prix destiné aux chercheurs «reconnus comme leaders dans leur discipline». Ses recherches, c'est du très solide.



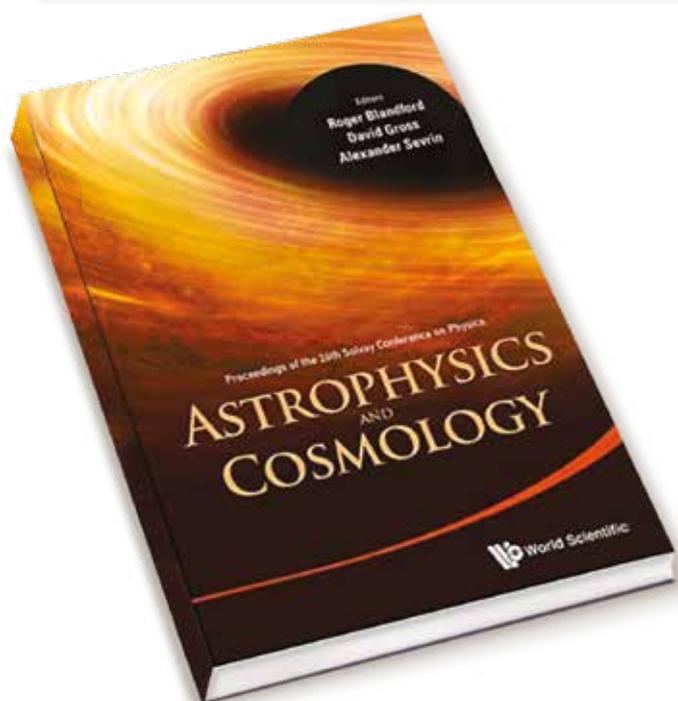
Marc Henneaux, professeur au service de physique théorique et mathématique de la faculté des sciences de l'Université Libre de Bruxelles (ULB) vient de recevoir un ERC Advanced Grant (bourse pour chercheur expérimenté), annonce l'université dans un communiqué mardi. Ce prix est remis par le Conseil européen de la recherche à des chercheurs «reconnus comme leaders dans leur discipline». Marc Henneaux avait déjà reçu cette bourse en 2010.

«Un des grands défis consiste à concilier les deux théories que sont la mécanique quantique (qui régit le monde microscopique) et la relativité générale (qui décrit les phénomènes aux échelles macroscopiques) en une théorie cohérente de la gravitation quantique», indique le communiqué. Établir une cohérence entre ces deux théories permettrait de comprendre «la physique des premiers instants après le Big Bang ou des régions proches du centre d'un trou noir».

Le professeur, également directeur des instituts Solvay, a été récompensé pour ses recherches sur ces questions physiques fondamentales et plus spécifiquement pour son étude sur les extensions de la théorie d'Einstein (la relativité générale).

L'ERC Advanced Grant est une bourse allouée pour cinq ans par le Conseil européen de la recherche. Elle peut atteindre jusqu'à 2,5 millions d'euros. Elle se destine aux chercheurs qui ont déjà «fait leurs preuves en tant qu'éminents chercheurs indépendants».

l'avenir.net – May 2016



*Proceedings of the 26th Solvay
Conference on Physics*

*ISBN: 978-981-4759-17-5 (hardcover)
380pp - June 2016*

The Solvay Meetings - Impact on Outreach Activities

By Prof. Alexander Sevrin

NEWS

Brief History

From Monday October 30 through Friday November 3, 1911, 23 leading physicists from all over Europe met at the Hotel Métropole in Brussels to discuss about "la théorie du rayonnement et les quanta", the theory of radiation and quanta. The initiative for this conference was taken by Ernest Solvay, a prominent Belgian industrialist with a keen interest in science, and the conference was chaired by Hendrik Lorentz.

In 1912 Ernest Solvay founded the International Institute for Physics followed in 1913 by the creation of the International Institute for Chemistry. In 1970 the Solvay family in association with the Université Libre de Bruxelles (ULB), and the Vrije Universiteit Brussel (VUB), merged both Institutes and established the "International Institutes for Physics and Chemistry, founded by Ernest Solvay".

For more than a century the tradition of scientific excellence continued and the activities of the International Solvay Institutes greatly expanded including an important emphasis on scientific outreach.



Photograph of participants of the first Solvay Conference, in 1911, Brussels, Belgium. Seated (L-R): Walther Nernst, Marcel Brillouin, Ernest Solvay, Hendrik Lorentz, Emil Warburg, Jean Baptiste Perrin, Wilhelm Wien, Marie Curie, and Henri Poincaré. Standing (L-R): Robert Goldschmidt, Max Planck, Heinrich Rubens, Arnold Sommerfeld, Frederick Lindemann, Maurice de Broglie, Martin Knudsen, Friedrich Hasenöhrl, Georges Hostenlet, Edouard Herzen, James Hopwood Jeans, Ernest Rutherford, Heike Kamerlingh Onnes, Albert Einstein, and Paul Langevin

Main Focus and Uniqueness

Today the main focus of the International Institutes for Physics and Chemistry founded by Ernest Solvay is still the organization of the International Solvay Conferences. It follows a three year cycle: in year one there is the Physics Conference, in year two there is no conference and in year three there is the Chemistry Conference. The last and 26th Solvay Physics Conference took place from October 9 through 11, 2014. Its theme was "Astrophysics and Cosmology" and it was chaired by Roger Blandford from Stanford University. The 23rd Solvay Conference on Chemistry will be held in October 2016.

The Solvay Conferences on Physics are unique among physics meetings and have followed the same setup since their very inception. The Scientific Committee for Physics of the Solvay Institutes is in charge of the Conferences. The Committee consists of ten outstanding physicists appointed for a six year period,

renewable once.¹ It defines a theme in physics of current interest and appoints a chair for the conference. From then on the chair assumes full responsibility. He or she drafts a list of 40 to 60 invitees, all leading experts in the theme addressed during the conference. In addition, five important questions within the theme are defined to each of which half a day is devoted. Each of these sessions is prepared by the session chair in close collaboration with the chair of the conference and starts with a brief review of the state of the art by the rapporteur. The bulk of the session is then fully devoted to a round table discussion, which makes the Solvay Conferences very different from other conferences in physics. Since the first Solvay Conference the discussions are reproduced verbatim in the proceedings thus providing a remarkable testimony on the thoughts and convictions of outstanding physicists at that given time. As an example, the last Solvay Conference on Physics held in 2014 addressed current problems in "Astrophysics and Cosmology" and the five sessions were devoted to: Neutron Stars, Black Holes, Cosmic Dawn, Dark Matter, and the Microwave Background. About 60 invited experts, coming from very different subdisciplines of astrophysics and cosmology, had over three days numerous lively, cross-fertilizing, and sometimes even contentious discussions.²

Other Highlights

While the Solvay Conferences on Physics and Chemistry remain the core business of the Solvay Institutes, numerous other initiatives are taken as well. Every year the Institutes organize four or five topical high level workshops that run over three to five days, focus on important developments in both physics and chemistry and are heavily attended by scientists from Belgium and its neighboring countries. Some topics recently covered were: Quantum Simulation with Cold Matter and Photons, Conceptual Quantum Chemistry, Bridging the Gaps at the PCB Interface - Multiscale Modeling in Physics, Chemistry and Biology, and Nonequilibrium and Nonlinear Phenomena in Statistical Mechanics.

The yearly International Jacques Solvay Chair in Physics and the International Solvay Chair in Chemistry attract eminent scientists who pass one or two months in Brussels, collaborating with the local scientists and giving Master Classes to doctoral students, postdoctoral fellows, and faculty from all over the country. The Master Class is preceded by an inaugural lecture aimed at a wider audience. The 2015 Jacques Solvay Chair in Physics was held by Peter Zoller who lectured on quantum information and quantum computing.

A monthly colloquium where hot topics are presented by eminent scientists serves the local physics and chemistry community. An extensive doctoral school "Quantum Field Theory, Strings and Gravity" is organized every year in collaboration with the ULB, the VUB, the University of Amsterdam, various institutions in Paris headed by Ecole Normale Supérieure, and various institutions in Switzerland led by the Swiss network "SwissMap" (ETH Zürich, U. Bern, U. Geneva, CERN) providing first-year PhD students with advanced courses in theoretical physics that help bridge the gap between Master-level courses and the most recent advances in the field.

In addition to this the International Solvay Institutes contribute both logistic and financial aid to numerous scientific and outreach events in and out of Belgium.

¹ The composition of the Scientific Committee for Physics, currently chaired by David Gross, can be found on the website of the International Solvay Institutes: www.solvayinstitutes.be where a lot of information on the International Solvay Institutes and its activities can be found.

² For the interested reader, the proceedings make a wonderful read and provide a timely account of some of the most pressing problems in the field: "The Proceedings of the 26th Conference on Physics, Astrophysics and Cosmology"; R. Blandford, D. Gross and A. Sevrin, editors; 2016 World Scientific; 13 + 357 pages.

Outreach Activities

One of the absolute highlights of the activities of the International Solvay Institutes are the yearly Solvay Public Lectures that take place in the magnificent setting of Studio 4 in the Flagey Building. The Flagey Building is a beautiful edifice in modernistic style constructed from 1935 through 1938 and located on the edge of the Flagey Square and next to the Ixelles ponds in Brussels. During the Solvay Public Lectures, which started in 2005 and are usually held on a Sunday afternoon in October, distinguished scientists deliver lectures on the state-of-the-art in their field of research with an overview of the most pressing current issues.

Organized jointly with the ULB, the VUB, and the Solvay Group, this event popularizes science and aims at making it more attractive to the younger generations. The talks are given in English but simultaneous translations into Dutch and French are provided. The lectures are followed by a debate where a panel consisting of renowned scientists address questions from the audience. The event closes with a drink offered to all the participants, allowing the public to interact directly with the invited scientists. The event is free and every year the 862 seats of Studio 4 are solidly packed!



Every year again the Solvay Public Lectures attracts more than 800 interested people in the magnificent Studio 4 of the Flagey Building in Brussels. Shown here: Reinhard Genzel in 2015 talking about "Massive Black Holes and the Evolution of Galaxies".

To give a flavor of the diversity of topics addressed during the Solvay Public Lectures and the excellence of the lecturers, I list the speakers and topics since the Centennial of the Solvay Institutes. In 2011 under the theme *The Future of Physics*, William Phillips talked on *Time and Einstein in the 21st century*, and Frank Wilczek on *Quantum Beauty*. In 2012 George Whitesides discussed *The Science of Simplicity*, Michael Freedman considered *Will our Thinking Become Quantum-Mechanical?*, and Kurt Wüthrich presented *Exploring the Postgenomic Protein Universe*. The next year the audience was entertained by presentations by Joachim Frank on *How proteins are made in the cell: Visualizing the ribosome in action* and Jason Chin on *Reprogramming the genetic code*. In 2014 three talks were delivered: Conny Aerts on *Starquakes and Exoplanets in our Milky Way galaxy*, Martin Rees on *From a 'simple' big bang to our complex cosmos*, and François Englert on *The Brout-Englert-Higgs mechanism and its scalar boson*. Last year one hundred years of Einstein's general relativity was celebrated by talks by Reinhard Genzel on *Massive Black Holes and the Evolution of Galaxies* and Viatcheslav Mukhanov on *From Nothing to the Universe*. This year's Public Event has *Chemistry for the World of Tomorrow* as its theme, and lectures by Robert Grubbs on *Green Chemistry for Sustainable Development* and Ben Feringa on *The Art of Building Small* will be delivered.

Since its start in 2005, the Solvay Public Lectures have grown into one of the most visible and popular scientific outreach events in Belgium. Its success clearly demonstrates that public outreach by physicists and other scientists is more than ever needed! As Jean-Marie Solvay, the great grand-son of Ernest Solvay and the President of the International Solvay Institutes states: "We need scientists to be heard and to be lauded, we need to show that science is a fascinating subject raising intriguing and captivating challenges, and we need to demonstrate that it is extraordinarily important for the future of humanity to pursue scientific advances, which are critical to the survival of human beings on earth. Hence our commitment to public events and lectures."



Viatcheslav Mukhanov presenting his outreach talk "From Nothing to the Universe" at the 2015 Solvay Public Event "One Hundred Years of Einstein's General Relativity".

The Hotel Métropole – European Physical Society (EPS) Historic Site

The Hotel Métropole was the venue of the first Solvay Council. After that both the Solvay Conferences on Physics and those on Chemistry moved to the campus of the Free University of Brussels (ULB). However since the 23rd Solvay Conference on Physics "The Quantum Structure of Space and Time" in 2005 the Solvay Conferences returned to the Hotel Métropole where they are being held ever since.

Recognizing the profound influence of the Solvay Conferences on physics, the EPS decided to bestow its Historic Site Award to the Hotel Métropole. On October 2015, a commemorating plaque was unveiled in the lobby of the hotel by Christophe Rossel, president of the EPS, and Jef Ongena, president of Belgian Physical Society (BPS). The ceremony was preceded by an academic session.³ The attendance included members of Belgian and European academic and political institutions. Guests of honor were fourteen direct descendants of the Nobel Laureates that were present in 1911, three descendants of Ernest Solvay, and Mr. Wielemans, heir to the family that founded this Brussels landmark hotel.



Christophe Rossel, President of the EPS, and Jef Ongena, President of the BPS, unveiling the EPS Historic Site plaque. It is now exhibited on top of the historic 1911 picture in the lobby of Hotel Métropole.

³The EPS Historic Site Award celebration was accompanied by the publication of a Special Topic Issue of the European Physical Journal: "The Early Solvay Councils and the Advent of the Quantum Era"; EPJ ST, Vol. 224, September 2015; F. Lambert, F. Berends and M. Eckert, editors.



More than a century later: the direct descendants of the participants to the 1911 Solvay Conference in Physics gather in October 2015 in the Hotel Métropole when the European Physical Society bestowed its Historic Site Award to the Hotel. Seated (L-R): Dieter Klingmüller [W. Nernst], Ursula Klingmüller [W. Nernst], Jean-Marie Solvay [E. Solvay], Anna de Haas [H. Lorentz], Yann Lapique [J.-B. Perrin], Françoise Chapuis [J.-B. Perrin], Paul Siebertz [W. Wien], Maria Rïchardt [W. Wien], Pierre Joliot [M. Curie]. Standing (L-R): Florian Baier [A. Sommerfeld], Monika Baier [A. Sommerfeld], Nathalie Ferrard [A. Einstein], Mary Fowler [E. Rutherford], Catherine Kamerlingh Onnes, Jeanne Kamerlingh Onnes.



The Solvay Public Event also provides a perfect forum for the ceremony attributing the Solvay Awards honoring outstanding young physicists and chemists for their Master and PhD theses.



Alexander Sevrin is a professor at the Free University Brussels (VUB) and founder of the Theoretical High Energy Physics Group whose members investigate aspects of elementary particle physics and cosmology. He is the deputy director and the scientific secretary for physics of the International Solvay Institutes for Physics and Chemistry. He sits on the board of directors of several organizations among which the Francqui Foundation, the largest Belgian private science foundation. He is member of the Royal Flemish Academy of Belgium for Science and the Arts.



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Introduction

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Accepted: 17 August 2016

One contribution of 17 to a theme issue 'Multiscale modelling at the physics–chemistry–biology interface'.

Subject Areas:

computational chemistry

Author for correspondence:

P. V. Coveney

e-mail: p.v.coveney@ucl.ac.uk

Bridging the gaps at the physics–chemistry–biology interface

P. V. Coveney¹, J. P. Boon² and S. Succi^{3,4}

¹Centre for Computational Science, University College London, Gordon Street, London WC1H 0AJ, UK

²Physics Department, Université Libre de Bruxelles, Campus Plaine, CP 231, Avenue F.D. Roosevelt 50, 1050 Bruxelles, Belgium

³Istituto Applicazioni del Calcolo-CNR, Viale del Policlinico 19, 00185 Roma, Italy

⁴Institute for Applied Computational Science, Harvard J. Paulson School of Engineering and Applied Sciences, Harvard University, 29 Oxford Street, Cambridge, MA 02138, USA

 PVC, 0000-0002-8787-7256

It is commonly agreed that the most challenging problems in modern science and engineering involve the concurrent and nonlinear interaction of multiple phenomena, acting on a broad and disparate spectrum of scales in space and time. It is also understood that such phenomena lie at the interface between different disciplines, such as physics, chemistry, material science and biology. The multiscale and multi-level nature of these problems commands a paradigm shift in the way they need to be handled, both conceptually and in terms of the corresponding problem-solving computational tools.

The triple interface between biology, chemistry and physics provides a most fertile ground for these kinds of phenomena; the design of environmentally friendly catalytic devices or smart-drug delivery devices for nanomedicine purposes being just two examples in point where atomic-scale details organize coherently.

The above phenomena take place far from equilibrium, where the organizing power of nonlinearity is fully exposed and macroscopic universality is compromised by the necessary degrees of microscopic (molecular) individualism. Indeed, the ability to integrate universality and molecular individualism is perhaps the most challenging task of modern multiscale modelling.

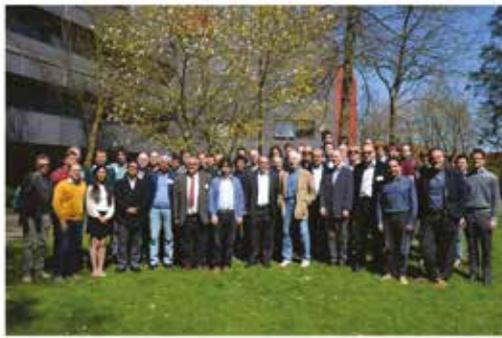


Figure 1. Participants at the Solvay Meeting 'Bridging the gap at the PC3 interface: multiscale modelling in physics, chemistry and biology', enjoying the excellent spring weather at the Université Libre de Bruxelles, 20 April 2016.

Computer science and technology, key to enabling the quantitative modelling of such complex phenomena across scales, have experienced an extraordinary and relentless growth in both computational processing power and memory, along with dramatic cost reduction, all encouraging increased access to these approaches. At the same time, the recent decades have also witnessed substantial progress in the development of modelling methodologies at all scales, including, for example, *ab initio* molecular dynamics and so-called QM/MM (quantum mechanics/molecular mechanics) techniques for atomic and nano-scales, lattice Boltzmann, Brownian and dissipative particle dynamics for mesoscales, and various grid-based methods for the several macroscales. The importance of all these efforts was recognized with the award of the 2013 Nobel Prize in Chemistry 'for the development of multiscale models for complex chemical systems' [1].

The papers contained in this theme issue of *Philosophical Transactions of the Royal Society A* are the peer-reviewed products of a call for papers under the title of the theme issue. They and their authors were in large part brought together under the auspices of an exciting and enjoyable Solvay Workshop (which was held between 19 and 21 April 2016 at the Université Libre de Bruxelles, Belgium; figure 1). The meeting itself was similarly centred on the rising multiscale modelling paradigm, with particular focus on emergent phenomena flourishing at the physics-chemistry-biology interface. The meeting helped not only to put a focus on the present state of art in the field, but, most importantly, also to foster and shape new cooperative research effort as to advance this exciting frontier of modern science.

The present theme issue starts with an opinion piece [2] discussing the 'big data' issue for conventional scientific methods of inquiry. Without conventional theoretical understand of the structural characteristics of the system under investigation, we lack the principles by which to guide the optimal acquisition of data which we would expect to be forthcoming any experimental design activity. The article provides a logical introduction to the trail of research topics discussed in the following papers [3–17], which report findings from full gamut of domains from physics and chemistry to biology. The first five research articles address issues associated with the development and implementation of a range of methods

schedule. As a result, the present issue has appeared in time for the Solvay Workshop to take place. One of us (P.V.C.) wishes to thank assistance in connection with the publication of this theme issue.

Lastly, two of us (P.V.C. and S.S.) wish to dedicate this issue to our friend, Juan Pierre Boon, on the occasion of his 80th distinguished and productive scientific career: we wish to express our sincere condolences.

Competing interests. We declare we have no competing interests. **Funding.** We received no funding for this study.

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Figure 2. Juan Pierre Boon (centre) with his fellow scientific committee members and Solvay workshop co-organizers Sauro Succi (left) and Peter Gaspard (right).

for handling multiscale problems in molecular and condensed matter physics as well as fluid dynamics. These include innovative combinations of consolidated atomistic and mesoscale techniques, such as adaptive molecular dynamics, direct simulation Monte Carlo and lattice Boltzmann. In particular, the notion of Chamaera simulation is introduced to denote the intriguing ability of mesoscale methods to 'morph' from continuum to quasi-atomistic tools by having the amount of molecular details. The following two articles [8,9] consider multiscale simulations arising in polymer and materials chemistry. The first eight articles [10–17] deal with the most complex and challenging aspects of multiscale modelling at the physics-chemistry-biology interface. The papers address problems which span many biologically relevant scales of organization, from the molecular and genomic levels through cellular to organ and organism levels.

According to Einstein's famous statement 'the most incomprehensible thing about our Universe is that it is comprehensible' [18]. Today, we appreciate that a principal ingredient of multiscale modelling is the hierarchical nature of multiple inter-connected layers of organization, as opposed to a scientific approach to comprehend such hierarchical observed processes. We hope that the present theme issue represents a valuable contribution along this fascinating road towards a better understanding of the marvellous complexity of the world around and within us.

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Overview of the Institutes through selected data

The Solvay Conferences on Physics

1911	Radiation theory and the quanta	1973	Astrophysics and gravitation
1913	The structure of matter	1978	Order and fluctuations in equilibrium and nonequilibrium statistical mechanics
1921	Atoms and electrons	1982	Higher energy physics: What are the possibilities for extending our understanding of elementary particles and their interactions to much greater energies?
1924	Electric conductivity of metals	1987	Surface science
1927	Electrons and photons	1991	Quantum optics
1930	Magnetism	1998	Dynamical systems and irreversibility
1933	Structure and properties of the atomic nuclei	2001	The physics of communication
1948	Elementary particles	2005	The quantum structure of space and time
1951	Solid state	2008	Quantum theory of condensed matter
1954	Electrons in metals	2011	The theory of the quantum world
1958	The structure and evolution of the universe	2014	Astrophysics and Cosmology
1961	Quantum Field Theory		
1964	The structure and evolution of galaxies		
1967	Fundamental problems in elementary particle physics		
1970	Symmetry properties of nuclei		



Chairs of the International Scientific Committee for Physics since the first Solvay Conference on Physics

1911 - 1928	Hendrik Lorentz 1902 Nobel Laureate in Physics, Haarlem (The Netherlands)	1967 - 1968	Christian Møller, Copenhagen (Denmark)
1928 - 1946	Paul Langevin, Paris (France)	1969 - 1980	Edoardo Amaldi, Rome (Italy)
1946 - 1962	Sir Lawrence Bragg 1915 Nobel Laureate in Physics, Cambridge (UK)	1980 - 1990	Léon Van Hove, Genève (Switzerland)
1962 - 1967	Robert Oppenheimer Princeton (USA)	1992 - 2006	Herbert Walther, Munich (Germany)
		2006 - present	David Gross 2004 Nobel Laureate in Physics Santa Barbara (USA)

The Solvay Conferences on Chemistry

1922	Five topical questions in chemistry	1976	Molecular Movements and Chemical Reactivity as conditioned by Membranes, Enzymes and other Molecules
1925	Chemical structure and activity	1980	Aspects of Chemical Evolution
1928	Topical questions in chemistry	1983	Design and Synthesis of Organic Molecules Based on Molecular Recognition
1931	Constitution and configuration of organic molecules	1987	Surface Science
1934	Oxygen : chemical and biological reactions	1995	Chemical Reactions and their Control on the Femtosecond Time Scale
1937	Vitamins and Hormons	2007	From Noncovalent Assemblies to Molecular Machines
1947	Isotops	2010	Quantum effects in chemistry and biology
1950	Oxidation mechanism	2013	New Chemistry and New Opportunities from the Expanding Protein Universe
1953	Proteins	2016	Catalysis in Chemistry and Biology
1956	Some problems in mineral chemistry		
1959	Nucleoproteins		
1962	Energy transfer in gases		
1965	Reactivity of the Photoexited Organic Molecule		
1969	Phase Transitions		
1972	Electrostatic Interactions and Structure of Water		

Chairs of the International Scientific Committee for Chemistry since the first Solvay Conference on Chemistry

1922 - 1939	Sir William Pope, Cambridge (UK)
1945 - 1958	Paul Karrer, 1937 Nobel Laureate in Chemistry, Zurich (Switzerland)
1958 - 1988	Alfred Ubbelohde, London (UK)
1989 - 2011	Stuart Rice, Chicago (USA)
2011 - present	Kurt Wüthrich, 2002 Nobel Laureate in Chemistry, Zurich (Switzerland) and La Jolla (USA)



Overview of the Institutes through selected data

The International Solvay Chairs in Physics and in Chemistry

Jacques Solvay Chair in Physics

2006	Ludwig Faddeev, Saint-Petersburg Russia	2011	Nathan Seiberg, Princeton, USA
2007	Michael Berry, Bristol, UK	2012	Jan Zaanen, Leiden, The Netherlands
2008	David Gross, Santa Barbara, USA 2004 Nobel Laureate in Physics	2013	Gian Giudice, CERN, Switzerland
2009	Valery Rubakov, Moscow, Russia	2014	Viatcheslav F. Mukhanov, LMU Munich, Germany
2010	Serge Haroche, Paris, France 2012 Nobel Laureate in Physics	2015	Peter Zoller, Innsbruck, Austria
		2016	Dam Thanh Son, Chicago, USA

Solvay Chair in Chemistry

2008	Richard Saykally, Berkeley, USA	2013	Egbert Meijer, Eindhoven The Netherlands
2009	Alexander Mikhailov, Berlin Germany	2014	Richard Schrock, MIT, USA 2005 Nobel Laureate in Chemistry
2010	Weitao Yang, Durham, USA	2015	Andreas Manz, KIST Europe, Saarbrücken, Germany
2011	Jean-Luc Brédas, Atlanta, USA	2016	Raymond Kapral, Toronto, Canada
2012	Viola Vogel, Zurich, Switzerland		

2011 Solvay Centenary Chair

David Gross, Santa Barbara, USA
2004 Nobel Laureate in Physics

Presidents and Directors

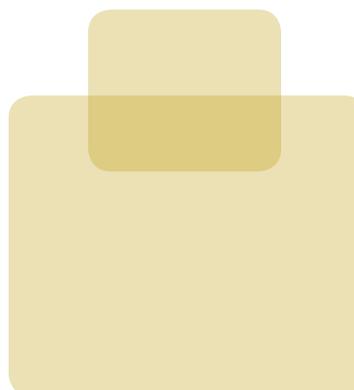
Ernest Solvay, his son Armand Solvay and his grand-son Ernest-John Solvay successively presided over the destiny of the International Solvay Institutes until 1958. In 1958, the Institutes were restructured with the creation of the positions of “President” and “Director”.

Presidents

1958 - 2010	Jacques Solvay
2010 - present	Jean-Marie Solvay

Directors

1958 - 2003	Ilya Prigogine 1977 Nobel Laureate in Chemistry Professor ULB
2003 - 2004	André Jaumotte Honorary Rector and Honorary President ULB
2004 - present	Marc Henneaux Professor ULB



The Solvay Public Lectures

22 June 2005

“From Quarks to the Quantization of Gravitation: Challenges and Obstacles in our Search for the Fundamental Forces”
by Gerard 't Hooft (Utrecht)
1999 Nobel Laureate in Physics

“From Structural Biology to Structural Genomics: New Challenges for Physics and Chemistry in the Post-Genomic Era”
by Kurt Wüthrich (Zurich and La Jolla)
2002 Nobel Laureate in Chemistry

4 December 2005

“Strings, Black Holes and the End of Space and Time”
by Robbert Dijkgraaf (Amsterdam)

“The Fabric of the Cosmos, Space, Time and the Texture of Reality”
by Brian Greene (New York)

20 May 2007

“The Origin of the Universe”
by Stephen Hawking (Cambridge, UK)

“Architecture in Nanospace”
by Harold Kroto (Brighton)
1996 Nobel Laureate in Chemistry

2 December 2007

Chemistry? More than ever!

“De la Matière à la Vie: la Chimie? La Chimie!”
by Jean-Marie Lehn (Paris and Strasbourg)
1987 Nobel Laureate in Chemistry

12 October 2008

Images from the Quantum World

“New Forms of Quantum Matter near Absolute Zero Temperature”
by Wolfgang Ketterle (Cambridge, USA)
2001 Nobel Laureate in Physics

“Visualizing Complex Electronic Quantum Matter at Atomic Scale”
by J.C. Seamus Davis (Ithaca, USA)

4 October 2009

“VIH/SIDA, une aventure scientifique et humaine en réponse à une épidémie émergente”
by Françoise Barré-Sinoussi (Paris)
2008 Nobel Laureate in Medicine

17 October 2010

Chemistry: at the crossroads of Physics and Biology

“The magnetic compass of birds and its physical basis”
by Wolfgang Wiltschko (Frankfurt am Main)

“Experimental surprises and their solutions in theory”
by Rudolph Marcus (Pasadena)
1992 Nobel Laureate in Chemistry

23 October 2011

The Future of Physics

“Time and Einstein in the 21st century”
by William Phillips (College Park)
1997 Nobel Laureate in Physics

“Quantum Beauty”
by Frank Wilczek (Cambridge, USA)
2004 Nobel Laureate in Physics

21 October 2012

“The Science of Simplicity”
by George Whitesides (Cambridge, USA)

“Will our Thinking Become Quantum-Mechanical?”
by Michael Freedman (Santa Barbara)
1986 Recipient of the Fields Medal

“Exploring the Postgenomic Protein Universe”
by Kurt Wüthrich (Zurich and La Jolla)
2002 Nobel Laureate in Chemistry

20 October 2013

“How proteins are made in the cell: Visualizing the ribosome in action”
by Joachim Frank (Columbia University, USA)

“Reprogramming the genetic code”
by Jason Chin (University of Cambridge, UK)

12 October 2014

“Starquakes and Exoplanets in our Milky Way galaxy”
by Conny Aerts (KU Leuven, Belgium)

“From a ‘simple’ big bang to our complex cosmos”
by Martin Rees (Cambridge, UK)

“The Brout-Englert-Higgs mechanism and its scalar boson”
by François Englert (ULB, Belgium)
2013 Nobel Laureate in Physics

18 October 2015

One hundred years of Einstein’s general relativity

“Massive Black Holes and the Evolution of Galaxies”
by Reinhard Genzel (Max Planck Institute Munich, Germany)

“From Nothing to the Universe”
by Viatcheslav Mukhanov (LMU Munich, Germany)

23 October 2016

Chemistry for the World of Tomorrow

“Translation of Academic Science into the Commercial”
by Robert Grubbs (California Institute of Technology, USA)
2005 Nobel Laureate in Chemistry

“The Art of Building Small”
by Ben Feringa (University of Groningen, The Netherlands)
2016 Nobel Laureate in Chemistry

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Postal address

International Solvay Institutes
Campus Plaine ULB / CP 231
Bd du Triomphe
B-1050 Brussels | Belgium

Delivery and visiting address

International Solvay Institutes
Campus Plaine ULB / Access 2
Bd de la Plaine
Building N.O.
5th Floor - Office 2N5 105A
B-1050 Brussels | Belgium



Ms Bogaerts: + 32 2 650 55 42
dominique.bogaerts@ulb.ac.be

Ms Van Geet: + 32 2 650 54 23
isabelle.vangeet@solvayinstitutes.be

Website: www.solvayinstitutes.be
Webdesigner: Thomas Philippe
Webmaster: Isabelle Van Geet



